Manifestation of spin nematic ordering in the spin-1 chain system

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Spin-1 chain material is considered. Recently, it was predicted that the spin nematic ordered phase can be realized due to the spin-elastic coupling. In this study we show that the appearance of the spin nematic ordering and phase transitions to such ordered states can be studied using magneto-acoustic experiments. One can observe such phases and phase transitions considering relative changes of the velocity of sound (related to the changes of the elastic modulus of the crystal) as a function of temperature and the external magnetic field. It is shown that those relative changes are proportional to the spin quadrupole susceptibility of the system. The results are obtained using the exact Bethe ansatz solution and Quantum Monte Carlo simulations for several typical values of the biquadratic spin-spin exchange interaction and for various values of the spin-elastic coupling and elastic modules.

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I. INTRODUCTION

Electron systems with nonconventional ordering connected with electron correlations, e.g., with the rotation symmetry breaking, attract attention of physicists. Such systems are similar to ordered states of molecules in liquid crystals [1]. In liquid crystals the distinguished orientation of molecules is present. The order parameter in the nematic system is a director [2], and it breaks the rotational O(3) symmetry. It is different from the magnetization (the order parameter in magnetically ordered systems), which is a vector violating the time-reversal symmetry. Nematic properties were observed in many correlated electron materials, like iron-based superconductors [3–6], heavy fermion systems [7], and rare-earth insulators [8]. For some electron systems the nematic ordering is related to orbital degrees of freedom of electrons [8], while for other systems it is connected with the spin subsystem. For the latter the spin nematic ordering is related to the spin multipole (e.g., quadrupole) ordering, unlike the usual magnetic ordering, which corresponds to the spin dipole ordering. The order parameters of the spin nematic phases are nonzero components of the expectation values of the second-rank spin traceless quadrupolar tensor $Q^{\alpha\beta} = S^\alpha S^\beta + S^\beta S^\alpha - [S(S+1)/3]\delta_{\alpha\beta}$, where S^α ($\alpha = x, y, z$) is the operator of the projection of the spin S, while magnetic order parameters are expectation values of the operators S^α or their combinations. The single-ion spin nematic ordering can exist for spin systems with $S \geqslant 1$, while the inter-ion spin nematic ordering can be present for any value of S, including $S = 1/2$, see, e.g., [9,10]. In magnetic systems the spin nematic ordering was predicted theoretically [11–13], in Refs. [14,15] the microscopic origin of the non-Heisenberg spin-spin interactions were considered. Nonetheless, the construction of the microscopic theory remains among important tasks for physicists. As a rule, the spin nematic ordering is caused by the exchange spin-spin coupling and with weaker relativistic interactions. In many cases the onset of the spin nematic ordering in magnetic material is connected with the geometrical frustration of the spin lattice, which suppresses the usual magnetic ordering [16–18]. For $S \geqslant 1$ the spin nematic ordering was predicted for systems with the biquadratic spin-spin exchange (quadrupole-quadrupole) interaction [19]. The biquadratic exchange coupling is considered to be small in usual magnetic systems. However, the analysis of the experiments with the Ni-based magnetic material [20–22], and ultracold atoms [23,24] implies that the biquadratic spin-spin interaction is essential.

Spin chain materials (or quasi-one-dimensional quantum spin systems) are magnetic systems in which the spin-spin interaction along one space direction is much larger than along other directions. In recent years many spin chain materials were synthesized due to the progress in fabrication of new materials with special properties. For many of one-dimensional spin models exact quantum mechanical solutions are known [25], and, therefore, that integrability permits to obtain theoretically exact characteristics of those models. It must be noted that peculiarities of the one-dimensional density of states yield an enhancement of quantum and thermal fluctuations. The latter results in the destruction of the long-range ordering for quantum systems with gapless excitations for nonzero temperatures [26]. Instead, in the ground state one-dimensional quantum systems can manifest a long-range ordering [27,28], with quantum phase transitions between ordered and disordered phases.

The spin nematic order parameter is not coupled to the external field directly. It is the reason why, despite many efforts [29–31], the results of experiments with magnetic materials often cannot be considered as a proof for existence of the spin nematic ordering. In the present paper we consider one-dimensional quantum spin-1 system coupled to the elastic subsystem of the spin-chain material. Recently it was shown [32] that such a system manifests phase transitions to the spin nematic ordered phase, in which quadrupole spin ordering take place. Here we show how the transitions to the spin nematic state and spin nematic ordered phases themselves can be observed when studying elastic characteristics of the system. Namely, we show that the temperature and external magnetic field dependencies of elastic modules and velocities of sound can reveal features, caused by the phase transitions to the spin nematic ordered state and between spin nematic ordered phases (spin nematic reorientation transitions).

II. RENORMALIZATION OF ELASTIC CHARACTERISTICS

Let us consider the spin-1 chain system described by the Hamiltonian

$$\mathcal{H} = \sum_n \left[J\mathbf{S}_n \cdot \mathbf{S}_{n+1} + J'(\mathbf{S}_n \cdot \mathbf{S}_{n+1})^2 - HS_n^z - D\big(O_2^0\big)_n\right] + CN\frac{\epsilon^2}{2}, \quad (1)$$

where $\mathbf{S}_n$ is the operator of the spin $S = 1$ in the nth site of the chain, $J > 0$ is the exchange parameter (here we limit ourselves with the most interesting antiferromagnetic linear spin-spin interaction), J' is the parameter of the biquadratic spin-spin exchange coupling (or spin quadrupole-quadrupole interaction), H is the external magnetic field (the units in which the effective magneton, $g\mu_B = 1$, are used; here g is the effective g factor and μ_B is the Bohr magneton), $(O_2^0)_n = (S_n^z)^2 - S(S+1)/3$ is the Stevens operator [25], related to the component of the spin quadrupole tensor $Q_n^{\alpha\beta}$, D is the value of the single-ion magnetic anisotropy coupled to that Stevens operator, C is the elastic modulus, ϵ is the strain (combination of strains), related to that modulus, and N is the number of spins in the chain. We can assume that $D = a\epsilon$, where a is the parameter of the magneto-elastic coupling. Physically, the ligands (nonmagnetic ions, surrounding the magnetic ones) produce the crystalline electric field. That field acts on the orbital moment of the magnetic ion, yielding the preferred direction of the orbital moment. Then, due to the spin-orbit interaction, such a mechanism creates the single-ion magnetic anisotropy for the magnetic ions. Suppose we start with the magnetically isotropic situation (e.g., the cubic symmetry of the crystal). Then the tetragonal strains ϵ produce the change of the elastic energy, see Eq. (1), reducing the symmetry of the crystal. On the other hand, those strains yield, according to the above, the magnetic anisotropy. If the energy of the magnetically anisotropic spin chain system is lower than the isotropic one, one has the gain of the energy, while the elastic subsystem loses the energy, and the phase transition of the Jahn-Teller type to the state with the nonzero magnetic anisotropy takes place [32]. The nonzero order parameter, which characterizes the state with the magnetic anisotropy is the expectation value of the Stevens operator (or the zth component of the spin quadrupole moment $Q_z = \langle\sum_n (O_2^0)_n\rangle$, and, correspondingly, the component of the spin quadrupole moment per site $q_z = N^{-1}Q_z$). In the ordered state with nonzero q_z the spin-rotational symmetry is violated, hence the ordered state is the spin nematic ordered state.

