Intersite spin nematic ordering in the spin-$\frac{1}{2}$ chain system

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A spin-1/2 chain system coupled to the elastic subsystem of the crystal is considered. Due to that coupling, the intersite spin nematic ordering in the spin subsystem takes place. The phase transition to the ordered phase is studied using the exact quantum-mechanical approach. It is shown how the nonzero temperature and the external magnetic field affect the transition to the intersite spin nematic phase and the phase itself.

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I. INTRODUCTION

Unconventional ordering and phases in correlated electron systems are attractive issues for researchers. They appear due to strong electron-electron coupling interactions, which often act together with weaker interactions or fluctuations. The important feature of some such systems is the possibility of violation of the rotation symmetry of the Hamiltonian. It leads to a fundamental change of properties of equilibrium states and dynamic processes, see, e.g., [1–4]. In particular, the nematic state in correlated electron systems is one of the most spectacular examples of such a new ordering. It is similar to the ordered phases of molecules in liquid crystals [5]. In a nematic ordered state the distinct orientation develops. The nematic order is very different from the conventional magnetic order, where the vector order parameter violates the time-reversal symmetry. It is instead similar to the ordered phases of molecules in liquid crystals [5]. The order parameter for the nematic state is not a vector but rather a director [6]. In the nematic phase the rotation of O(3) symmetry is broken. Among the examples of nematicity in correlated electron systems one can mention, e.g., heavy-fermion systems [7], rare-earth insulators [8], or iron-based superconductors [9–13]. It turns out that the spin nematic order parameter is not coupled to the external field directly. This is why, despite numerous efforts (see, e.g., Refs. [14,15]), the experimental proof of the spin nematic ordering in magnets is often under debate.

Spin nematicity in correlated electron systems is connected with spin multipoles [16–18]. The quadrupole order parameters in spin S systems is connected with the nonzero components of the expectation values of the second-rank spin traceless quadrupolar tensor $Q_i^{\alpha\beta} = S_i^\alpha S_i^\beta + S_i^\beta S_i^\alpha - [S(S+1)/3]\delta_{\alpha\beta}$, where S_i^α $(\alpha = x, y, z)$ is the operator of the projection of the spin S in site i [19]. On the other hand, for spin-1/2 systems such components are zero. However, obviously, quantum effects are mostly pronounced for spin-1/2 systems. This is why it is necessary to introduce the intersite quadrupole order parameters as the expectation values of the operators $Q_{ij}^{\alpha\beta} = (1/2)[S_i^\alpha S_j^\beta \pm S_i^\beta S_j^\alpha] - (1/3)\mathbf{S}_i\mathbf{S}_j$, which can be nonzero for systems with spins 1/2 [20–22]. The observables of those operators are the intersite spin nematic order parameters.

Spin chain materials are systems in which spin-spin couplings along one space direction are stronger than interspin interactions in other directions. Such systems are interesting for researchers because of several reasons. First, many spin-chain materials have been manufactured in recent decades. Second, such systems often manifest special properties compared to other spin systems. In particular, quantum phase transitions [23] are characteristic for these materials, a consequence of the enhancement of fluctuations due to enhanced one-dimensional density of states [24]. And, maybe most importantly, one-dimensional quantum systems are distinguished from others because of known exact quantum-mechanical solutions for them [25]. Exact solutions permit one to obtain theoretically exact characteristics of many-body quantum systems. Among many known spin systems, the spin-1/2 chain materials are, perhaps, most attractive for researchers, because they reveal the largest quantum effects and they can be used in a large variety of applications, from the modern spintronics to quantum information and computing. This is why it is important to get information about the possibility and details of spin nematic ordering there.

The present work is devoted to the study of a one-dimensional quantum spin-1/2 system coupled to the elastic subsystem of the spin-chain material. The integrability of the spin subsystem permits us to obtain characteristics of the many-body quantum spin subsystem exactly. We show that there can exist Jahn-Teller-like phase transitions to the intersite spin nematic ordered phases. In those phases the intersite quadrupole spin ordering of various types can take place. The

influence of the external magnetic field and nonzero temperature on the spin nematic ordering is studied.

II. EXACT QUANTUM SOLUTION FOR THE SPIN SUBSYSTEM

The Hamiltonian of the considered spin-chain subsystem is

$$\mathcal{H}_0 = \sum_n \left[J\left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z\right) - H S_n^z\right], \quad (1)$$

where $S_n^{x,y,z}$ are the operators of the x, y, z components of spins $1/2$ situated at site n of the chain, J is the exchange integral, the parameter Δ determines the spin anisotropy of the exchange, and H is the external magnetic field (we use units in which $g\mu_B = 1$, where g is the effective g factor and μ_B is the Bohr magneton). In what follows we can use the exchange parameter $J = 1$, since static characteristics of the system with the Hamiltonian $\mathcal{H}_0$ do not depend on the sign of J [26]. We can also introduce the normalized value of the magnetic field $h = H/J$. Notice that eigenvalues of the Hamiltonian (1) are odd functions of H and thus of h. Thus, the Hamiltonian (1) can be written as

$$\mathcal{H}_0 = \sum_n \left[S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta S_n^z S_{n+1}^z - h S_n^z\right]. \quad (2)$$

It is known [27] that the system described by the Hamiltonian (1) is integrable, i.e., all eigenvalues and eigenfunctions can be obtained solving the Bethe ansatz equations for the quantum numbers, see, e.g., [25]. For the periodic boundary condition for the general case of any M, the Bethe ansatz equations can be written as

$$e^{ik_j L} = (-1)^{M-1} e^{-i\sum_{l=1,\, l\neq j}^{M} \theta(k_j,k_l)}, \quad j = 1, \ldots, M, \quad (3)$$

where k_j is the quasimomentum of the eigenstate,

$$\theta(k_j, k_l) = \tan^{-1}\left(\frac{\Delta \sin[(k_j - k_l)/2]}{\cos[(k_j + k_l)/2] - \Delta \cos[k_j - k_l)/2]}\right), \quad (4)$$

L is the number of sites in the chain, and M is the number of spins down. The general form of the eigenfunction in the co-ordinate representation as the superposition of the plane waves is

$$\Psi(x_1, \ldots, x_M) = \sum_P A_P \exp\left(i \sum_{j=1}^{M} k_{P_j} x_j\right), \quad (5)$$

where $x_1, \ldots, x_M$ are the co-ordinates of down spins, and P denotes a permutation of M indices $1, 2, \ldots, M$. Amplitudes A_P are related to $A_{1,2,\ldots,M}$ (which is determined from the normalization condition) as

$$A_P = \pm A_{1,2,\ldots,M} \exp\left[i \sum \theta(k_j, k_l)\right]. \quad (6)$$

Here the summation is performed over all pairs of indices j, l obtained from the initial arrangement of them for A_P, which is necessary to interchange in order to get $A_{1,2,\ldots,M}$. The sign is determined by the parity of those permutations. The eigenvalue of the Hamiltonian (1), which corresponds to the eigenfunction Eq. (5), is

$$E = -\frac{h(L-2M)}{2} + \frac{L\Delta}{4} - \sum_{j=1}^{M} (\Delta - \cos k_j). \quad (7)$$

Let us start with the ground-state properties. The ground state of the considered spin subsystem corresponds to the total filling of eigenstates with negative energies. The ground state depends on the values of Δ and h.

