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Electric field- and strain-induced quantum phase transitions in a spin chain

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The effect of the external electric field and/or the external strain on the low-temperature behavior of the quantum spin chain model is studied. The external electric field or the strain can cause the quantum magnetic structural phase transition between two magnetically ordered phases with different order parameters. Such a quantum critical point can be observed in the special behavior of the low-temperature specific heat: At the critical value the low-temperature specific heat manifests linear in temperature behavior instead of the exponentially small one for other values of the field. The magnetic susceptibility also manifests the special behavior, in which quantum phase transitions are revealed.

Keywords: quantum spin chain, electric field, external strain.

The coupling between the electric, magnetic and elastic subsystems can be seen in magneto-electric, piezoelectric and magneto-elastic effects. The attention of researchers is attracted by application of those effects in microelectronics, e.g., spintronics [1, 2], for instance as switching devices, or as writing and reading devices for memory storages, which can be governed by external fields and strains. Also, such an attention is determined by the interesting physics behind them. The most known systems in which such effects take place are the so-called multiferroics, i.e., systems, where both magnetic and ferroelectric properties are manifested, see, e.g., [3–9]. Therefore, most of studies were performed on magnetically ordered systems, like ferro- and antiferromagnets (like ferroborates, for the recent studies see [10–13]). However, from general grounds it is clear that similar effects can exist in spin systems without magnetic ordering.

Recently magneto-electric, piezoelectric, electro-magnetic and magneto-acoustic effects in the quantum paramagnet (a single spin) have been studied [14, 15], where the quadrupole spin moment has the single-ion nature. It is interesting to investigate the quantum many-body spin insulating system, in which similar effects can take place. The ligands surrounding magnetic ions determine the anisotropy of the orbitals, and, together with the spin-orbit interaction and the exchange one, it 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 interesting behavior in the external electric field, or under the action of the external strain.

Quantum spin chain systems can be used as the testing ground for investigation of many-body effects together with the coupling between electric, magnetic and elastic subsystems. On the one hand, the reduced dimensionality preserves the system against magnetic ordering at nonzero temperatures [16]. On the other hand, those systems manifest quantum many-body effects. Also important, spin-1/2 chains permit to obtain many exact theoretical results [17], which give the opportunity to use those results for comparison with the data of experiments in spin chain systems, and with the results of approximate theoretical calculations for more realistic systems.

In the present study, we consider the behavior of static thermodynamic characteristics of the quantum spin chain model, which interacts with external electric field or strain. Using the exact analytic result, we have shown that the external electric field and/or strain can cause additional quantum phase transition in the spin chain system between two ordered magnetic phases with different order parameters.

Consider the Hamiltonian of the model, which can be written as [11, 18]

$$\mathcal{H} = -H\sum_n S_n^z + I\sum_n (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y)$$
$$+ J\sum_n (S_n^x S_{n+1}^x - S_n^y S_{n+1}^y) - aE\sum_n (S_n^x S_{n+1}^x - S_n^y S_{n+1}^y)$$
$$+ b(u-u_0)\sum_n (S_n^x S_{n+1}^x - S_n^y S_{n+1}^y)\,, \qquad (1)$$

where $S_n^{x,y,z}$ are the operators of spin projections of the spins 1/2 situated at the site n, with the magnetic field H directed along the z axis (we use units in which $g\mu_B = 1$, where μ_B is the Bohr magneton, and g is the effective g-factor), $I = (J_x + J_y)/2$, $J = (J_x - J_y)/2$, $J_{x,y}$ are the parameters of the magnetically anisotropic exchange interaction, $E \equiv E_x \geq 0$ is the electric field directed along the x axis, u is the strain ($u \equiv u_{xx} - u_{yy}$, and u_0 is the static strain), a and b are the coefficients of the magneto-electric and magneto-elastic couplings, respectively (all issues are connected with the x coordinate). In what follows, the energy of the electric field and the energy of the elastic subsystem (classical values) do not play roles, and we do not write them.

The form of the electro-magnetic, strain-spin and piezoelectric coupling is the special case of the general interactions between spin, electric and elastic degrees of freedom $\sum_{m,n}\sum_{ipq} a_{ipq} E_i S_n^p S_m^q$, and $\sum_{m,n}\sum_{ijpq} b_{ijpq} u_{ij} S_m^p S_n^q$, where n, m numerate lattice sites, and $i, j, p, q = x, y, z$ [18] with a, and b, being the components of the tensors a_{ipq}, and b_{ijpq}. We use the form of magneto-electric and magneto-elastic couplings similar to [11], where the studied effects were observed in the magnetically ordered multiferroic. The effect is related to the orientation of the magnetic anisotropy axes of the spin-spin interaction in the chain. The latter is determined mostly (if not take 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 inter-spin interactions in the chain.