Notice that here we consider the onset of the single-ion magnetic anisotropy in the spin-chain material. There exists the possibility of the exchange-striction mechanism, in which the exchange parameter depends on changes of the positions of magnetic ions themselves or of nonmagnetic ions, which participate in the nondirect exchange, see, e.g., [31,33–35]. Such a situation can also produce spin nematic ordering in a spin chain material. We do not consider here that case; notice that below all obtained results are presented in units of J.

Following [35–37], according to the elasticity theory [38] we can write

$$\frac{\partial u}{\partial t} = \frac{\partial \sigma}{\partial x}, \quad (2)$$

where u are displacements, and σ are stresses, related to the strains ϵ. (Notice that in [36,37] displacements and strains were denoted by the same letter, however it did not affect the correctness of the results of [36,37], because in the calculations only the right-hand side of Eq. (2) was used.). The stress can be obtained as the derivative of the free energy of the system per site f with respect to ϵ,

$$\sigma = \frac{\partial f}{\partial \epsilon} = C\epsilon - aq_z. \quad (3)$$

Then we obtain

$$\frac{\partial \sigma}{\partial x} = C\frac{\partial \epsilon}{\partial x} - a\frac{\partial q_z}{\partial \epsilon}\frac{\partial \epsilon}{\partial x}, \quad (4)$$

from which the renormalized elastic modulus is

$$C_{\text{eff}} = C - a\frac{\partial q_z}{\partial \epsilon} = C - a^2\chi_q, \quad (5)$$

where χ_q is the related component of the spin nematic (quadrupole) susceptibility $\chi_q = (\partial q_z/\partial D) = a^{-1}(\partial q_z/\partial \epsilon)$. The relative change of the elastic modulus, hence, can be written as

$$\frac{\Delta C}{C} = \frac{C_{\text{eff}} - C}{C} = -\frac{a^2}{C}\chi_q. \quad (6)$$

In magneto-acoustic experiments [39] one often measures the absolute values and the relative changes of the velocity of the sound v. For highly symmetric crystals the latter is related to the elastic modulus via $C = \rho v^2$, where ρ is the density of the crystal. Then, according to the above, one can extract the spin nematic susceptibility χ_q from the magneto-acoustic experiments, which measure the relative changes of the sound velocities (or the elastic modules). The spin nematic ordering manifests itself in the changes of the behavior of χ_q, and, therefore, one can directly observe the phase transitions to the spin nematic ordered phase in such magneto-acoustic experiments. For convenience we can define, following [32] $\alpha = C/a^2$, so that $\chi_q = -\alpha(\Delta C/C)$.

The ground-state energy at the fixed magnetic field H and constant α corresponds to the minimum of the energy of the system with the Hamiltonian (1) at zero temperature with respect to D,

$$E_{\min}(H,\alpha) = \min_D E(H,D,\alpha) = E(H,D_{\min},\alpha), \qquad (7)$$

so that

$$\frac{\partial E(H,D,\alpha)}{\partial D}|_{D=D_{\min}} = 0, \qquad (8)$$

and, therefore

$$q_z = \alpha D_{\min}. \qquad (9)$$

Hence, in the case of zero temperature $T = 0$ the spin quadrupole susceptibility (per site) is

$$\chi_q = -N^{-1}\frac{\partial^2 E}{\partial D^2}\bigg|_{D=D_{\min}} = \frac{\partial q_z}{\partial D}\bigg|_{D=D_{\min}} = \mathbf{Var}\{q_z^*\}. \qquad (10)$$

Here $q_z^* = N^{-1}Q_z(D_{\min})$. Actually, in condensed matter physics the measurement of the dispersion $\mathbf{Var}\{x\} = \langle x^2\rangle - \langle x\rangle^2$ of a variable x is often used as the powerful tool to obtain the important information about possible ordering in a subsystem, corresponding to $\langle x\rangle$, phase transitions, etc. (Here $\langle x\rangle$ is the mean over the distribution function of x.)

In the case of finite temperatures T we can write

$$\chi_q(T) = T^{-1}\big(\langle q_z^2\rangle_G - \langle q_z\rangle_G^2\big). \qquad (11)$$

Here $\langle\ldots\rangle_G$ is the thermodynamic (Gibbs) mean.

A. Bethe ansatz solution of the SU(3) symmetric spin-1 model

The spin-1 chain model is exactly solvable in the SU(3) symmetric situation at which $J' = J$ (so-called Uimin-Lai-Sutherland model [40–42]). For that spin model all components of the spin moment $\sum_n S_n^{x,y,z}$ and the Stevens operators $\sum_n (O_2^m)_n$ $(m = 0, \pm 1 \pm 2)$ commute with the exchange part of the Hamiltonian, hence they have the same set of eigenfunctions. One can classify all the states of the SU(3) symmetric Hamiltonian according to values of projections of the components of the SU(3) fields.

Within the Bethe ansatz method the eigenvalues and eigenfunctions of the model can be described by two sets of quantum numbers called rapidities $u_{j=1}^{n_a+n_b}$, and $v_{m=1}^{n_a}$. Here $n_{a,b,c}$ with $a, b, c = \pm 1, 0$ are the numbers of states with each possible values of the z-projection of the site spin S_j^z, i.e., ± 1, 0. They are related to each other via the obvious constrain $n_1 + n_0 + n_{-1} = N$. One can suppose that $n_a \leqslant n_b \leqslant n_c$. For periodic boundary conditions the rapidities satisfy the following set of Bethe ansatz equations (BAE):

$$(-1)^N X_1^{-N}(u_j) = \prod_{m=1}^{n_a} X_1(u_j - v_m)\prod_{q=1}^{n_a+n_b} X_2(u_j - u_q),$$
$$j = 1,\ldots,n_a+n_b, \prod_{b=1}^{n_a} X_2(v_m - v_b)$$
$$= \prod_{q=1}^{n_a+n_{-b}} X_1(v_m - u_q), m = 1,\ldots,n_a, \qquad (12)$$

