Electromagnetic, piezoelectric, and magnetoelastic characteristics of a quantum spin chain system

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Electric, piezoelectric, and elastic characteristics of the quantum spin-1/2 chain system are calculated. Using the exact analytical solution we show that electric permittivity, piezoelectric and elastic modules, and magnetic characteristics can manifest strong dependencies on the values of the external magnetic, electric field, external strain, and temperature.

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I. INTRODUCTION

Magnetoelectric, piezoelectric, and magnetoelastic effects are the manifestation of the coupling between the electric, magnetic, and elastic subsystems of the studied compounds. Possible uses of those effects in micro- and nanoelectronics, e.g., spintronics [1,2], as switching devices, or as writing and reading devices for memory storage, which can be governed by external fields and strains attract the attention of researchers. On the other hand, such attention to those effects is caused by the interesting physics behind them. The best known subjects for such a purpose are so-called multiferroics, i.e., substances which have both magnetic and ferroelectric properties (see, e.g., [3–9]). As such, most of the studies were performed on magnetically ordered systems, like ferro- and antiferromagnets (like ferroborates; for the recent studies see [10–13]). However, it is clear from general grounds that similar effects can exist in spin systems without magnetic ordering.

Recently we have studied magnetoelectric, piezoelectric, electromagnetic and magnetoacoustic effects in the quantum paramagnet (a single spin) [14,15], where the quadrupole spin moment, the key subject for such systems, has a single-ion nature. It is also interesting to study the quantum many-body spin insulating system, in which similar effects can take place; however, the quadrupole spin moment is of interspin nature. Quantum spin chain compounds can serve as a very good testing ground for consideration of the interaction between electric, magnetic, and elastic subsystems. Here the reduced dimensionality preserves the system against magnetic ordering at nonzero temperatures [16]. On the other hand, those systems manifest quantum many-body effects. Last but not least, for spin-1/2 chains there exist many exact theoretical results [17], which give the opportunity to check them in comparison with the data of experiments in spin chain compounds.

The goal of the present study is to find the effects of the renormalization of the magnetic, electric, and elastic characteristics of an insulating spin chain system due to the coupling between the electric, magnetic, and elastic subsystems of the crystal. The ligands surrounding magnetic ions determine the crystalline electric field, which acts on magnetic ions and, together with the spin-orbit interaction and the exchange one, defines the magnetic anisotropy of the effective (indirect superexchange in nature) interaction between spins in the considered spin model. Then the interaction between the spin, charge, and elastic subsystems of the crystal can yield magnetoelectric, piezoelectric, and magnetoelastic effects in such a quantum many-body spin system. Below we calculate how such an interaction can be observed in the temperature, magnetic field, electric field, and external strain dependencies of the characteristics of such a crystal, like the magnetic moment, magnetic susceptibility, electric permittivity, and piezoelectric and elastic modules.

II. CONSIDERED SYSTEM

The Hamiltonian of the considered model can be written as [11,18]

$$\begin{aligned}\mathcal{H} = &-g\mu_B H \sum_n S_n^z - I\sum_n \left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y\right)\\ &-J\sum_n \left(S_n^x S_{n+1}^x - S_n^y S_{n+1}^y\right) - J_z \sum_n S_n^z S_{n+1}^z + \frac{Cu^2}{2}\\ &-\varepsilon \frac{E^2}{8\pi} + eEu + aE\sum_n \left(S_n^x S_{n+1}^x - S_n^y S_{n+1}^y\right)\\ &+b(u-u_0)\sum_n \left(S_n^x S_{n+1}^x - S_n^y S_{n+1}^y\right), \end{aligned} \tag{1}$$

where $S_n^{x,y,z}$ are the operators of spin projections of the spins 1/2 situated at the site n, g is the effective g factor for the magnetic field H (supposed to be directed along the z axis), μ_B is the Bohr magneton, $I = (J_x + J_y)/2$ and $J = (J_x - J_y)/2$, $J_{x,y,z}$ are the parameters of the magnetically anisotropic exchange interaction (we consider the case with $-|I| \leqslant J_z \leqslant |I|$; the most interesting effects are related to the antiferromagnetic spin-spin interactions), $E \equiv E_x$ is the electric field directed along the x axis, ε is the electric permittivity, e is the piezoelectric modulus (do not confuse with the charge of the electron), C is the elastic modulus, u is the strain ($u \equiv u_{xx} - u_{yy}$, and u_0 is the static strain), and a and b are the coefficients of the magnetoelectric and magnetoelastic couplings, respectively (all issues are connected with the coordinate x).

The form of the electromagnetic and strain-spin and piezoelectric coupling is the particular case of the general interactions between spin, electric, and elastic degrees of freedom $\sum_{m,n}\sum_{ipq} a_{ipq}E_i S_n^p S_m^q$, $\sum_{m,n}\sum_{ijpq} b_{ijpq}u_{ij}S^pS^q$, and $\sum_{ipq} e_{ipq}E_i u_{pq}$, where n, m numerate the lattice sites, and $i, j, p, q = x, y, z$ [18] with a, b, and e being the components of the tensors a_{ipq}, b_{ijpq}, and e_{ipq}. Here we use the form of magnetoelectric and magnetoelastic couplings similar to [11] where the studied effects were observed in the magnetically ordered multiferroic. Generally speaking, according to the above, the considered effect does not depend on the orientation of the spin chain directly. It is rather related to the orientation of the axes of the magnetic anisotropy of the spin-spin interaction in the chain. The latter is determined mostly (if not taking into account rather weak magnetic dipole-dipole interaction) by the distribution of nonmagnetic ligands, surrounding magnetic ions, through which the indirect exchange between spins of magnetic ions is realized. The spin-orbit interaction together with the orientation of orbitals of ligands and magnetic ions affects the anisotropy of the interspin interactions in the chain, the key issue of the present study. However, e.g., the effect of the electric field will be maximal for the orientation of the chain perpendicular to the direction of the electric field (x axis). On the other hand, the strain must be in the xy plane of the crystal; i.e., in that case, we deal with the strains of ligands in the plane, perpendicular to the direction of the chain.