Using the well-known Jordan–Wigner transformation [19], the Hamiltonian of the spin chain can be exactly mapped onto the one of the quadratic form of spinless Fermi operators. Then, using the Fourier transformation and the Bogolyubov transformation that fermionic Hamiltonian can be diagonalized [17], and the free energy of the system can be written as

$$F = -TN^{-1}\sum_k \ln\left[2\cosh(\varepsilon_k/T)\right], \qquad (2)$$

where T is the temperature (we use the units in which the Boltzmann constant is equal to unity, $k_B = 1$), and

$$\varepsilon_k = \left[(H - I\cos k)^2 + [J - aE + b(u-u_0)]^2 \sin^2 k\right]^{1/2}. \quad (3)$$

All features of thermodynamic behavior of the spin chain are determined by the dispersion law ε_k. It is known that for $a = b = 0$ the dispersion law is gapped, with the gap value $|H \pm I|$ at $k = 0, \pi$ and $\sqrt{H^2 + J^2}$ at $k = \pi/2$. The spectrum becomes gapless at $J = 0$, i.e., in the uniaxial case, and for $H < I$. In the uniaxial case $J = 0$, the spin chain is disordered at any temperature, including the ground state [17]. At $H = H_c = I$, the ground state magnetic susceptibility has the square root singularity. On the other hand, for $J \neq 0$, the system can be in the magnetically ordered state at $T = 0$. Suppose $I, J > 0$, then, according to [20], one can see that in the ground state $T = 0$ the static pair spin-spin correlation functions behave in a different way. Namely, the correlation function $\langle S_n^x S_{n+r}^x \rangle$ does not decay with the distance r, manifesting for $H < I$ nonzero behavior at the infinite distance, while it is zero for $H > I$. On the other hand, $y-y$ and $z-z$ pair correlation functions decay with distance r (except of the trivial case $J = 0$ and $H > I$, where the spin chain is in the magnetic field-induced phase with all $\langle S_n^z \rangle = 1/2$, hence z–z correlation function is 1/4), so that in the limit $r \to \infty$ they are zero. It means that for $H < I$, the spin chain is in the magnetically ordered state in the ground state $T = 0$. The order parameter is antiferromagnetic; it is the (staggered) x projection of the magnetic moment. The point $H = H_c = I$ is known as the quantum critical point, at which the quantum phase transition takes place. Here the gap of the dispersion law ε_k is closed at one value of the quasimomentum, $k = 0$. For that reason, the ground state magnetic susceptibility has the logarithmic feature. It is the transition between the spontaneously ordered and disordered phases.

That quantum phase transition can manifest itself, e.g., in the behavior of the spin specific heat c, which can be calculated, as usual, as $c = -T\partial^2 F/\partial T^2$. In general, the temperature dependence of the specific heat of the spin chain manifests the growth with temperature at low temperatures, then the maximum (the Schottky-type anomaly for the many-body quantum system) and finally, decays with T at high temperatures [17]. Figure 1 shows the behavior of the low-temperature part of the specific heat of the spin chain with $a = b = 0$ and $I = 1$, $J = 0.3$ for several values of the external magnetic field.

We see that the low-temperature part of the specific heat behaves differently at the quantum critical point $H = H_c$: It grows linearly with T, while for $H \neq I$ the specific heat is exponentially small.

Let us consider the effect of the external electric field with $a \neq 0$ (while $b = 0$). One can see that the electric field renormalizes the value of the exchange integral $J \to J - aE$. It means that at the critical field $E_c = J/a$ the spin chain becomes effectively uniaxial. In that case, as

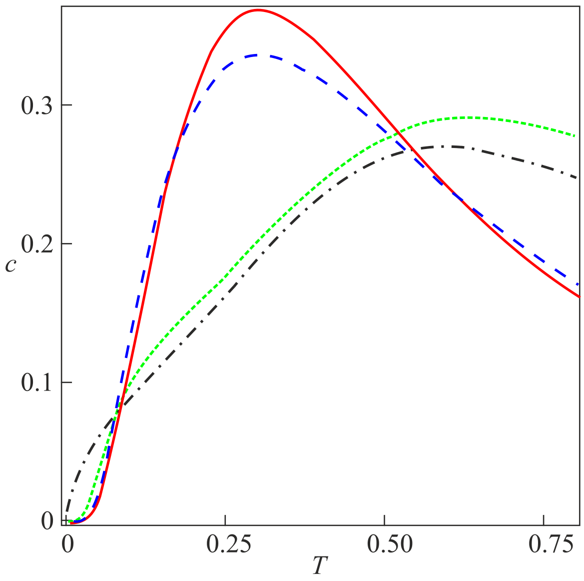

Fig. 1. (Color online) The low-temperature part of the specific heat of the spin-1/2 chain for $I = 1$ and $J = 0.3$ with $a = b = 0$ for $H = 0$ (red solid line), $H = 0.3$ (blue dashed line), $H = 1$ (black dashed-dotted line), and $H = 1.2$ (green dotted line).