TABLE I. Values of $n_{a,b,c}$, M_z, and Q_z for various relations between n_1, n_0, and n_{-1} for the ground state of the SU(3) symmetric spin-1 chain.

n_a	n_b	n_c	M_z	Q_z
n_{-1}	n_0	n_1	$N - 2n_a - n_b$	$N/3 - n_b$
n_{-1}	n_1	n_0	$n_b - n_a$	$n_a + n_b - 2N/3$
n_0	n_{-1}	n_1	$N - 2n_b - n_a$	$N/3 - n_a$
n_0	n_1	n_{-1}	$n_a + 2n_b - N$	$N/3 - n_a$
n_1	n_{-1}	n_0	$n_a - n_b$	$n_a + n_b - 2N/3$
n_1	n_0	n_{-1}	$2n_a + n_b - N$	$N/3 - n_b$

where $X_n(y) = (2y + in)/(2y - in)$. The eigenvalue of the system is

$$E = J\left[N - \sum_{j=1}^{n_a+n_b}\frac{4}{u_j^2+1}\right] - HNm_z - DNq_z, \qquad (13)$$

where $m_z = N^{-1}\langle\sum_n S_n^z\rangle$ is the eigenvalue of the z projection of the total spin of the system.

In the ground state for the antiferromagnetic case $J > 0$ in the thermodynamic limit $N, n_{a,b,c} \to \infty$ with the ratios $n_{a,b,c}/N$ fixed the rapidities, which satisfy the BAE, are real [40]. The equations for the densities of rapidities $\rho(u)$ and $\sigma(v)$ are

$$2\pi\rho(u) = a_1(u) - \int_{-A}^{A} dy a_2(u-y)\rho(y)$$
$$+ \int_{-B}^{B} dz a_1(u-z)\sigma(z),$$
$$2\pi\sigma(v) = \int_{-A}^{A} dy a_1(v-y)\rho(y)$$
$$- \int_{-B}^{B} dz a_2(v-z)\sigma(z), \qquad (14)$$

where $a_1(x) = 4/(1+4x^2)$, $a_2 = 2/(1+x^2)$. The limits of integration are determined from the condition

$$\frac{n_a}{N} = \int_{-B}^{B} dy\sigma(y),$$
$$\frac{n_a+n_b}{N} = \int_{-A}^{A} dx\rho(x). \qquad (15)$$

The ground-state energy is

$$E = N\left[J - J\int_{-A}^{A} dx a_1(x)\rho(x) - Hm_z - Dq_z\right]. \qquad (16)$$

There exist six following possibilities [32], see the Table I, to determine the values $n_{a,b,c}$ via $n_{\pm 1,0}$, For instance, for $n_a = n_{-1}$, and $n_b = n_0$, one has $n_c = n_1 = N - (n_a + n_b)$ so that $M_z \equiv Nm + z = N - (n_a + n_b) - n_a$ (i.e., $m_z = 1 - \int_{-A}^{A} du\rho(u) - \int_{-B}^{B} dv\sigma(v)$), and $Q_z \equiv Nq_z = N - (n_a + n_b) + n_a - (2N/3)$ (i.e., $q_z = (1/3) - \int_{-A}^{A} du\rho(u) + \int_{-B}^{B} dv\sigma(v)$). [This case is related to the situation of large positive values of the magnetic field H.] At fixed values of the fields D and H we minimize the ground state energy with

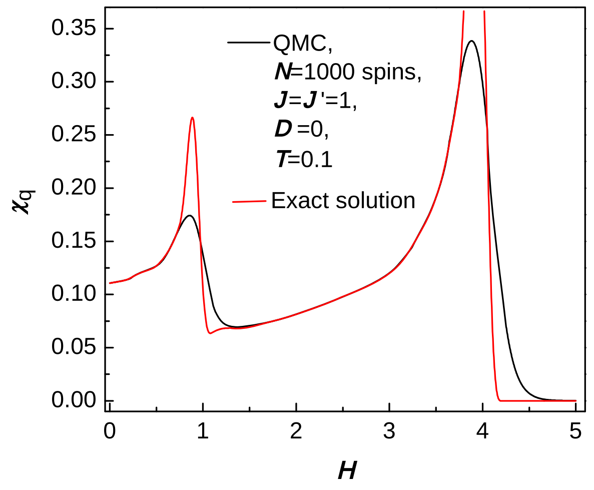

FIG. 1. The dependence of the spin nematic (quadrupole) susceptibility (per site) χ_q on the magnetic field H at $T = 0$ (red curve) and $T = 0.1$ (black curve) for the case $J' = J = 1$ at $a = 0$.

respect to $0 \leqslant A, B < \infty$ and $(M_z)_i$, $(Q_z)_i$. Here the index $i = 1, 2, \ldots, 6$ enumerates possible combinations, connecting $n_{a,b,c}$ and $n_{\pm 1,0}$ for given values of the fields D and H as it is shown in the Table I.

In what follows all numerical calculation were performed in dimensionless units, so that $J = 1$.

In our calculations we mostly used the finite temperature Quantum Monte Carlo (QMC) method [43–45]. To check the correctness of such numerical simulations in Fig. 1 the results for the spin nematic (quadrupole) susceptibility of the spin-1 chain decoupled from the elastic subsystem as a function of the magnetic field H obtained using the exact Bethe ansatz (the red curve) and the low-temperature QMC method (the black curve) are presented. One can see that the QMC results agree very well with the exact ones, except of the vicinity of phase transitions caused by the external magnetic field [32]. In our calculations the zero-temperature dependencies of χ_q were obtained by the numerical differentiation of q_z [see Eq. (10)],

$$\chi_q \approx \frac{q_z(D_{\min} + \delta D) - q_z(D_{\min})}{N\delta D}, \quad \delta D \ll 1. \tag{17}$$

B. The effect

We have pointed out in the Introduction that the main goal of this study is to propose the mechanism of the experimental observation of the spin nematic phase and the phase transition to the spin nematic ordered phase. To realize that goal we propose to measure the magnetic field H and the temperature T dependencies of the spin nematic (quadrupole) susceptibility, which, as it was shown above, determines the changes of the elastic modules and the velocities of sound. The latter can be measured in magneto-acoustic experiments.