III. GENERAL APPROACH

Using the standard formulas of the elasticity theory [19]

$$\sigma = \frac{\partial F}{\partial u} = Cu + eE + bQ, \tag{2}$$

where F is the free energy of the system, σ is the elastic deformation, $Q = (1/N)\langle\sum_n (S_n^x S_{n+1}^x - S_n^y S_{n+1}^y)\rangle$ (the brackets denote the averaging with the density matrix, and N is the length of the chain) is the average value of the operator of the component of the quadrupolar spin moment of the chain [20], and the definition

$$e = \frac{d\sigma}{dE}, \tag{3}$$

for the effective piezoelectric modulus [18], we get

$$e_{\rm eff} = e + b\frac{\partial Q}{\partial E}. \tag{4}$$

Then using the equation for the electric induction D,

$$D = -4\pi\frac{\partial F}{\partial E}, \tag{5}$$

and the definition of the electric permittivity,

$$\varepsilon = \frac{\partial D}{\partial E}, \tag{6}$$

we find the effective permittivity

$$\varepsilon_{\rm eff} = \varepsilon - 4\pi a\frac{\partial Q}{\partial E}. \tag{7}$$

Finally, according to the elasticity theory [19] we have

$$\rho\frac{\partial^2 u}{\partial t^2} = \frac{d\sigma}{dx}, \tag{8}$$

where ρ is the density of the crystal. Calculating the right-hand side of that equation we get

$$\frac{\partial\sigma}{\partial x} = C\frac{\partial u}{\partial x} + e\frac{\partial E}{\partial x} + b\left(\frac{\partial Q}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial Q}{\partial E}\frac{\partial E}{\partial x}\right). \tag{9}$$

Then using the equation of the electric neutrality (we use here only the necessary component of the electric induction)

$$(\nabla\cdot D) = \varepsilon\frac{\partial E}{\partial x} - 4\pi e\frac{\partial u}{\partial x} - 4\pi a\left(\frac{\partial Q}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial Q}{\partial E}\frac{\partial E}{\partial x}\right) = 0 \tag{10}$$

we obtain

$$\frac{\partial\sigma}{\partial x} = \left(\frac{\partial u}{\partial x}\right)\left[C + 4\pi\frac{ee_{\rm eff}}{\varepsilon_{\rm eff}} + \left(b + 4\pi a\frac{e_{\rm eff}}{\varepsilon_{\rm eff}}\right)\frac{\partial Q}{\partial u}\right]. \tag{11}$$

The right-hand side of the latter can be presented via the effective elastic modulus $C_{\rm eff}$. Let us denote $J^{\rm eff} = J - aE - b(u - u_0)$. We obtain $Q = -\partial F/\partial J^{\rm eff}$, and $\partial Q/\partial E = -a(\partial Q/\partial J^{\rm eff})$ and $\partial Q/\partial u = -b(\partial Q/\partial J^{\rm eff})$. Then we can take into account that $\partial Q/\partial J^{\rm eff} = \chi_Q$ is the component of the tensor of the quadrupolar susceptibility. It yields

$$e_{\rm eff} = e - ab\chi_Q,$$
$$\varepsilon_{\rm eff} = \varepsilon + 4\pi a^2\chi_Q, \tag{12}$$

and

$$C_{\rm eff} = C - b^2\chi_Q + 4\pi\frac{e_{\rm eff}^2}{\varepsilon_{\rm eff}}$$
$$= C + \frac{4\pi e^2 - b(8\pi ae + b\varepsilon)\chi_Q}{\varepsilon + 4\pi a^2\chi_Q}. \tag{13}$$

Taking into account that the component of the quadrupolar susceptibility is positive, we see that the change of the electrical permittivity $\varepsilon_{\rm eff} - \varepsilon$ is positive. The change of the elastic modulus $C_{\rm eff} - C$ exists even for $a = 0$, i.e., for the absent magnetoelectric coupling (in that case, however, the piezoelectric coupling produces the constant term). The change obviously consists of two contributions (see the first line of the above formula). The first contribution (the magnetoelastic contribution) is negative; it manifests the softening of the elastic modulus due to the magnetoelasticity. The second term is positive; it manifests the hardening of the elastic modulus, caused by the piezoelectricity. Hence, the softening or the hardening of the elastic modulus (the sign of the change) of the considered system depends on whether the quadrupole susceptibility is larger or smaller than $4\pi e^2/b(8\pi ae - b\varepsilon)$ (see the second line). Finally, the sign of the change of the piezoelectric modulus $e_{\rm eff} - e$ depends on the sign of $(-ab)$.

For convenience one can introduce the relative changes of the electric permittivity $\Delta\varepsilon = \varepsilon_{\rm eff} - \varepsilon$, the piezoelectric modulus $\Delta e = e_{\rm eff} - e$, and the elastic modulus $\Delta C = C_{\rm eff} - C$ (the latter is connected with the relative change of the sound velocity $\Delta v/v \approx \Delta C/2C$ for high symmetric lattices).