It is easy to show that the free energy of the system is $F(\Delta, T)$ for $\Delta > 0$ (i.e., for the antiferromagnetic interactions) and $-F(|\Delta|, -T)$ for $\Delta < 0$ (i.e., for the ferromagnetic interactions).

The ground-state energy of the system in the thermodynamic limit ($L \to \infty$, $M \to \infty$ with M/L fixed) is obtained from the solution of the following set of integral equations. Let us consider the antiferromagnetic region $\Delta > 0$ and parametrize $\Delta = \cosh(\Phi)$ (i.e., we have the "easy-axis" magnetic anisotropy $|\Delta| \geqslant 1$; for the "easy-plane" anisotropy one has $\Phi = i\theta$ with $0 \leqslant \mathrm{Re}\Theta \leqslant \pi$,

$$\varepsilon(x) + \frac{1}{2\pi}\int_{-A}^{A} dy \frac{\varepsilon(y)\sinh(2\Phi)}{\cosh(2\Phi) - \cos(x-y)} = h - \frac{\sinh^2(\Phi)}{\cosh(\Phi) - \cos(x)}, \quad (8)$$

where the "dressed" energy of the spinon $\varepsilon(x) < 0$ in the region $(-A, A)$. Hence $\pm A$ plays the role of the Fermi points, and the ground-state energy per site is

$$e_0 = \frac{\Delta}{4} + \frac{1}{2\pi}\int_{-A}^{A} dx \varepsilon(x) \frac{\sinh(\Phi)}{\cosh(\Phi) - \cos(x)}. \quad (9)$$

It is possible to introduce the density function $\rho(x)$ via the relation

$$\rho(x) = \frac{1}{2\pi \sinh(\Phi)}\left(h\frac{\partial \varepsilon}{\partial h} - \varepsilon\right). \quad (10)$$

The density function satisfies the following integral equation:

$$\rho(x) + \frac{1}{2\pi}\int_{-A}^{A} dy \frac{\rho(y)\sinh(2\Phi)}{\cosh(2\Phi) - \cos(x-y)} = \frac{\sinh(\Phi)}{2\pi[\cosh(\Phi) - \cos(x)]}, \quad (11)$$

and the ground-state energy per site is

$$e_0 = \frac{\Delta}{4} + \sinh^2(\Phi)\int_{-A}^{A} dx \frac{\rho(x)}{\cosh(\Phi) - \cos(x)} - mh. \quad (12)$$

The magnetic moment per site is

$$m = \frac{L-2M}{2L} = \frac{1}{2} - \int_{-A}^{A} dx \rho(x) = \frac{1}{2} - \frac{1}{2\pi}\int_{-A}^{A} dx \frac{\sinh(\Phi)}{\cosh(\Phi) - \cos(x)} \frac{\partial \varepsilon}{\partial h}. \quad (13)$$

For $h > \Delta + 1$ we get $A = 0$, and $m = 1/2$. For $h \leqslant \sinh(\Phi)\sum_{k=-\infty}^{\infty} e^{i\pi k}/\cosh(k\Phi)$ the magnetic moment is zero.

For $-1 < \Delta < 1$ we can introduce the parametrization $\Delta = \cos(\theta)$. Then the integral equation for the density, the ground-state energy, and the magnetic moment (per site) are

$$\rho(x) + \frac{1}{2\pi}\int_{-A}^{A} dy \frac{\rho(y)\sin(2\theta)}{\cosh(x-y)-\cos(2\theta)} = \frac{\sin(\theta)}{2\pi[\cosh(x)-\cos(\theta)]}, \tag{14}$$

$$e_0 = \frac{\Delta}{4} + \sin^2(\theta)\int_{-A}^{A} dx \frac{\rho(x)}{\cosh(x)-\cos(\theta)} - mh, \tag{15}$$

and

$$m = \frac{1}{2} - \int_{-A}^{A} dx \rho(x). \tag{16}$$

In the terms of the "dressed energy" of a spinon we have

$$\varepsilon(x) + \frac{1}{2\pi}\int_{-A}^{A} dy \frac{\varepsilon(y)\sin(2\theta)}{\cosh(x-y)-\cos(2\theta)} = h - \frac{\sin^2(\theta)}{\cos(x)-\cos(\theta)}, \tag{17}$$

where the "dressed" energy of the spinon $\varepsilon(x) < 0$ in the region $(-A, A)$. Hence $\pm A$ plays the role of the Fermi points. and the ground-state energy per site is

$$e_0 = \frac{\Delta}{4} + \frac{1}{2\pi}\int_{-A}^{A} dx \varepsilon(x) \frac{\sin(\theta)}{\cosh(x)-\cos(\theta)}. \tag{18}$$

For example, the ground-state energy at $h = 0$ per site e_0 for $-1 < \Delta < 1$ is equal to

$$e_0 = \frac{\Delta}{4} - \sin(\theta)\int_0^{\infty} dx \left(1 - \frac{\tanh(\theta x)}{\tanh(\pi x)}\right), \tag{19}$$

where $\Delta = \cos(\theta)$. For $\Delta > 1$ we can write

$$e_0 = -\frac{\Delta}{4} - \sinh(\Phi)\sum_{n=0}^{\infty} e^{-2n\Phi}\tanh(n\Phi), \tag{20}$$

where $\Delta = \cosh(\Phi)$. Finally, for $\Delta < -1$ the ground-state energy per site is $e_0 = \Delta/4$.