To remind, the physics is as follows. The strain ϵ of the elastic subsystem reduces the symmetry of the crystal down to the tetragonal one. For some values of the strain, and, hence, of the related parameter of the single ion anisotropy $D = a\epsilon$, the energy of the spin subsystem becomes smaller than the one

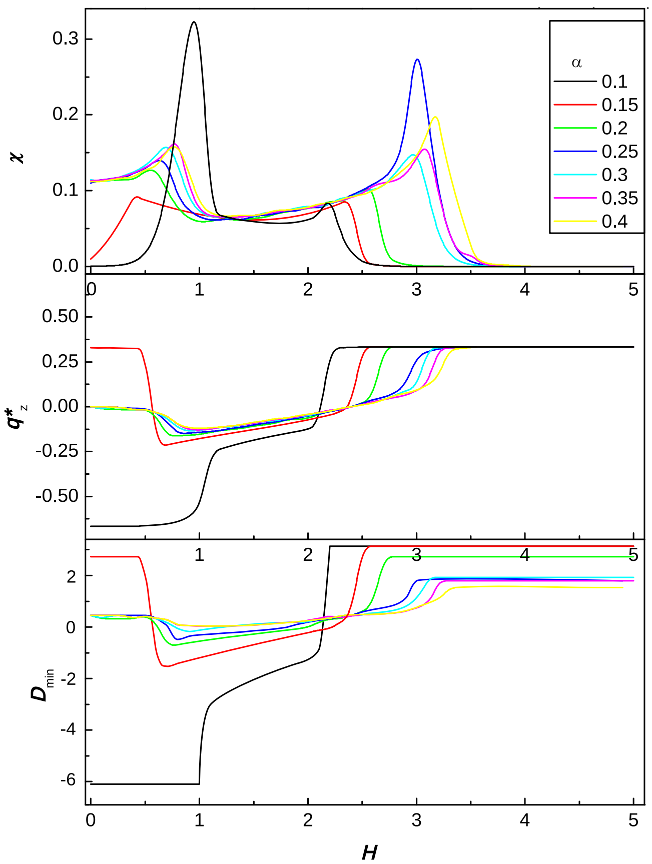

FIG. 2. The dependencies of the spin nematic (quadrupole) susceptibility per site, χ_q (upper panel), the spin quadrupole moment per site q_z^* (central panel), and the quadrupole field (the parameter of the single-ion magnetic anisotropy) $D_{\min}$ (lower panel) on the magnetic field H at different values of the parameter α. All results have been obtained by the QMC method for the system of $N = 1000$ spins at the temperature $T = 0.1$. The exchange parameter is $J = 1$, the parameter of the biquadratic spin-spin exchange coupling is $J' = 1$.

at $D = 0$. Hence, such a strain produces the energy loss of the elastic subsystem, and, at the same time, the energy gain in the spin subsystem of the crystal. The situation is reminiscent of the Jahn-Teller effect, however, for the spin subsystem: The strain lifts the degeneracy of the spin subsystem, because in the absence of the magnetic anisotropy, caused by the strain, the direction of the spin nematic order parameter is arbitrary. Depending on the parameter $\alpha = C/a^2$, transitions to the spin nematic ordered phases can be realized. The external magnetic field H affects the spin nematic ordering caused by the interaction with the elastic subsystem. Notice that the magnetic field itself can cause the spin nematic ordering without the coupling to the elastic subsystem [32].

C. The magnetic field dependence

Due to the good agreement between the results of exact solution and QMC for the SU(3) symmetric case (see Fig. 1) we have used the QMC simulation for our further calculations. The reason is the following: The QMC method allows us to perform calculation at arbitrary value of J', while the exact solution is valid for the case of $J' = J$ only.

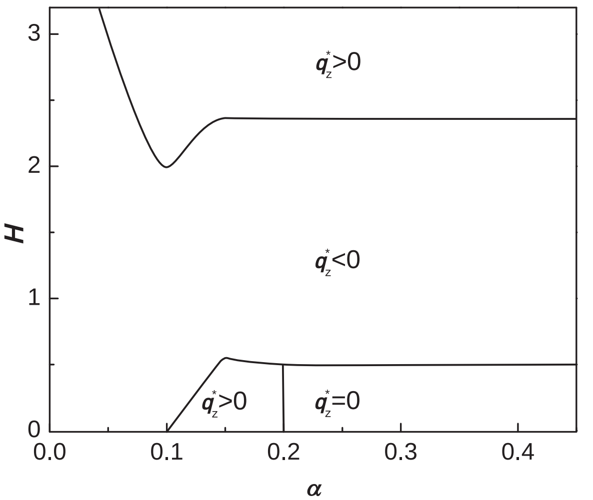

FIG. 3. The ground-state phase diagram for the SU(3) symmetric spin-1 system.

First of all, we have performed the analysis of $q_z^*(H) = -\frac{\partial E(H)}{\partial D}|_{D=D_{\min}}$ dependencies for different values of α (see the central panel of Fig. 2). At $H = 0$ we have established that

(i) For $\alpha < \alpha' \approx 0.15$ the spontaneous spin quadrupole moment exists and $q_z^* < 0$. It is the case of the strong coupling between the magnetic and elastic subsystems.

(ii) For $\alpha' \leqslant \alpha < \alpha'' \approx 0.2$ the spontaneous spin quadrupole moment also exists, but $q_z^* > 0$. It is the case of the intermediate coupling.

(iii) For $\alpha \geqslant \alpha''$ the spontaneous spin quadrupole moment is absent. It is the case of the weak coupling.

Actually, as it is seen from Fig. 2, at $\alpha = 0.1$ (the black curve) the spontaneous spin quadrupole moment [i.e., the nonzero $q_z^*(H = 0)$] is $q_z^* = -2/3$, and the quadrupole field (the parameter of the single-ion magnetic anisotropy) is nonzero, $D_{\min} \neq 0$, for $\alpha = 0.15$ (the red curve) we have $q_z^* = 1/3$, and $D_{\min} \neq 0$, finally, for $\alpha > 0.15$ one sees that $q_z^* = 0$ and $D_{\min} = 0$.

In the case of $H > 0$ the ground-state phase diagram becomes more complicated. For SU(3) symmetric spin-1 system, it is presented in Fig. 3. The diagram was obtained using the exact solution of the Bethe ansatz equations. The lines correspond to quantum phase transitions between the phase without the spin nematic ordering ($q_z^* = 0$), and two spin nematic ordered phases with the easy-plane ($q_z^* < 0$) and easy-axis ($q_z^* > 0$) magnetic anisotropy.

The series of curves $\chi_q(H)$ is presented in the upper panel of Fig. 2. One can see that if the spontaneous spin quadrupole moment is present then the value of $\chi_q(H)$ decreases at $H \to 0$ and even tends to zero. This result seems to be reasonable, because the ordering in the spin quadrupole subsystem suppresses fluctuations due to the onset of long-range correlations. Vice versa, if the spontaneous spin quadrupole moment is absent then $\chi_q(0) \neq 0$. Thus, the measurement of $\chi_q(H = 0)$ should be a powerful indicator of the spin nematic ordered phase.