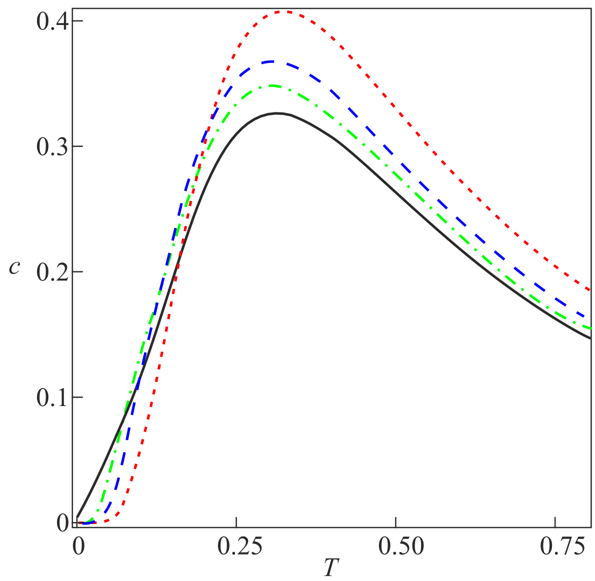

Fig. 2. (Color online) The low-temperature part of the specific heat of the spin-1/2 chain for $I = 1$ and $J = 0.3$ with $a = 1$ and $b = 0$ at $H = 0$ and for $E = 0$ (blue dashed line), $E = 0.1$ (green dashed-dotted line), $E = 0.3$ (black solid line), and $E = 0.8$ (red dotted line).

we know [17], in the ground state all spin-spin correlation functions decay; they decay algebraically for $H < I$ at $T = 0$ (the dispersion law is gapped for any value of k), and exponentially for $H > I$ at $T = 0$, and for any H at nonzero temperatures. On the other hand, for $E < E_c$, the eigenstates of the spin chain are gapped for $H < I$, and the correlation function $(-1)^r \langle S_n^x S_{n+r}^x \rangle$ is nonzero in the limit $r \to \infty$, cf. [20],

$$\lim_{r\to\infty} (-1)^r \langle S_n^x S_{n+r}^x \rangle = \left[\frac{(J - aE)^2 [1 - (H/I)^2]}{2I(I + J - aE)} \right]^{1/4} . \quad (4)$$

Other pair spin-spin correlation functions decay with the growth of distance r. The spin chain is in the magnetically ordered state with the antiferomagnetic order parameter being the x projection of the staggered magnetic moment. Then, for $E > E_c$, the system is again in the magnetically ordered state. However, now the correlation function $(-1)^r \langle S_n^y S_{n+r}^y \rangle$ is nonzero at $r \to \infty$,

$$\lim_{r\to\infty} (-1)^r \langle S_n^y S_{n+r}^y \rangle = \left[\frac{(J - aE)^2 [1 - (H/I)^2]}{2I(I - J + aE)} \right]^{1/4} , \quad (5)$$

while other pair spin-spin correlation functions decay with the growth of distance r. It means that the quantum critical point $E = E_c$ divides two magnetically ordered (in the ground state) phases, one with the nonzero x-component of the site staggered magnetization, and the second one with the y-component. The ground state phase transition at $E = E_c$ is the magnetic structural phase transition between two ordered phases with different order parameters.

The quantum critical point $E = E_c$ can be also manifested in the low-temperature part of the specific heat of the spin chain. Figure 2 shows the low-temperature specific heat of the spin chain with $I = 1$ and $J = 0.3$ in zero magnetic field for $b = 0$ and $a = 1$ for several values of the external electric field.

Notice that the external electric field almost does not change the position of the maximum of the specific heat (its height depends on E), while the electric field drastically changes its low-temperature behavior. For $E = E_c$, the low-temperature specific heat manifests the linear in T behavior, while for other values of E the behavior is exponential.

Consider the common effect of the external electric and magnetic fields. The quantum critical line in the H–E plane at $T = 0$ is determined by the formula

$$H^2 + (J - aE)^2 = I^2 . \quad (6)$$

Figure 3 shows the behavior of the low-temperature specific heat of the spin chain with $I = 1$, $J = 0.3$ at $a = 1$ and $b = 0$ for several values of the external electric and magnetic fields.