In Fig. 1 the exact result for the ground-state energy of the spin-1/2 chain at $h = 0$ is presented. For the description of the properties of the spin subsystem at nonzero temperatures within the Bethe ansatz scheme one can use several methods. For our purpose the most convenient one is the so-called quantum transfer matrix approach [28]; see also, e.g., [25,29–35]. For the considered spin subsystem at finite temperatures we use a suitable lattice representation by a mapping which preserves the integrability. Let $R^{m_i m_{i+1}}_{a_i b_i}(u)$ be the standard R matrix of the spin-1/2 antiferromagnetic chain with the uniaxial magnetic anisotropy (let us consider the easy-plane magnetic anisotropy, $1 \leqslant \Delta \leqslant 1$, for concreteness). The nonzero matrix elements of that R matrix are $R^{21}_{12} = R^{12}_{21} = 1$, $R^{11}_{11} = R^{22}_{22} = \sin[(\theta(u+2)/2]/\sin(\theta)$, and $R^{12}_{12} = R^{21}_{21} = \sin[(\theta u)/2]/\sin(\theta)$, where the index 1 is related to the state with spin-up, and the index 2 is related to the state with spin-down. Here u is the spectral parameter, the indices a_i and b_i denote states in the Hilbert space of the spin at site i, and m denotes states in the auxiliary Hilbert space. The standard

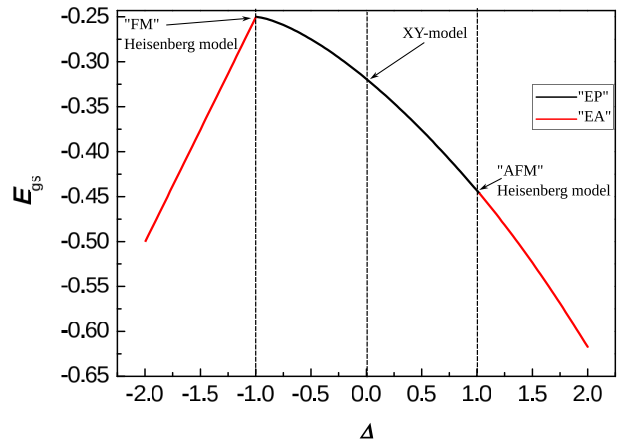

FIG. 1. The ground-state and free energy of the spin-1/2 chain as a function of the parameter Δ. Red lines–the "easy-axis" magnetic anisotropy; black line–the "easy-plane" magnetic anisotropy.

(row-to-row) transfer matrices $\tau^b_a(u)$ have the form of a trace over the auxiliary space of the product of R matrices,

$$\tau^b_a(u) = \sum_{\{m_i\}}\prod_{i=1}^{L} R^{m_i m_{i+1}}_{a_i b_i}(u). \tag{21}$$

The R matrices satisfy the Yang-Baxter equations, and thus the transfer matrices with different spectral parameters commute [25]. Then we introduce R matrices of different types, related to the initial one by the anticlockwise rotation $\bar{R}^{mn}_{ab}(u) = R^{ab}_{nm}(u)$ and by the clockwise rotation $\tilde{R}^{mn}_{ab}(u) = R^{ba}_{mn}(u)$. The transfer matrix $\bar{\tau}(u)$ can be constructed in a way similar to the case of $\tau(u)$. It is straightforward to show that the partition function Z of the considered quantum one-dimensional system is identical to the partition function of the inhomogeneous classical vertex model with alternating rows on the square lattice of size $L \times N$ (N is the Trotter number):

$$Z = \lim_{N\to\infty} \mathrm{Tr}\prod_{i=1}^{N/2} \tau(u_i)\bar{\tau}(0), \tag{22}$$

with suitable spectral parameters u_i (of order of N^{-1}). The interactions on the two-dimensional lattice are four-spin interactions with the coupling parameters depending on $(N/\beta)^{-1}$. (Here β^{-1} is the inverse temperature; in what follows we use the units in which the Boltzmann constant is unity $k_B = 1$. Also, notice that the temperature T is measured in units of J.) The system is studied in the thermodynamic limit $N, L \to \infty$ using the approach based on a transfer matrix describing transfer in a horizontal direction. The corresponding column-to-column transfer matrices are referred to as quantum transfer matrices. The magnetic field h is included via twisted boundary conditions:

$$\tau_{\mathrm{QTM}}(u) = \sum_{\{m_i\}} e^{m_1 h/T}\prod_{i=1}^{N/2} R^{m_{2i-1}m_{2i}}_{a_{2i-1}b_{2i-1}}(u-u_i)\tilde{R}^{m_{2i}m_{2i+1}}_{a_{2i}b_{2i}}. \tag{23}$$

The quantum transfer matrix posses a gap between the largest eigenvalue and the next-largest ones. Thus the free energy of the spin subsystem per site f can be calculated from the

largest eigenvalue of the quantum transfer matrix $\Lambda_0(u)$ as $f = -T \lim_{N\to\infty} \ln[\Lambda_0(u=0)]$.

Let us use the notations $\phi_+(x) = \prod_{l=1}^{N/2} \sinh[\theta(x+ix_l)/2]$, $\phi_1(x) = \sinh^{N/2}[\theta x/2]$, and $Q(x) = \prod_{j=1}^{M^*} \sinh[\theta(x-x_j)/2]$. The rapidities x_j (related to the quasimomenta $k_j = i\ln(\sinh[\theta(x_j - i/2)]/\sinh[\theta(x_j+i/2)])$ can be obtained from the solution of the Bethe ansatz equations written in the form

$$\frac{\phi_-(x_j)\phi_+(x_j+2i)}{\phi_+(x_j)\phi_-(x_j-2i)} = e^{2h/T}\frac{Q(x_j+2i)}{Q(x_j-2i)}, \quad j = 1,\dots M^*. \tag{24}$$

From the algebraic Bethe ansatz (or the quantum inverse scattering method) we can write [34,35] $\Lambda_{\rm QTM}(ix) = \Lambda(x)/\sinh^N(i\theta)$, where $\Lambda(x) = \lambda_1(x) + \lambda_2(x)$, and

$$\lambda_1(x) = \phi_+(x)\phi_-(x-2i)e^{h/T}\frac{Q(x+2i)}{Q(x)},$$
$$\lambda_2(x) = \phi_-(x)\phi_+(x+2i)e^{-h/T}\frac{Q(x-2i)}{Q(x)}. \tag{25}$$

The largest eigenvalue of the quantum transfer matrix (QTM) Λ_0 is related to $M^* = L/2$. Let us introduce the auxiliary functions $b(x) = \lambda_1(x+i)/\lambda_2(x+i)$, and $\bar b(x) = \lambda_2(x-i)/\lambda_1(x-i)$. It is easy to see that

$$\Lambda(x+i) = [1+b(x)]\lambda_2(x+i), \ \Lambda(x-i) = [1+\bar b(x)]\lambda_1(x-i). \tag{26}$$

Then we can write

$$b(x) = e^{2h/T}\prod_{\pm}\frac{\phi_\pm(x\pm i)}{\phi_\pm(x+2i\pm i)}\frac{Q(x+3i)}{Q(x-i)},$$
$$\bar b(x) = e^{-2h/T}\prod_{\pm}\frac{\phi_\pm(x\pm i)}{\phi_\pm(x-2i\pm i)}\frac{Q(x-3i)}{Q(x+i)}. \tag{27}$$