On the other hand, we can see that the magnetic moment of the system depends on the value of the external electric field E and on the static and the internal strains u_0 and u (i.e., on the characteristics of the elastic subsystem).

IV. SPIN CHAIN FEATURES

Below we consider the cases which permit analytical solutions. For example, let us consider the case $J_z = 0$, for which we can use the well-known exact solution for the spin-1/2 XY chain (see, e.g., [17]). Here we have

$$\chi_Q = -\frac{\partial^2 F}{\partial J^2}, \tag{14}$$

and the z projection of the average magnetic moment $M = (g\mu_B/N)\sum_n \langle S_n^z\rangle$ can be written as

$$M = -\frac{\partial F}{\partial H}, \tag{15}$$

with the magnetic susceptibility $\chi = \partial M/\partial H$, where the free energy of the system can be written as

$$F = N^{-1}\left[\frac{Cu^2}{2} - \varepsilon\frac{E^2}{8\pi} + eEu - k_B T\sum_k \ln 2\cosh(\varepsilon_k/k_B T)\right], \tag{16}$$

where T is the temperature, k_B is the Boltzmann constant, and

$$\varepsilon_k = [(g\mu_B H - I\cos(k))^2 + [J - aE - b(u-u_0)]^2\sin^2 k]^{1/2}. \tag{17}$$

Namely, the projection of the magnetic moment is

$$M = \frac{g\mu_B}{2N}\sum_k \frac{(g\mu_B H - I\cos k)}{\varepsilon_k}\tanh(\varepsilon_k/2k_B T). \tag{18}$$

It is also easy to show that the component of the magnetic susceptibility χ depends on the values of the external electric field and the static and internal strains too.

The effect of the z-z spin-spin interaction can be analytically taken into account, e.g., utilizing the well-known exact result [21] for $H = T = 0$. The energy of the ground state of the system with the Hamiltonian $\mathcal{H}_{\rm chain}$,

$$\mathcal{H}_{\rm chain} = -\sum_j \left(J_x S_j^x S_{j+1}^x + J_y S_j^y S_{j+1}^y + J_z S_j^z S_{j+1}^z\right) - g\mu_B H\sum_j S_j^z, \tag{19}$$

can be exactly obtained at $H = 0$ by using the known Baxter solution [21]. Two exchange constants can be expressed via the third one as $J_z = \mathrm{cn}(2\zeta, k)J_x$ and $J_y = \mathrm{dn}(2\zeta, k)J_x$ so that the parameter ζ is determined by the anisotropy of spin-spin interactions. Here $\mathrm{cn}(\zeta, k)$, $\mathrm{dn}(\zeta, k)$ [and $\mathrm{sn}(\zeta, k)$, see below] are Jacobi elliptic functions of the argument ζ with the modulus k. The latter determine the magnetic anisotropy of the system. The modulus k is equal to

$$k = \left[\frac{J_x^2 - J_y^2}{J_x^2 - J_z^2}\right]^{1/2}. \tag{20}$$

The ground-state energy can be written as [21]

$$E_{gs} = \frac{J_x}{8} + \frac{\pi J_x}{2K_k'}\mathrm{sn}(2\zeta, k)\sum_{n=1}^{\infty} X, \tag{21}$$

where

$$X = \sinh^2[(\tau-\lambda)n]\tanh(\lambda n)/\sinh 2\tau n), \tag{22}$$

with $\tau = \pi K_k/K_k'$, $\lambda = \pi\zeta/K_k'$ $(0 < \lambda < \tau)$, and K_k and K_k' being the complete elliptic integrals of the first kind with the modulus k and $k' = \sqrt{1-k^2}$, respectively. Then, by differentiating twice the ground-state energy E_{gs} with respect to $J = (J_x - J_y)/2$ (see also [20]), we get the value of the necessary component of the ground-state quadrupolar susceptibility χ_Q of the XYZ spin-1/2 chain. However, such an approach permits to obtain the analytic (however, exact) result, only for $H = 0$, in the ground state and for low temperatures (see [20,22]). It is also possible (and for practical purposes more convenient) to use the Hartree-Fock-like approximation to take into account the nonzero J_z coupling constant. The result can be obtained using the consideration of the Hamiltonian $\mathcal{H}_{\rm chain}$ in the Hartree-Fock-like approximation as the XY part of the spin-1/2 Hamiltonian of the one-dimensional spin-1/2 chain with the renormalized parameters. After the well-known Jordan-Wigner transformation [23] and the Fourier transformation the total Hamiltonian of the interacting spin-1/2 chain, $\mathcal{H}_{\rm chain}$, can be written as

$$\begin{aligned}\mathcal{H}_{\rm chain} = &-\frac{N[J_z + 2g\mu_B H]}{4} - \sum_k\Big[(g\mu_B H - I\cos(k) - J_z)a_k^\dagger a_k \\ &+ \frac{J}{2}\sin(k)(a_{-k}a_k + \mathrm{H.c.}) \\ &+ \frac{J_z}{N}\sum_{k_1+k_2=k_3+k_4}\cos(k_1-k_4)a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}a_{k_4},\end{aligned} \tag{23}$$

where the fermion operators a_k $(a_k^\dagger)$ are destruction (creation) operators, and N is the length of the chain. Let us introduce the parameters [24]

$$\begin{aligned} s &= \langle S_j^z\rangle, \\ r &= 2\langle S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\rangle, \\ q &= 2\langle S_j^x S_{j+1}^x - S_j^y S_{j+1}^y\rangle,\end{aligned} \tag{24}$$

which satisfy the self-consistency equations

$$\begin{aligned} s &= \frac{1}{2N}\sum_k \frac{\tilde{A}_k}{\tilde{\epsilon}_k}\tanh\left(\frac{\tilde{\epsilon}_k}{2k_B T}\right), \\ r &= -\frac{1}{N}\sum_k \frac{\tilde{A}_k\cos(k)}{\tilde{\epsilon}_k}\tanh\left(\frac{\tilde{\epsilon}_k}{2k_B T}\right), \\ q &= -\frac{i}{N}\sum_k \frac{\tilde{B}_k\sin(k)}{\tilde{\epsilon}_k}\tanh\left(\frac{\tilde{\epsilon}_k}{2k_B T}\right).\end{aligned} \tag{25}$$