The field dependencies of χ_q, q_z^*, and $D_{\min}$ for $J' = 1/2$ and $J' = 0$ are shown in Fig. 4 and Fig. 5, respectively. Notice that for the pure Heisenberg case $J' = 0$ the gap for spin

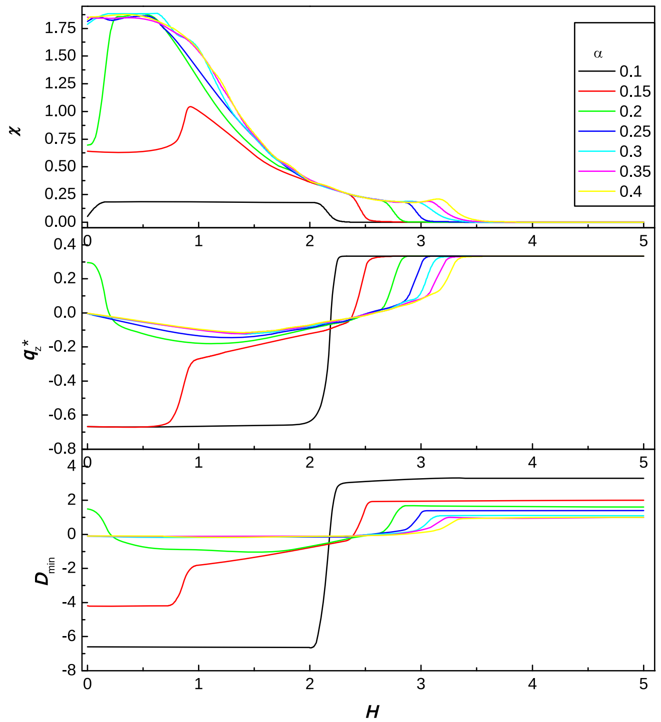

FIG. 4. The same series of the dependencies as in Fig. 2, but for $J' = 0.5$.

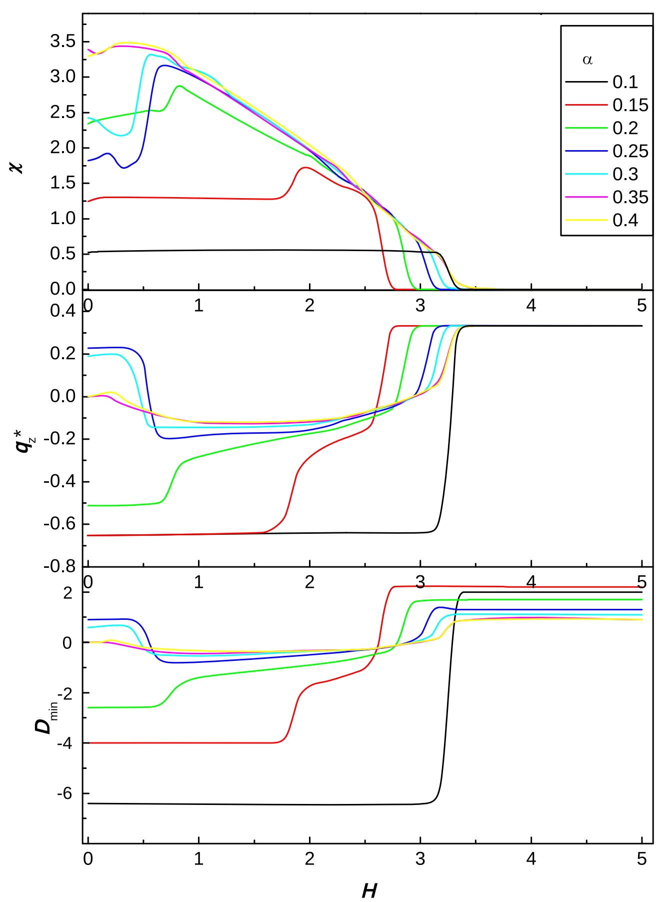

FIG. 5. The same series of the dependencies as in Fig. 2, but for $J' = 0$.

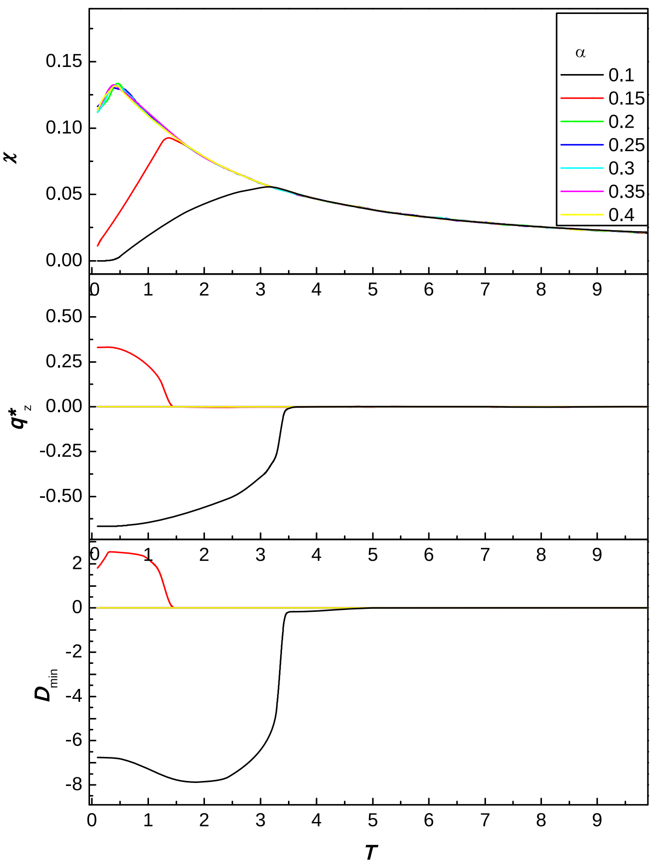

FIG. 6. The dependencies of the spin nematic (quadrupole) susceptibility per site χ_q (upper panel), the quadrupole spin moment per site q_z^* (central panel), and the quadrupole field (the parameter of the single-ion magnetic anisotropy) $D_{\min}$ (lower panel) on the temperature T at different values of the parameter α. All the results have been obtained by the QMC method for the system of $N = 1000$ spins at zero magnetic field $H = 0$. The exchange parameter is $J = 1$, the parameter of the biquadratic spin-spin exchange coupling is $J' = 1$.