One can see that these auxiliary functions are analytic, and nonzero, and the functions $b(x)$ and $1+b(x)$ have constant asymptotic behavior for the strip $-1 < {\rm Im}x \leqslant 0$. The functions $\bar b(x)$ and $1+\bar b(x)$ have constant asymptotic behavior for the strip $0 \leqslant {\rm Im}x < 1$. Then we can introduce functions $a(x) = b[(2/\pi)(x+i\epsilon)]$ and $\bar a(x) = \bar b[(2/\pi)(x-i\epsilon)]$ with an infinitesimal $\epsilon > 0$. By taking the logarithmic derivative of these functions, Fourier transforming the equations, eliminating the functions $Q(x)$, and then inverse-Fourier transforming, we obtain the final set of two nonlinear integral equations [28,29,32–35]. Then we take the limit $N \to \infty$. Proceeding this way, we find for our system the following set of nonlinear integral equations, see below. For $f(x) = -T\lim_{N\to\infty}\ln\Lambda(x)$ we can write

$$f(ix) = e_0(x) - \frac{T}{2\pi}\int dy \frac{\ln([1+a(y)][1+\bar a(y)])}{\cosh(x-y)}. \tag{28}$$

Taking the limit $x = 0$, we get the free energy per site $f(0)$, with $e_0(0)$ being the ground-state energy per site. In the case $|\Delta| > 1$, it is possible to perform a similar procedure.

The nonzero temperature thermodynamics for $\Delta > 1$ is determined by the solution of the following set of nonlinear integral equations with respect to the functions $a(x)$ and $\bar a(x)$:

$$\ln a = -\frac{2\pi\sinh(\Phi)c(x)}{T} + \frac{h}{T} + \int_{-\pi}^{\pi} dy g(x-y)\ln(1+a) - \int_{-\pi}^{\pi} dy g(x-y-i[2\Phi-\epsilon])\ln(1+\bar a),$$
$$\ln \bar a = -\frac{2\pi\sinh(\Phi)c(x)}{T} - \frac{h}{T} + \int_{-\pi}^{\pi} dy g(x-y)\ln(1+\bar a) - \int_{-\pi}^{\pi} dy g(x-y+i[2\Phi-\epsilon])\ln(1+a), \tag{29}$$

where ϵ is an infinitesimally small number,

$$c(x) = \frac{1}{2\pi}\left[\frac{1}{2} + \sum_{n=1}^{\infty}\frac{\cosh(inx)}{\cosh(n\Phi)}\right], \tag{30}$$

and

$$g(x) = \frac{1}{2\pi}\left[\frac{1}{2} + \sum_{n=1}^{\infty}\frac{e^{-n\Phi}\cosh(inx)}{\cosh(n\Phi)}\right], \tag{31}$$

with $\cosh(\Phi) = \Delta$. The free energy per site is

$$f = e_0 - T\int_{-\pi}^{\pi} dx c(x)\ln[(1+a)(1+\bar a)]. \tag{32}$$

For $-1 < \Delta < 1$ we have the same set of integral equations for a and $\bar a$ with the replacements $\sinh(\Phi) \to \sin(\theta)$, $h \to \pi h/(\pi-\theta)$, with $\Phi \to \theta$ in the shift of the kernel, and the replacement in the limits of integration $\pi \to \infty$, with

$$c(x) = \frac{1}{2\theta\cosh(\pi x/\theta)}, \tag{33}$$

and

$$g(x) = \frac{1}{4\pi}\int_{-\infty}^{\infty} dy \frac{\sinh[(\pi-2\theta)y/2]\cos(xy)}{\cosh(\theta y/2)\sinh[(\pi-\theta)y/2]}, \tag{34}$$

where $\cos(\theta) = \Delta$. The free energy per site is again described by Eq. (32) but with different values of a, $\bar a$, and e_0, determined for $-1 < \Delta < 1$.

Let us consider the deviation of the spin-chain system from the SU(2) symmetric case [the Heisenberg situation, in which $\mathcal{H}_0 = \sum_n(\mathbf{S}_n\cdot\mathbf{S}_{n+1})$, see (2)] with the addition $d\sum_n S_n^z S_{n+1}^z$. The parameter d is related to Δ by the relation $\Delta = {\rm sign}(\Delta) + d$.

It is convenient to distinguish four possibilities. For the ferromagnetic (FM) situation (for the isotropic exchange one has $\Delta = -1$) the system with the parameter $d < 0$ describes the ferromagnetic spin chain with the "easy-axis" (EA) magnetic anisotropy. On the other hand, the case with $d > 0$ describes the ferromagnetic spin chain with the "easy-plane" (EP) magnetic anisotropy. For the antiferromagnetic (AFM) situation (for the isotropic exchange one has $\Delta = 1$), the case $d > 0$ describes the easy-axis spin-chain antiferromagnet, while the case with $d < 0$ is related to the antiferromagnetic spin chain with the easy-plane magnetic anisotropy.

III. INTERACTION WITH THE ELASTIC SUBSYSTEM

Now let us show how the intersite spin nematic ordering (related to the one distinguished axis) can appear in spin-1/2 chain materials. It is known that the interion magnetic anisotropy is caused due to two factors. First, the crystalline electric field of nonmagnetic ions (ligands) surrounding the magnetic ion affects the orbital moment of the latter. Then, the spin-orbit interaction taken in the lowest approximation yields the anisotropy of the exchange interaction [36], see also [25].