For the biaxial spin-1/2 chain we can write in the Hartree-Fock-like approximation as

$$\tilde{A}_k = g\mu_B H + 2sJ_z - (I - rJ_z)\cos(k),$$
$$\tilde{B}_k = -i(J + qJ_z)\sin(k), \quad (26)$$
$$\tilde{\epsilon}_k = \sqrt{\tilde{A}_k^2 + |\tilde{B}_k|^2},$$

where brackets denote the Gibbs distribution with the Hamiltonian $\mathcal{H}_{\text{chain}} \approx \sum_k \tilde{\epsilon}_k c_k^\dagger c_k + C$, the fermion operators c_k $(c_k^\dagger)$ are destruction (creation) operators in which $\mathcal{H}_{\text{chain}}$ is diagonal in the Hartree-Fock-like approximation, and C is the operator-independent value. In the general case of nonzero $J_{x,y,z}$ we can solve Eqs. (25) analytically, e.g., for high temperatures $k_BT \gg \max(\tilde{\epsilon}_k)$. The solution is

$$s = \frac{g\mu_B H}{4k_BT - 2J_z},$$
$$r \approx \frac{I}{2k_BT + J_z},$$
$$q \approx \frac{J}{2k_BT - J_z}, \quad (27)$$
$$\tilde{A}_k \approx g\mu_B H\left(1 + \frac{J_z}{2k_BT}\right) - I\cos(k)\left(1 - \frac{J_z}{k_BT}\right),$$
$$\tilde{B}_k \approx -iJ\sin(k)\left(1 + \frac{J_z}{4k_BT}\right),$$

where $J_z \ll k_BT$. The low-temperature regime is more interesting. There correlations of the one-dimensional spin system can manifest themselves. Unfortunately, even in the ground state the analytical solution of Eqs. (25) is complicated (it can be presented as the combination of elliptic integrals, which is clear, taking into account the above presented exact solution [21]). However, the simple solution, as we show below, reveals some main features of exact results for spin-1/2 chains, at least in the ground state. We can consider the case $H = 0$ (with $s = 0$), in which the following relation holds:

$$J + qJ_z = \pm(I - rJ_z). \quad (28)$$

These relations mean that $(r + q)J_z = J_y$ for the plus sign, and $(r - q)J_z = -J_x$ for the minus sign. The self-consistency equations are simplified to

$$r = \pm q = \frac{1}{2}\tanh\left(\frac{I \mp rJ_z}{k_BT}\right),$$
$$s = 0, \quad (29)$$

with $q = r$ for the plus sign, and $q = -r$ for the minus sign. The transcendental equations (29) can be solved graphically, and the solution exists for any temperature range. It is easy to show that solution leads to the onset of a critical temperature, below which the magnetic ordering can take place. It is, of course, the artifact of the mean-field nature of the Hartree-Fock-like consideration. The critical nonzero temperature must not exist for a one-dimensional spin system with the nearest-neighbor interactions with gapless excitations [16]. For $J_x \neq J_y \neq J_z$, on the other hand, excitations are gapped. There are no exact results for gapped spin chain models with nearest-neighbor interactions which manifest spontaneous magnetic ordering at nonzero temperatures. We know that the Ising chain and the XY chain reveal ordering in the ground state [25,26]. For $T = 0$ the simple solution of the self-consistency equation (29) corresponds to $r = q = 1/2$, or $r = -q = 1/2$. The solution manifests the spin ordering for x (y), components of spins at $T = 0$, expected [26] for $J_y \neq J_x$. Such an ordering is similar to the ones of the Ising or XY chains [25,26]. Notice, however, that mean-field features of the used approximation imply mean-field values of correlation exponents. The renormalization of those exponents can be taken into account, e.g., in the bosonization approach [27]. The main features of the above shown results will be kept, though.

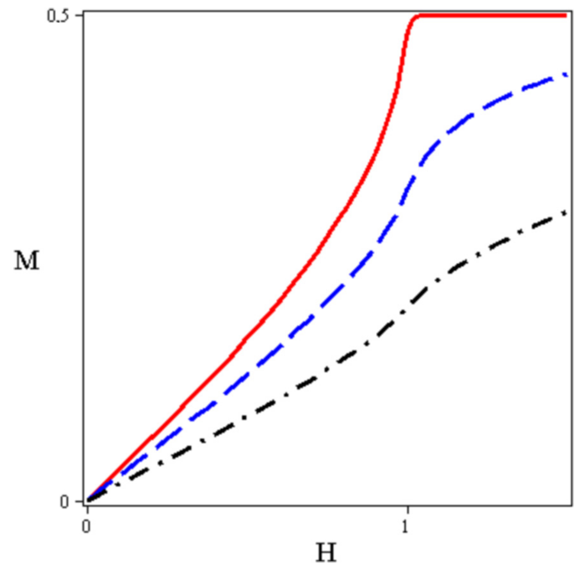

FIG. 1. Magnetic moment of the spin-1/2 chain for $I = a = 1$ with $J = J_z = 0$ for $T = 0.01$ as a function of the external magnetic field H for the external electric field $E = 0$ (red solid line); $E = 1$ (blue dashed line) and $E = 3$ (black dashed-dotted line).