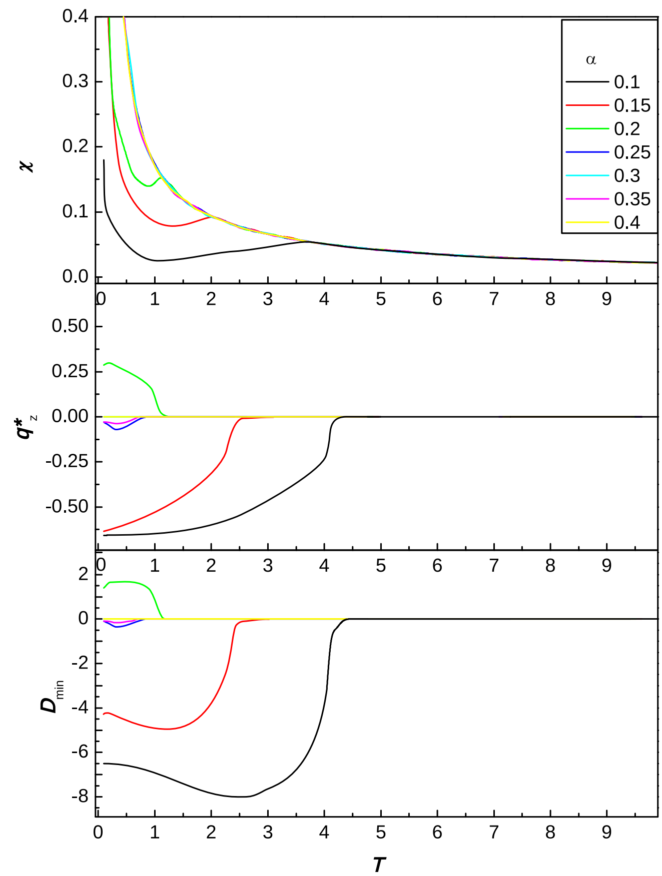

FIG. 7. The same series of the dependencies as in Fig. 6, but for $J' = 0.5$.

excitations $\sim J \exp(-\pi S)$ is predicted [46]. We can see the shifts of α' and α'' values with respect to the SU(3) symmetric case. For example, for $J' = 1/2$ the critical values are $\alpha' \approx 0.2$, $\alpha'' = 0.25$ and for $J' = 0$ the critical values are $\alpha' \approx 0.3$ and $\alpha'' = 0.35$. Besides, in these non-SU(3) symmetric systems the well-defined area of the transition from $q_z^* = 0$ to $q_z^* \neq 0$ is absent. As the result, the peaks in the dependencies $\chi_q(H)$ are absent or, at least, they are strongly suppressed.

At the same time, the trend established by us in the SU(3) symmetric case still remains: If the spontaneous spin quadrupole moment is present, then the value of $\chi_q(H)$ decreases at $H \to 0$. Whereas, the absence of peaks in the $\chi_q(H)$ dependencies and the finite value of $\chi_q(0)$ at $q_z^* \neq 0$ make non-SU(3) symmetric systems less suitable for spin nematic state detection.

D. The temperature dependence

The temperature dependencies of χ_q, q_z^*, and $D_{\min}$ are presented in Figs. 6–8. Figure 6 corresponds to the SU(3) symmetric model ($J' = 1$ with $J = 1$), and Figs. 7 and 8 describe the cases with $J' = 1/2$ and $J' = 0$, respectively.

As for the magnetic field dependencies, presented in the previous subsection, the spin nematic order parameter, the spin nematic (quadrupole) susceptibility, and the related to the strain quadrupole field (the parameter of the single-ion magnetic anisotropy), related to the minimal free energy of the spin and the elastic subsystems are shown as a function of the temperature. Analysis of the situation is performed similar to the magnetic field dependence. For all considered cases at high temperature the system is in the state with zero spin nematic order parameter (see the central panels of Figs. 6–8). With the decrease of the temperature the system can appear in the spin nematic ordered phase with nonzero value of the order parameter q_z^* for strong enough coupling (small enough α) between the elastic and spin subsystems. For large α the system remains in the state with zero spin nematic ordering. Depending on the value of α the spin nematic ordering can be of the easy-axis or the easy-plane type (different signs of $q_z^* \neq 0$). It is interesting to see that for the Heisenberg case $J' = 0$ at intermediate values of the coupling parameter α one can observe the temperature-governed phase transition between two spin nematic ordered phases, with the easy-plane like magnetic anisotropy and with the easy-axis one, see blue lines ($\alpha = 0.25$) in Fig. 8.

One can see from the figures that there are several types of peculiarities in $\chi_q(T)$ curves. The first type is observable in all series, even in the case of the absence of the quadrupole-quadrupole (biquadratic spin-spin) interaction

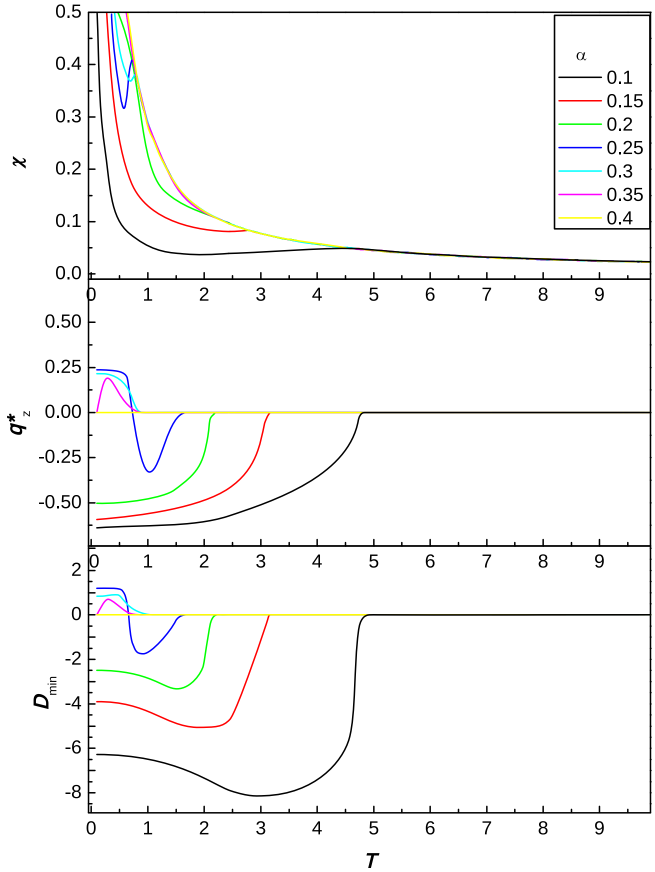

FIG. 8. The same series of the dependencies as in Fig. 6, but for $J' = 0$.