On the other hand, the change of the co-ordinates of magnetic ions can renormalize the value of the exchange interaction. In the main linear approximation a strain ϵ_{zz} renormalizes the exchange parameter J_z of a spin system as $J_z \to J_z(1 - a\epsilon_{zz})$, where $a = (\partial J_z/\partial R_z)$ is the component of the tensor of the magnetoelastic interaction and R is the co-ordinate of the magnetic ion. Suppose initially the spin chain had the isotropic exchange interaction, and the strain ϵ_{zz} introduces the renormalization of the exchange constant for the $z-z$ spin-spin coupling in the chain, as described above. It is clear that in our notations the parameter d is caused by the related strain ϵ_{zz} of the elastic subsystem of the spin-chain crystal with the initially isotropic exchange, $d = a\epsilon_{zz}$, where a is the spin-elastic coupling parameter. The strain reduces the symmetry of the crystal surrounding of magnetic ions, e.g., from the cubic to the tetragonal one. Such a strain enlarges the energy of the system as $C\epsilon_{zz}^2/2$, where C is related elastic modulus [37] (notice that we measure C in units of the exchange interaction for $J = 1$). We consider the elastic subsystem classically and in the ground state, because the characteristic elastic energy, the Debye temperature, is much stronger than characteristic exchange coupling in spin-chain materials. Then the total Hamiltonian can be written as $\mathcal{H}_0 + Nd^2\alpha/2$, where $\alpha = C/a^2$. Small values of α correspond to the strong coupling between the spin and elastic subsystems, while large α values describe the weak coupling. For some values of the parameter d the energy of the spin subsystem becomes smaller than the one at $d = 0$, i.e., in the isotropic SU(2) symmetric situation. This is why the nonzero strain ϵ_{zz} 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 similar to the Jahn-Teller effect (however, for the spin subsystem): The strain of the elastic subsystem, by reducing the symmetry, lifts the degeneracy of the spin subsystem. The degeneracy of the latter is caused by the fact that for $d = 0$ the direction of the spin nematic order parameter is arbitrary. Unlike Ref. [38], in which we considered the spin-1 chain material with antiferromagnetic interactions with respect to the single-ion spin nematic ordering, here we study the spin-1/2 subsystem for both ferro- and antiferromagnetic interactions and the onset of the interion spin nematic ordering.

Taking into account that $\langle S_j^z S_{j+1}^z\rangle = \partial f/\partial d$ (and similar definition for the ground state), we calculate the value of $\langle S_j^z S_{j+1}^z\rangle$, using the exact Bethe ansatz solution, as a function of d at several values of the external magnetic field and temperature together with the lines $-\alpha d$ (the derivative of the elastic contribution to the energy with respect to d) for the SU(2) symmetric case. The points of crossing the lines correspond to the phase transitions to the state with nonzero d. These states are the intersite spin nematic states, because the intersite spin nematic order parameters $\langle S_j^z S_{j+1}^z\rangle$ are nonzero.

It is important to point out that the effect similar to that of the strain of ligands in spin-chain crystals can be also realized for organic spin-chain materials. Our theory can be applied for that situation too: In our notations ϵ plays the role of vibrations of organic molecules. The spin nematic ordering can take place due to the coupling between the spin and the vibronic subsystems of the organic spin-chain materials.

A. Spin nematicity of the antiferromagnetic spin-1/2 chain with the easy-axis anisotropy

In this case the exact solution shows that the addition to the ground-state energy and the free energy of the spin subsystem is negative for $d \neq 0$. We plot in Fig. 2 the results of calculations for the spin-1/2 chain material with the antiferromagnetic coupling between spins for positive d. We see that depending on the parameter α (which measures the effective strength of the coupling between the elastic and the spin subsystems of the material), temperature and the external field several situations can be realized.

In zero external magnetic field (see Fig. 2), the crossings at $d \neq 0$ exist for low temperatures. With the growth of the temperature the value of the magnetic anisotropy caused by the distortion is decreased. Then for high enough temperatures (stronger than the spin-spin interactions) the crossing exists at zero value of d only, because the intersite spin-spin coupling is much smaller than the temperature. Large values of the parameter α (large slopes of the line $-\alpha d$) correspond to smaller values of d in the spin nematic ordered phase and hence to smaller magnetic anisotropy.

For small values of the external magnetic field the situation is similar to the case $h = 0$, see Fig. 2. The external magnetic field causes the decrease of the anisotropy parameter in the spin nematic ordered phase and the decrease of the temperature, at which the spin nematicity becomes zero.

On the other hand, for larger values of the external magnetic field (see Fig. 2), the crossings (at $d \neq 0$) exist only in the ground state or at low temperatures. Notice that the crossing (and hence the phase transition to the spin nematic ordered phase) exists only for small enough values of the parameter α, i.e., for strong spin-lattice couplings. The behavior is clear, because at such values of the magnetic field the nonzero d produces positive addition to the energy of the spin subsystem, see Fig. 2, and there is no energy gain for the coupled spin-lattice system due to the strain.

B. Spin nematicity of the antiferromagnetic spin-1/2 chain with the easy-plane anisotropy

In this case the signs of the additions to the ground-state energy and the free energy of the system depend on the value of the applied magnetic field. For $h = 0$ those additions are positive, and there is no gain in the energy of the spin subsystem due to nonzero d. However, for large enough values of h, the addition to ground-state energy and the free energy caused by $d \neq 0$ becomes negative, which implies the possibility of a phase transition to the spin nematic phase.

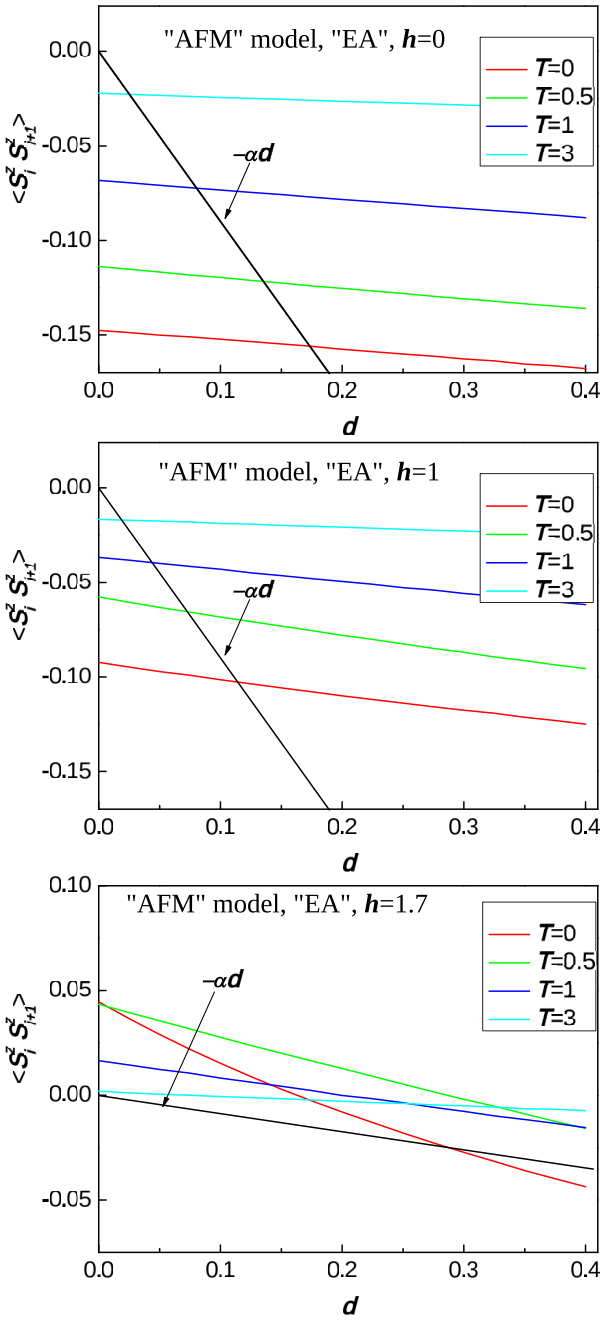

FIG. 2. Derivatives of the spin and elastic contributions to the ground-state energy and free energy of the coupled spin-elastic subsystems for the antiferromagnetic coupling as a function of d. Upper panel corresponds to $h = 0$ and $\alpha = 0.9$, middle panel–to $h = 1$ and $\alpha = 0.9$, and lower panel–to $h = 1.7$ and $\alpha = 0.085$.