Summarizing, the spin-spin interaction with $J_z \neq 0$ in the Hartree-Fock-like approximation yields the dependence of the magnetic moment, and the magnetic and the quadrupolar susceptibility of the XY spin-1/2 chain, on J_z.

V. RESULTS

Now let us present some results, to illustrate the features of the electromagnetic, piezoelectric, and magnetoacoustic characteristics of the spin chain system.

First, let us consider the electromagnetic effect; i.e., let us see how the external electric field can change the magnetic field behavior of the magnetic characteristics of the spin chain (first without the effect of the elastic subsystem; see below). In what follows we use the units in which $g\mu_B = k_B = 1$ with $J_z = 0$, and $I = 1$ for simplicity. Figures 1 and 2 show the magnetic field behavior of the magnetic moment and the magnetic susceptibility for the case $J = 0$ at $T = 0.01$ and

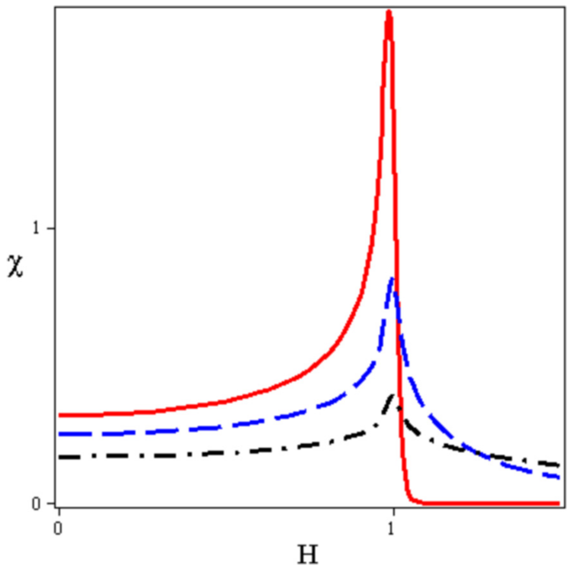

FIG. 2. Magnetic susceptibility for the spin-$1/2$ chain as a function of the external magnetic field H and various values of the external electric field E. The parameters and notations are the same as in Fig. 1.

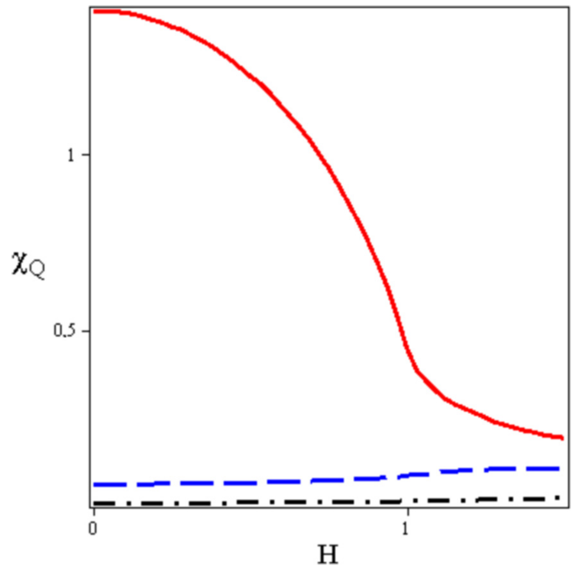

FIG. 3. The component of the quadrupolar susceptibility for the spin-$1/2$ chain as a function of the external magnetic field H and various values of the external electric field E. The parameters and notations are the same as in Fig. 1.

for several values of the electric field E. We see that the external electric field can drastically change the behavior of magnetic characteristics. For example, for $E = 0$ the magnetic moment in the ground state shows the saturation behavior for $g\mu_B H > g\mu_B H_c = I$. At the critical field the ground-state magnetic susceptibility manifests the square-root divergence. On the other hand, for $E \neq 0$ for $H > H_c$ the magnetic moment is not saturated at $T = 0$, and the magnetic susceptibility is finite there. At $H = H_c$ the magnetic susceptibility shows the weaker logarithmic feature in the ground state. For higher temperatures the effect becomes less strong.

Naturally, similar behavior is kept for $J \neq 0$. There is a critical value of the external electric field $E_c = J/a$, at which the system becomes effectively uniaxial (there is no anisotropy in the "easy" spin plane). However, for any other value of the external electric field the system is biaxial. That is manifested in the different behavior of magnetic characteristics of the spin chain for various values of the external field.

Consider now other effects, the magnetoelectric, magnetoelastic, and the piezoelectric ones in the spin chain. Figure 3 shows the magnetic field behavior of the mentioned component of the quadrupolar susceptibility for various values of the external magnetic field at $T = 0.01$ (the values of the parameters of the spin chain are the same as in Figs. 1 and 2).

Figure 4 shows the magnetic field behavior of the quadrupolar susceptibility of the spin chain as a function of the magnetic field for the external field $E = 1$ for several values of the temperature.

Now let us consider the magnetoelectric effect, namely, the dependence of the electric permittivity of the spin chain with the coefficient of the magnetoelectric coupling $a = 1$ on the external electric and magnetic fields. We see from Fig. 5 that the application of the magnetic field reduces the effective electric permittivity of the spin chain.