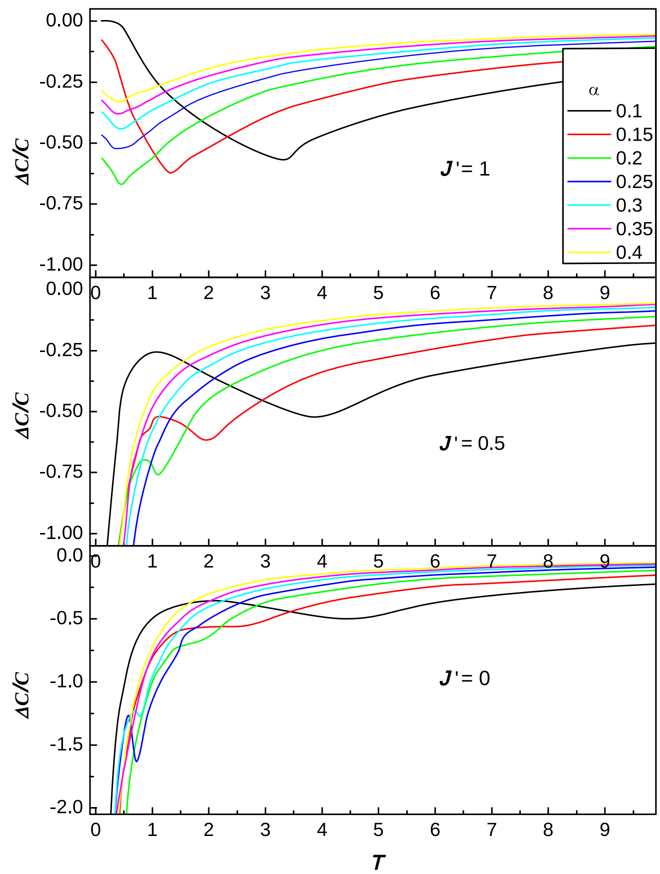

FIG. 9. The dependencies of the relative changes of the elastic modulus $\Delta C/C$ on the temperature T at zero magnetic field $H = 0$ for different values of the parameter α. Upper panel corresponds to $J' = 1$; central panel corresponds to $J' = 0.5$ and lower panel corresponds to $J' = 0$. All the results were obtained by the QMC method for the system of $N = 1000$ spins.

($J' = 0$). Therefore, this peculiarity is determined just by the appearance of nonzero quadrupole field ($D_{\min} \neq 0$). Such a situation is typical for the strong coupling between the magnetic and elastic subsystems, i.e., for small α (see, for example, the black curves corresponding to $\alpha = 0.1$). That is why for this type of peculiarity a weak shift of the transition temperature on J' is typical. It should be noted that such a behavior is similar to the temperature behavior of the magnetic susceptibility of paramagnets in an external magnetic field H.

Similar to the previous case, the second type of peculiarities is also determined by a nonzero quadrupole field (the parameter of the single-ion magnetic anisotropy). However, in this case the jump in the quadrupole field is accompanied by the changes both in the value and the sign of $D_{\min}$. This type of peculiarities is observable in the model with $J' = 0$ only. Such a situation is typical for intermediate values of α (see, for example, the blue curve corresponding to $\alpha = 0.25$ in Fig. 8). The typical temperature of peculiarities is about $T \approx 1$.

The third type of peculiarities seems to be the most interesting for the experimental detection, because it is realized in the most common systems with the weak coupling between the magnetic and elastic subsystems. This peculiarity is caused by the quadrupole-quadrupole (biquadratic spin-spin) interaction and it appears in the SU(3) symmetric model only (see the curves corresponding to $\alpha = 0.25, 0.3, 0.35$, and 0.4 in Fig. 6). As it can be seen, for these values of the parameter α the values of q_z^* and $D_{\min}$ are equal to zero in the total temperature range. The temperature dependence of $\chi_q(T)$ in this case can be well described in the terms of the Curie-Weiss law.

Note that, as it can be expected, if the peculiarities are absent (for large values of α), then the temperature dependence of $\chi_q(T)$ with the high accuracy can be described by the Curie law [$\chi_q(T) \sim T^{-1}$] in the total temperature range.

III. ELASTIC AND MAGNETO-ACOUSTIC CHARACTERISTICS

Using the results of previous sections here we present the results for the temperature and magnetic field behavior of the relative changes of the elastic modulus $\Delta C/C$. Notice that such dependencies can be observed in magneto-acoustic experiments, which measure relative changes of sound velocities [39], since $C = \rho v^2$. Figures 9 and 10 present the temperature and the magnetic field dependencies of the relative changes of the elastic modulus for several typical values of the spin-spin biquadratic exchange (quadrupole-quadrupole)

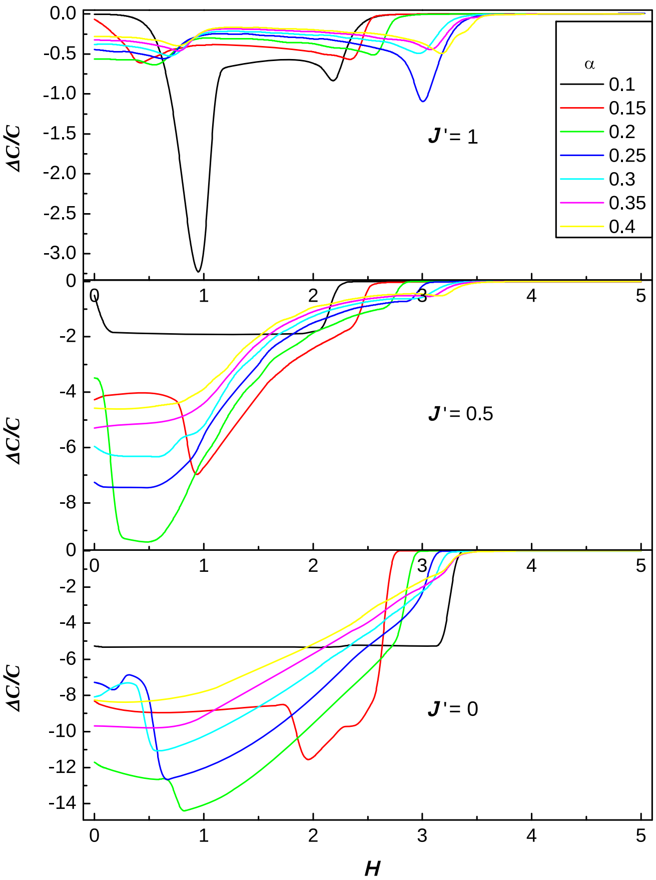

FIG. 10. The low-temperature dependencies of the relative changes of the elastic modulus $\Delta C/C$ on the magnetic field H for different values of the parameter α. Upper panel corresponds to $J' = 1$; central panel corresponds to $J' = 0.5$ and lower panel corresponds to $J' = 0$. All the results were obtained by the QMC method for the system of $N = 1000$ spins at the temperature $T = 0.1$. (The temperature and the magnetic field are measured in units of the exchange constant J).

interaction. For potential experiments the cases with $J = J'$ [the SU(3) symmetric case], and with $J' = 0$ (it is often believed that the exchange interaction even between spins $S > 1/2$ is of standard Heisenberg bilinear in spins form) are most interesting.