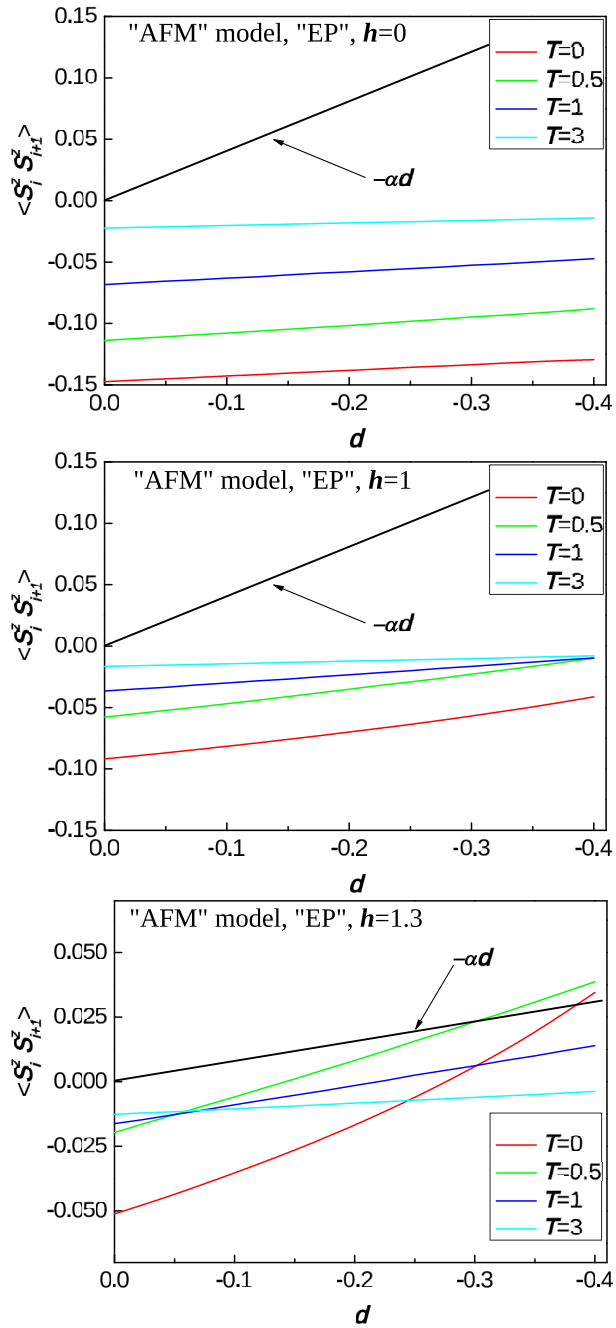

FIG. 3. The derivatives of the spin and the elastic contributions to the ground-state energy and the free energy of the coupled spin-elastic subsystems for the antiferromagnetic coupling as a function of d. Upper panel corresponds to $h = 0$, and $\alpha = 0.4$, middle panel–to $h = 1$, and $\alpha = 0.4$, and lower panel–to $h = 1.3$, and $\alpha = 0.08$.

Figure 3 manifests the results of calculations for the spin-1/2 chain material with the antiferromagnetic coupling between spins for negative d. In zero and in the weak enough magnetic field there are no crossings. This means that the spin-1/2 with the antiferromagnetic Heisenberg interactions between neighboring spins coupled to the lattice is stable with respect to the transition to the spin nematic phase. On the other hand, for larger values of the magnetic field crossings appear. Again, the phase transition to the spin nematic ordered state takes place for large values of the coupling between the spin and lattice subsystems. The values of the easy-plane magnetic anisotropy are larger for larger values of the external magnetic field and decrease with the growth of temperature.

C. Spin nematicity of the ferromagnetic spin-1/2 chain with the easy-axis anisotropy

The exact solution evidences that for the spin chain with the ferromagnetic coupling between spins, the addition to

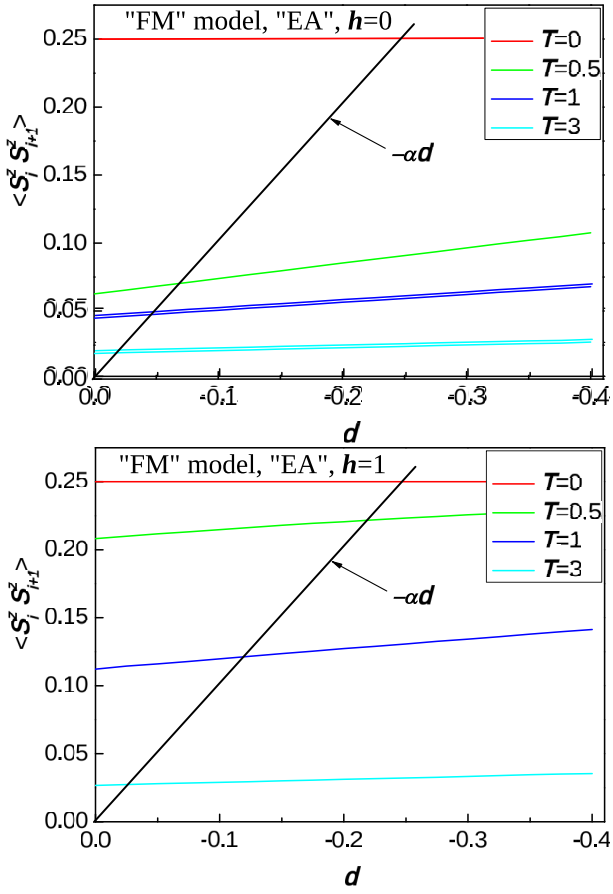

FIG. 4. The derivatives of the spin and the elastic contributions to the ground-state energy and the free energy of the coupled spin-elastic subsystems for the ferromagnetic coupling as a function of d. Upper panel corresponds to $h = 0$, and $\alpha = 1$, lower panel–to $h = 1$, and $\alpha = 1$.