Figure 6 shows the change of the piezoelectric modulus of the spin chain with $I = 1$, $J = 0.5$, and the coefficients of the magnetoelectric and magnetoelastic couplings $a = 0.5$, $b = -0.5$, respectively, as a function of the applied external electric field for several values of the external magnetic field. The magnetic field reduces the change of the piezoelectric modulus. Figure 7 shows the piezoelectric modulus as a function of the electric field for $H = 0$ for several values of the

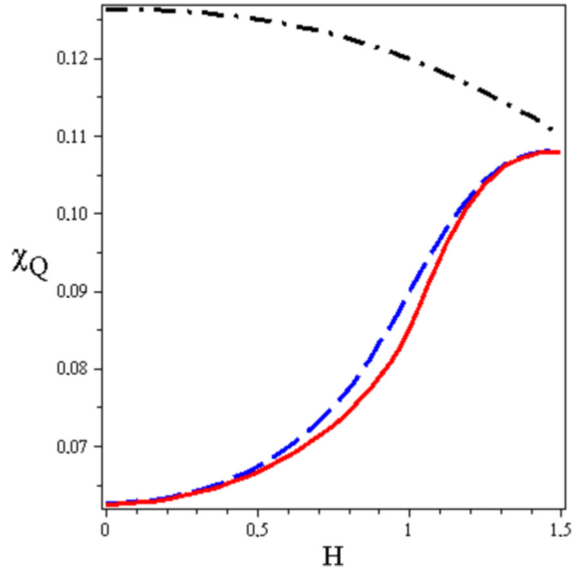

FIG. 4. The component of the quadrupolar susceptibility for the spin-$1/2$ chain as a function of the external magnetic field H and various values of temperature ($T = 0.01$, solid red line; $T = 0.1$, dashed blue line; and $T = 0.5$, dash-dotted black line) for the external electric field $E = 1$. The parameters are the same as in Fig. 3.

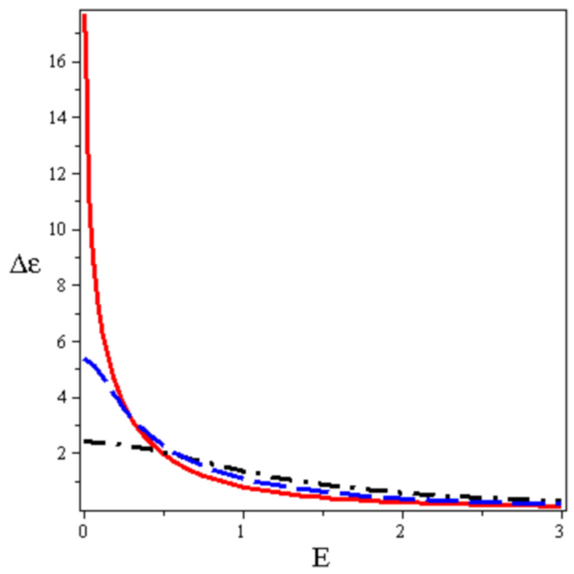

FIG. 5. The change of the electric permittivity for the spin-1/2 chain as a function of the external electric field E at $T = 0.01$ for $a = 1$ and various values of the external magnetic field ($H = 0$, solid red line; $H = 1.01$, dashed blue line; and $H = 1.5$, dash-dotted black line). Other parameters are the same as in previous figures.

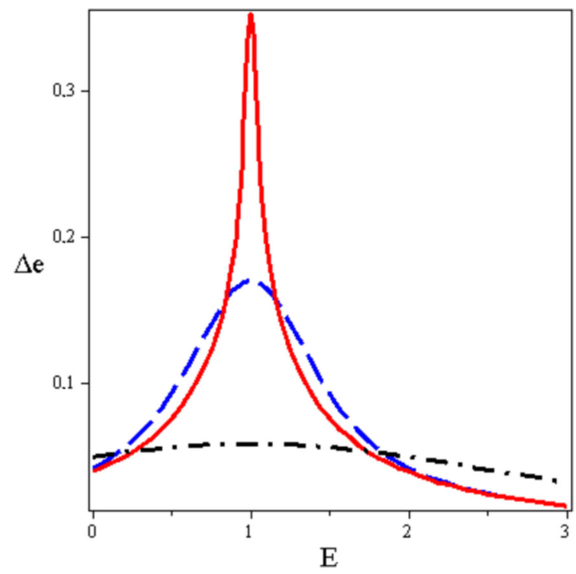

FIG. 7. The change of the piezoelectric modulus for the spin-1/2 chain as a function of E and $H = 0$ for different values of the temperature ($T = 0.01$, solid red line; $T = 0.1$, dashed blue line; and $T = 0.5$, dash-dotted black line).

temperature. At $E_c = J/a$ the piezoelectric modulus manifests the second-order quantum phase transition at $T = 0$.

Finally, let us consider the change of the elastic modulus of the spin chain. Figure 8 shows the temperature dependence of the elastic modulus for zero electric field for several values of the external magnetic field for the initial values of the electric permittivity $\varepsilon = 20$ and of the elastic modulus $e = 2$. We see that the application of the magnetic field shifts the position and the value of the minimum in the temperature dependence of ΔC. Figure 9 shows the temperature dependence of the change of the elastic modulus at $H = 0$ for several values of the external electric field E.

Then Figs. 10 and 11 show the magnetic field dependence of the change of the elastic modulus of the spin chain.