First of all from the temperature dependence of the relative changes of elastic modules we see that for $T \gg J$ the changes of elastic modules behave according the Curie-Weiss law for all values of the parameter α: $\Delta C/C$ is softening with the decrease of the temperature. The transition to the spin nematic ordered phase manifest itself at relatively large values of the temperature of order of several values of the exchange constant, and not like the exchange parameter itself, usual for spin-1/2 chain systems. It is physically clear, because we consider spin-1 situation, and, besides, the single-ion magnetic anisotropy, and not the inter-ion exchange anisotropy. The transition is manifested most sharply for the SU(3) symmetric case. Notice that for that case the transition to the spin nematic ordered phase exists only for $\alpha = 0.1, 0.15$: The minima at larger values of α are caused by the quantum phase transition, cf. Fig. 1, between the SU(3) symmetric phase and the SU(2) symmetric one [32], characteristic for the $J' = J$ case only. It is interesting to notice that the value of the temperature, at which the phase transition to the spin nematic ordered phase becomes smaller with the decrease of the parameter α, is small. However, for smaller values of α the feature, related to the phase transition, becomes more pronounced. Also it is interesting to point out that with the decrease of the temperature for small α the spin nematic ordered phase is related to the easy-plane magnetic anisotropy, while for larger values of α the easy-axis magnetic anisotropy appears. The most interesting situation can be realized for the Heisenberg case $J' = 0$, at intermediate $\alpha \sim 0.25$. With the temperature decrease down to $T \sim 1.5J$ the phase transition from the state without spin nematic ordering to the easy-plane spin nematic ordered phase takes place, and then, at further temperature lowering to $T \sim 0.8J$ the reorientation phase transition for the spin nematic order parameter takes place from the easy-plane to the easy-axis situation. Those transitions can be clearly seen from the features of the temperature dependence of $\Delta C/C$. For large enough values of α the reentrant situation can be realized: First, with the decrease of the temperature the system enters the spin nematic ordered phase, and for lower temperatures it goes to the state without spin nematic ordering. The case with $J' = 0.5J$ is intermediate between the two mentioned situations. Here mostly the transition to the spin nematic phase with the easy-plane anisotropy takes place, however, at intermediate values of $\alpha \sim 0.3$ the spin nematic easy-axis situation is realized. The features, related to those phase transitions, can be observed in the temperature dependence of velocities of sound in magneto-acoustic experiments.

The magnetic field dependencies of the relative changes of elastic modules reveal the following features. At large values of the field H the transition to the spin polarized phase takes place. In that phase the spin nematic ordering is also present, however, it has the trivial nature. For small values of the parameter α (strong spin-elastic coupling), when the value of the magnetic field is decreased, the transition to the spin nematic phase with the easy-plane anisotropy takes place for the values of the biquadratic exchange $J' \neq J$. For the SU(3) symmetric case the transitions between three spin nematic ordered phase take place: For large H the easy-axis phase is realized, and for smaller values of H two easy-plane spin nematic phases appear with different values of the spin nematic order parameter. For larger values of α (smaller values of the spin-elastic interaction) the transition between those phases takes place in two steps: First, when decreasing the value of H the system goes from the spin nematic easy-axis ordered phase to the state with smaller or almost zero spin nematic order parameter, and then, for lower values of H the spin nematic easy-plane ordering takes place. For intermediate values of the parameter α for $J' = J$ and $J' = 0.5J$ when the magnetic field is decreased the transition from the spin nematic easy-plane ordered state to the easy-plane ordered state with the small value of the order parameter takes place, and then, at lower values of H the spin nematic order parameter becomes zero. The features, related to those phase transitions, can be clearly seen from the magnetic field dependence of velocities of sound in magneto-acoustic experiments.

IV. SUMMARY

Summarizing, in this study we have shown how the spin nematic ordered phase and the phase transition to such a phase can be observed in experiments. As the example we have considered the spin-1 chain system. Due to the coupling of the spin subsystem with the elastic one, the Jahn-Teller like transition to the spin nematic ordered phase can take place [32], in which the spin degeneracy is lifted by the elastic strain. We have shown that the onset of the spin nematic ordering can be studied using magneto-acoustic experiments, by considering relative changes of the velocity of sound, which are related to the relative changes of the elastic modulus of the crystal. We have shown that those relative changes are proportional to the spin nematic (quadrupole) susceptibility of the system. We have calculated the temperature and the magnetic field dependencies of the latter using the exact Bethe ansatz solution and Quantum Monte Carlo simulations for several typical values of the biquadratic spin-spin exchange interaction. It has been shown that for the SU(3) symmetric case of the spin-spin coupling in the chain the phase transition to the spin nematic ordered phase manifests itself in the change of the temperature behavior of the elastic modulus from softening (at high temperatures according the Curie-Weiss law) to hardening with the decrease of T. For the intermediate biquadratic exchange and for the absence of the latter (the Haldane situation with only Heisenberg coupling between spins) one or two phase transitions can be observed. The highest temperature feature is related to the transition to the spin nematic ordered state, while the other corresponds to the transition between spin nematic ordered states with different spin nematic order parameters (for example, between the state with the easy-plane to the easy-axis spin anisotropy, i.e., spin nematic reorientation phase transitions). In the magnetic field dependence of the relative change of the elastic modulus (sound velocity) one can observe features related to the phase transition between the spin-polarized state (the paramagnetic phase, in which spin nematic ordering is trivial) and the spin nematic ordered phase, or the state with zero-spin nematic order parameter, depending on the strength of the coupling between the spin and the elastic subsystems and the value of the elastic modulus. For some values of the biquadratic spin-spin exchange interaction and for the intermediate values of the spin-lattice coupling and elastic modulus we have predicted additional phase transitions between spin nematic ordered phases with different orderings, or between the phase with zero-spin nematic order parameter and the phase with nonzero spin nematic ordering. One can observe such phase transitions as features in the magnetic field behavior of the relative change of the sound velocity. Our predictions can be checked in magneto-acoustic experiments with spin-1 chain compounds like [47–57] containing magnetic ions with $3d^2$ electron configuration for V^{3+}, Cr^{4+}, Mn^{5+}, Ti^{2+} ions, or $3d^8$ electron configuration for Ni^{2+}, Cu^{3+}, or Co^{+} ions with the isotropic g factors.

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