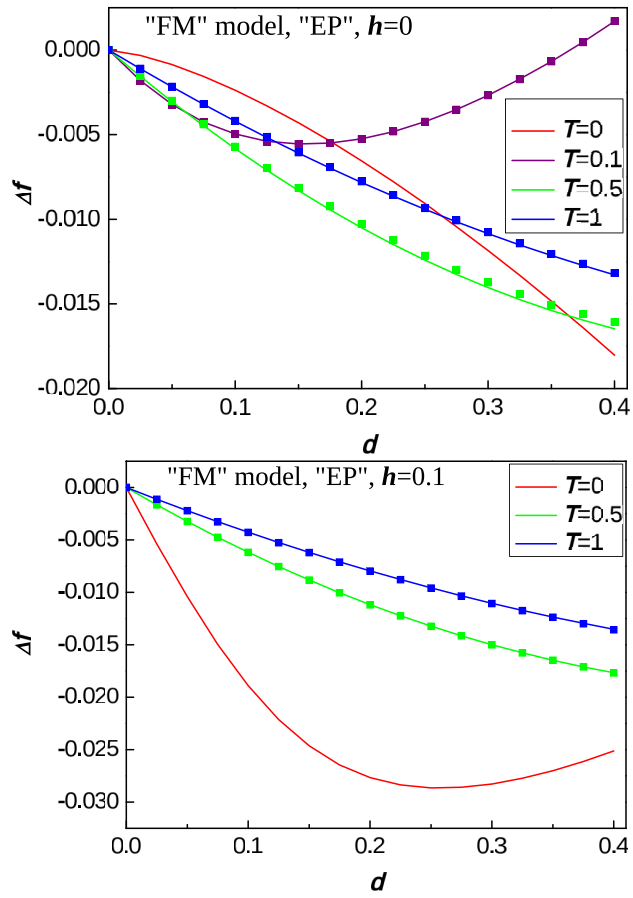

FIG. 5. The derivation from the isotropic case (i.e., $d = 0$) of the ground state and free energy $\Delta f = f(T, h, d) - f(T, h, d = 0)$ at $T = 0, 0.1, 0.5, 1$ for the ferromagnetic spin-1/2 chain with easy-plane magnetic anisotropy. The boxes correspond to quantum Monte Carlo simulations. Upper panel corresponds to $h = 0$, lower panel–to $h = 0.1$.

the ground-state energy and the free energy is negative for nonzero $d < 0$ (i.e., for the easy-axis magnetic anisotropy).

In Fig. 4 the results for the spin-1/2 chain material with the ferromagnetic coupling between spins for negative values of d are presented. Hence, for the case of the ferromagnetic spin-spin interactions and negative values of d (the easy-axis magnetic anisotropy), the coupling between the spin and the elastic subsystem of the material yields the intersite spin nematic ordering for any values of the applied magnetic field. One can see that again, the larger (absolute) values of the parameter of the anisotropy (and hence the spin nematic order parameter) correspond to smaller values of the effective coupling between the spin and the elastic subsystems α and smaller values of temperature (at high enough temperatures the crossing exists at $d = 0$). For nonzero temperatures the external magnetic field in general reduces the (absolute) value of the magnetic anisotropy; however, in general the magnetic field dependence of the induced d is nonmonotonic.

D. Spin nematicity of the ferromagnetic spin-1/2 chain with the easy-plane anisotropy

The exact solution manifests that for the ferromagnetic interaction between spins the addition to the ground-state energy caused by nonzero d is negative for any value of the magnetic field. However, for nonzero temperatures the addition to the free energy can be positive or negative, depending on the values of the temperature and the applied magnetic field.

Figure 5 illustrates how the temperature and the external magnetic field act. At $h = 0$, see Fig. 5, the addition to the free energy $\Delta f = f(T, h, d) - f(T, h, d = 0)$ of the spin subsystem at low temperature can become positive; however, with the growth of T the addition to the free energy becomes negative. An already weak external magnetic field yields the negative sign to the addition to the free energy caused by $d \neq 0$, and further growth of h does not change the situation.

To check our calculations we performed additional quantum Monte Carlo (QMC) simulations [39,40]. The equations obtained in the framework of the Bethe ansatz approach are exact, but these are nonlinear integral equations, and hence they can be solved, generally, numerically only. The numerical solution of such equations has its own limitation (the stability boundary, etc.). The quantum Monte Carlo method, in turn, is the approximate method with its own limitation—depending on the realization, it can have

temperature limitations, anisotropy limitations, etc. That is why we used both methods to improve the reliability of the obtained results. As far as the direct measurements of free energy are impossible in this QMC method, we calculated free-energy derivation as $\Delta f(d) = \int_0^d c(x)dx$, where the correlator $c = \langle S_j^z S_{j+1}^z \rangle$ was measured in QMC calculations as

$$c = \frac{1}{L-1}\left\langle \sum_{j=1}^{L-1} S_j^z S_{j+1}^z \right\rangle_{\text{QMC}}. \tag{35}$$

Here $\langle \ldots \rangle_{\text{QMC}}$ means averaging over the QMC sampling.

Figure 6 presents the results for the spin-1/2 chain material with the ferromagnetic coupling between spins for positive values of d. Note that for convenience we plot αd in these figures. Hence, for the case of the ferromagnetic spin-spin interactions and positive values of d (the easy-plane type of the magnetic anisotropy), the interaction between the spin and the elastic subsystem of the material produces the intersite spin nematic ordering for any values of the applied magnetic field and temperature. One can see that, again, the larger (absolute) values of the parameter of the anisotropy (and hence the spin nematic order parameter) correspond to smaller values of the effective coupling between the spin and the elastic subsystems α and smaller values of temperature (at high enough temperatures the crossing exists at $d = 0$). For nonzero temperatures the external magnetic field in general reduces the (absolute) value of the magnetic anisotropy; however, in general the magnetic field dependence of the induced d is nonmonotonic, in particular at low temperatures and small values of the external magnetic field.

In summary, for the ferromagnetic spin-1/2 chain material the spin nematic ordering exists for any value of the coupling α between the spin and the elastic subsystems, the temperature, and the magnetic field. It is different from the spin-1 chain material [38], where critical values of α exist. The same is true for the antiferromagnetic spin-1/2 chain material with the easy-axis magnetic anisotropy, for any values of α, T, and h. The situation is different for the antiferromagnetic spin chain with the easy-plane anisotropy. In the absence of the magnetic field there is no spin nematic ordering for any values of α and T. If the magnetic field is nonzero, there are two possibilities. First, if the field is large enough, for any coupling parameter α there exists a temperature range where the spin nematic order exists. This situation is described in Fig. 7, where the h-T phase diagram is presented. The physical meaning of the line in Fig. 7 is clear: Without the magnetic field and for small enough values of h, the spin-spin correlation function $\langle S_n^x S_{n+1}^z \rangle$ is negative, and for larger values of h it becomes positive. There is also another solution for $d \neq 0$ of the self-consistency equation, but it corresponds to very large values of the magnetic field and very strong coupling between the spin and elastic subsystems.