We can see that with the growth of the temperature the minimum in the magnetic field dependence of the change of the elastic modulus is shifted to lower values of H. On the

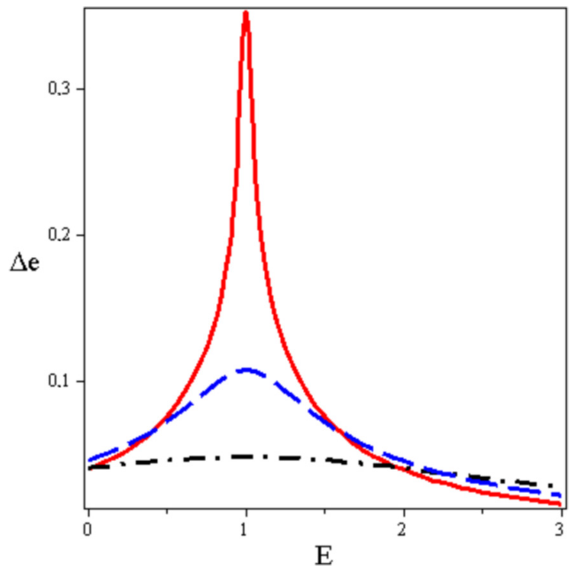

FIG. 6. The change of the piezoelectric modulus for the spin-1/2 chain as a function of the external electric field E at $T = 0.01$ for $a = 1$ and various values of the external magnetic field ($H = 0$, solid red line; $H = 1.01$, dashed blue line; and $H = 1.5$, dash-dotted black line).

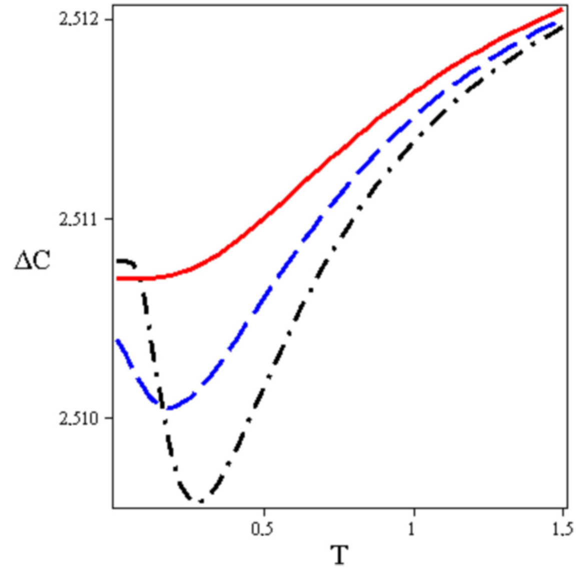

FIG. 8. The change of the elastic modulus for the spin-1/2 chain as a function of the temperature at $E = 0$ and various values of the external magnetic field ($H = 1.5$, solid red line; $H = 1.01$, dashed blue line; and $H = 0$, dash-dotted black line). Other parameters are the same as in Fig. 6.

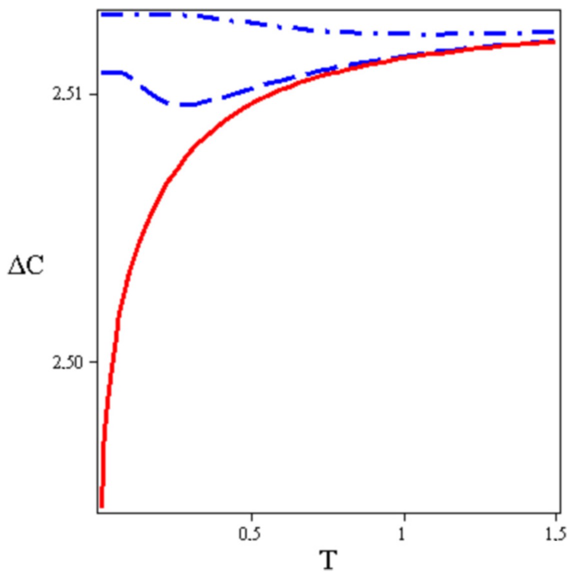

FIG. 9. The change of the elastic modulus for the spin-1/2 chain as a function of the temperature at $H = 0$ and various values of the external electric field ($E = 1.01$, solid red line; $E = 0$, dashed blue line; and $E = -3$, dash-dotted black line). Other parameters are the same as in Fig. 8.

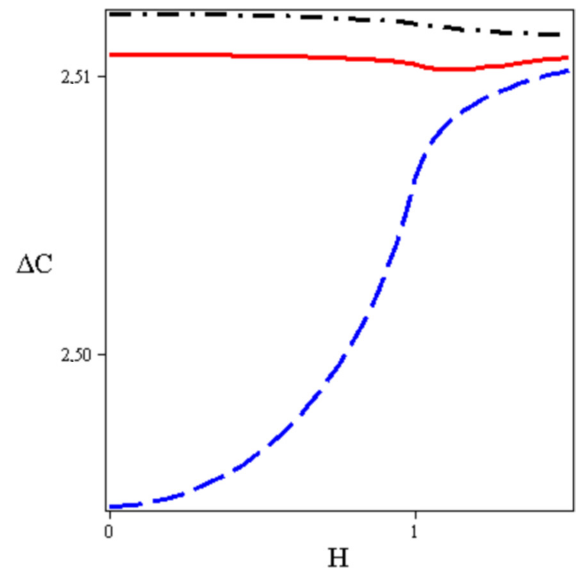

FIG. 11. The change of the elastic modulus for the spin-1/2 chain as a function of the external magnetic field H at $T = 0.01$ for various values of the external electric field ($E = 0$, solid red line; $E = 1.01$, dashed blue line; and $E = -3$, dash-dotted black line).

other hand, at the critical value of the external field $E = E_c$ the magnetic field dependence manifests the deeper minimum at low values of the field H (see Fig. 11).

Our Hartree-Fock-like analysis shows that for nonzero values of $-I \leqslant J_z \leqslant I$ the magnetoelectric, piezoelectric, and magnetoelastic effects in the spin chain manifest qualitatively similarly to the case $J_z = 0$ behavior.

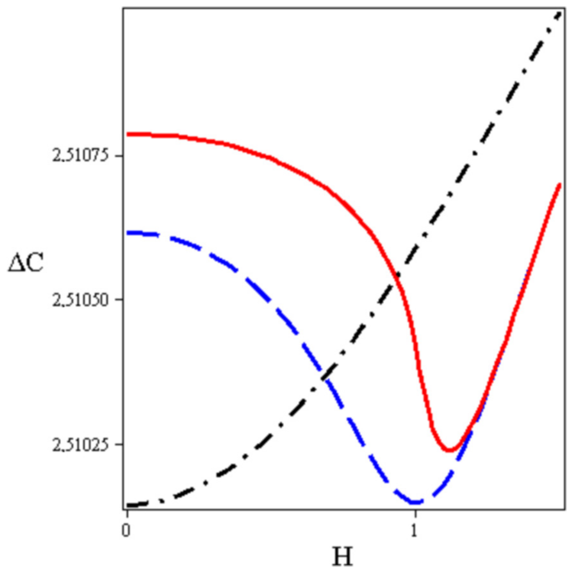

FIG. 10. The change of the elastic modulus for the spin-1/2 chain as a function of the external magnetic field H at $E = 0$ for various values of the external magnetic field ($T = 0.01$, solid red line; $T = 0.1$, dashed blue line; and $T = 0.5$, dash-dotted black line). Other parameters are the same as in Figs. 8 and 9.

Now, let us turn to the external strain behavior of magnetic, acoustic, and electric characteristics of the spin chain. Looking at Hamiltonian (1) we see that the external strain u_0 plays a role similar to the external electric field E: It renormalizes the effective parameter of the in-plane anisotropy of spin-spin interaction J. Then, the effect of the external strain is similar to the effect of the external electric field. As for the internal strain, the following relation holds:

$$\frac{\partial^2 u}{\partial t^2} - \left[C - \frac{be}{a}\right]\frac{\partial u}{\partial x} = \left[e + \frac{b\varepsilon}{4\pi a}\right]\frac{\partial E}{\partial x}, \qquad (30)$$

i.e., the dynamics of the internal strain in the system depends on the spatial changes of the external electric field. Notice, however, that the realistic values of the external electric field can be much larger than the one for the external strain, caused by the external pressure. This is why it is possible that for realistic values of the external pressure one cannot reach the values of u_0 at which the crossover to the uniaxial behavior can take place.

VI. SUMMARY

In summary, we have studied the magnetoelectric, electromagnetic, piezoelectric, piezomagnetic, and magnetoelastic effects in the insulating spin chain system. We have shown that electric, magnetic, and elastic characteristics of the considered system manifest interesting behavior, especially in the low-temperature region. Important features of that behavior are determined by two quantum critical points, H_c and E_c, which govern the low-energy sector of the considered model. The critical value of the magnetic field for the antiferromagnetic chain is related to the phase transition to the (almost) spin-polarized phase, where no magnetic ordering exists in the ground state. It can be approximately determined by the value $(J_x + J_y)/2 + J_z$; i.e., it is large enough (of order of the exchange coupling). Unfortunately, no exact results are known for the XYZ spin chain in the magnetic field; hence the critical value is defined only by approximate methods or numerically. Nonetheless, that value is known exactly for the cases of $J_x = J_y$, where $g\mu_B H_c = I + J_z$, or for $J_z = 0$, where $g\mu_B H_c = I$. On the other hand, the critical value of the external electric field is related to the value of the external electric field, at which the effective magnetic xy anisotropy is vanished. It is determined by the value of the anisotropy of the spin-spin interaction, $J_x - J_y$, and by the value of the electromagnetic coupling coefficient a (supposed to be small enough). For the case $J_z = 0$ we have $E_c = J/a$ (or $u_0^c = -J/b$). All that results in the difference between the values of those critical fields (strains). Such a behavior is different from the one of multiferroics, in which one or more order parameters exist at low temperatures [3,4,7], and in the ordered phases quantum effects are suppressed (one has classical vectors of magnetic moments instead of spins with spin waves, small deviations from the classical equilibrium). On the other hand, the behavior differs from the one which takes place in a (single-ion) paramagnet with the interaction between electric, spin, and elastic subsystems, where many-body effects are absent [14,15]. Some of the effects theoretically considered here qualitatively agree with the ones observed in rare-earth (paramagnetic) alumoborates [28], for example, the temperature behavior of the electric permittivity, the piezoelectric modulus, and the elastic modulus, and the general suppression of the features by the external magnetic field. It implies the generic nature of the considered effects for systems in which magnetic, electric, and elastic subsystems are strongly coupled. On the other hand, the manifestation of quantum phase transitions in the behavior of calculated characteristics of the spin chain are related to the low-dimensional nature of the considered many-body quantum spin system. The effects predicted in this study can be useful for the application in some devices of modern microelectronics.

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