Unfortunately, it is impossible to measure the value of α in experiments. However, α is related to the constant of the magnetoelastic coupling. The latter can be determined in magnetoacoustic experiments that study the magnetic field dependence of relative changes of the sound velocity. Using the data of magnetoacoustic experiments with known spin-chain materials, see, e.g., [15,41,42], we can estimate the values

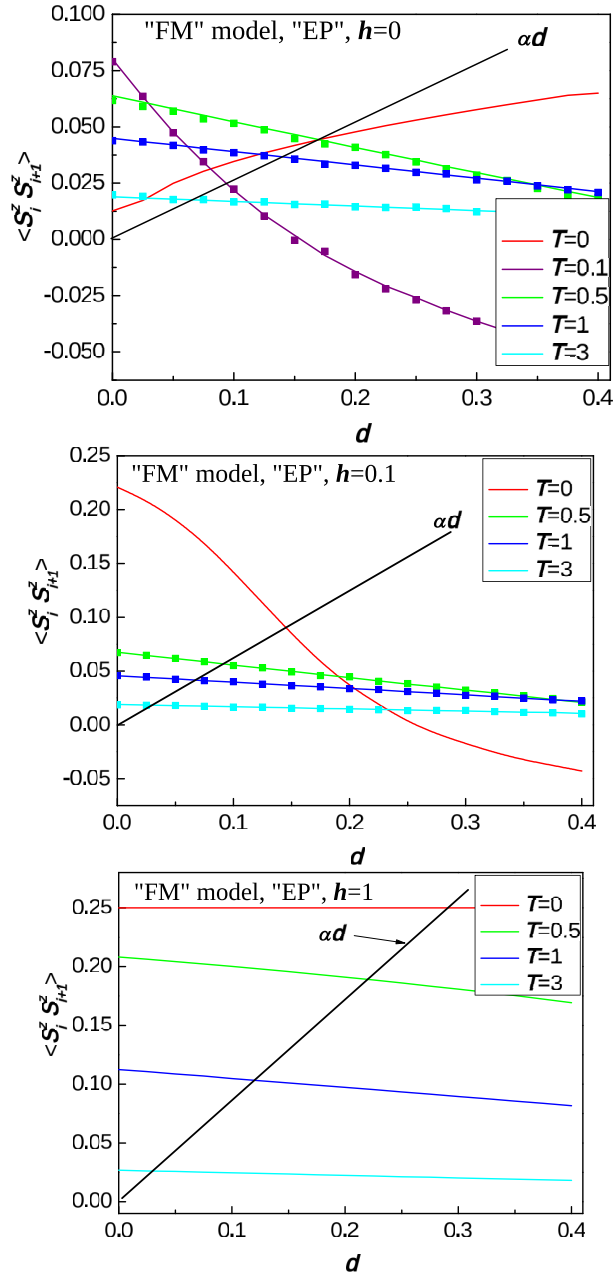

FIG. 6. The derivatives of the spin and the elastic contributions to the ground-state energy and the free energy of the coupled spin-elastic subsystems for the ferromagnetic coupling as a function of d. The boxes correspond to quantum Monte Carlo simulations. Upper panel corresponds to $h = 0$, and $\alpha = 0.25$, middle panel–to $h = 0.1$, and $\alpha = 0.6$, and lower panel–to $h = 1$, and $\alpha = 0.85$.

of α (we restore the value of the exchange coupling J in those estimations). The estimations imply $\alpha \sim 10^2 - 10^3$ for systems with antiferromagnetic interactions along chains, i.e., the couplings between the spin and elastic degrees of freedom were small. Notice that in Refs. [15,41,42], antiferromagnetic spin-1/2 chain materials with the easy-plane magnetic anisotropy were studied. For large α (small spin-elastic couplings) the value of the spin nematic order parameter and the magnetic anisotropy d is small, $Jd \sim 0.01J$. For such a situation, the spin nematic ordering must exist for large values

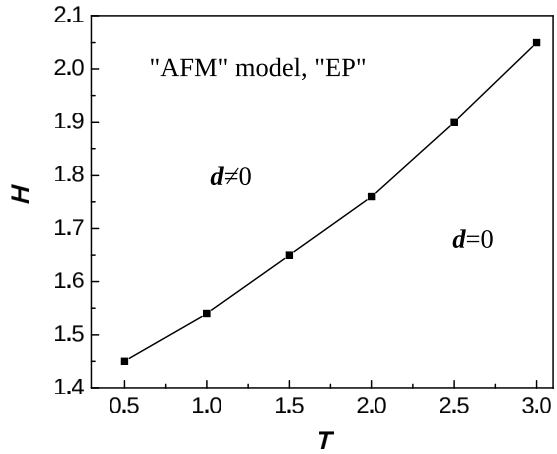

FIG. 7. h-T phase diagram for the antiferromagnetic spin-1/2 chain material with the easy-plane magnetic anisotropy. The line describes the exact results, the boxes show the results of the QMC simulations.

of the magnetic field and low temperatures. It looks like such a situation was observed in Ref. [15], where the spin nematic ordered phase existed in the strong magnetic field close to the transition to the spin-polarized phase. However, for spin-chain systems with stronger interactions between spin and lattice degrees of freedom the effect must be larger.

IV. SUMMARY

In summary, we have studied the onset of the intersite spin nematic ordering in the spin-1/2 chain material. The integrability of the spin subsystem of the coupled spin-lattice systems of those materials permits us to show that these materials can be unstable with respect to the spin nematic ordering. Using the exact solution, we have analyzed how the coupling between the spin and the elastic subsystems, temperature, and the external magnetic field can affect the intersite spin nematic ordering. Namely, we have shown that for the ferromagnetic interactions between spins, the system is unstable with respect to the appearance of the spin nematicity, related to the magnetic anisotropy of the easy-axis and the easy-plane type. The nonzero external magnetic field does not change the situation qualitatively. We have also shown that for the antiferromagnetic spin-spin coupling the system is unstable with respect to the onset of the spin nematic ordering related to the easy-axis magnetic anisotropy. On the other hand, the spin nematic ordering related to the easy-plane magnetic anisotropy is absent for $h = 0$ and can appear only for high enough values of the magnetic field.

ACKNOWLEDGMENT

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