While in the absence of the fields the low-temperature part of the specific heat is exponentially small, for $H = 0$ at the critical field $E = E_c$ it becomes linear in T with the position of the maximum situated approximately at the same value as for $E = 0$. On the other hand, for $H = H_c$, the maximum of the specific heat is shifted for higher values of the temperature. At the point $H = H_c$ and $E = E_c$, the Sommerfeld coefficient (before the linear in T part of the specific heat) is maximum. At this point, the dispersion

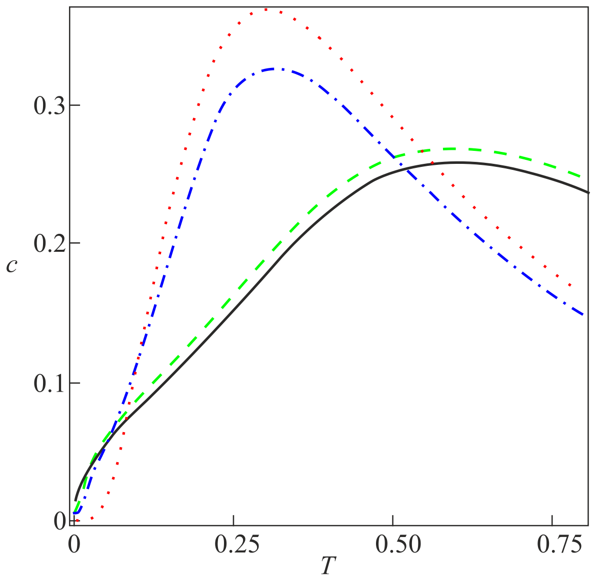

Fig. 3. (Color online) The low-temperature part of the specific heat of the spin-1/2 chain for $I = 1$ and $J = 0.3$ at $a = 1$ and $b = 0$ for $H = E = 0$ (red dotted line), $H = 0$, $E = 0.3$ (blue dashed-dotted line), $H = 1$, $E = 0$ (green dashed line), and $H = 1$, $E = 0.3$ (black solid line).

law is $\varepsilon_k = I \sin(k/2)$, and the magnetic susceptibility manifests the square root singularity in the ground state.

Also the quantum phase transition at $E = E_c$ reveals itself in the zero magnetic susceptibility for $H > H_c = I$ in the ground state. It is interesting to see how the low-temperature magnetic susceptibility of the spin chain depends on

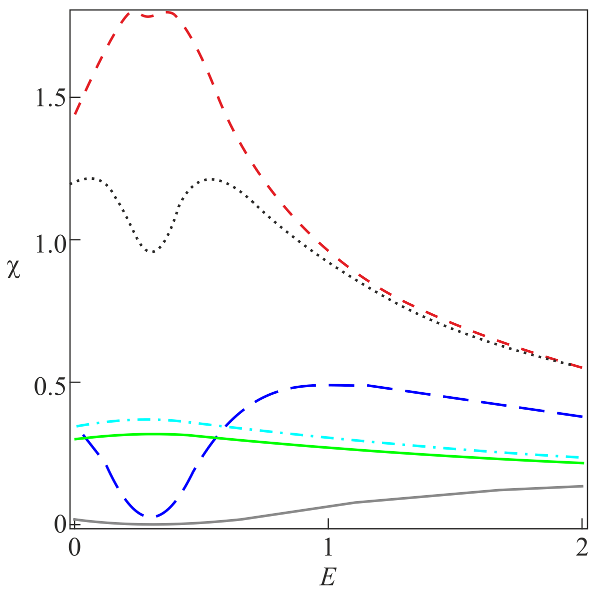

Fig. 4. (Color online) The low-temperature magnetic susceptibility of the spin-1/2 chain as a function of the applied electric field E for $I = 1$ and $J = 0.3$ at $a = 1$ and $b = 0$ for $H = 0$ (green solid line), $H = 0.5$ (cyan dashed-dotted line), $H = 0.99$ (red dashed line), $H = 1.01$ (black dotted line), $H = 1.05$ (blue long-dashed line), and $H = 1.5$ (grey solid line).

the applied external electric field. Figure 4 manifests the low-temperature ($T = 0.01$) the electric field behavior of the magnetic susceptibility of the spin chain with $I = 1$ and $J = 0.3$ for $a = 1$, $b = 0$, and for several values of the applied magnetic field. We can see that for small fields, approximately $H < H_c$, the magnetic susceptibility grows with E at low values of E, then it has the maximum at $E = E_c$, and then it decays with the growth of E. On the other hand, at $H \approx H_c$, a minimum is developed at $E = E_c$ instead of the maximum, and it becomes deeper with the growth of H. Finally, for $H > H_c$, the magnetic susceptibility is small and first decays with E, and then the maximum appears with the small hight, and the position shifted to large values of E.

Let us turn to the external strain behavior of characteristics of the spin chain for $b \neq 0$. Looking at the Hamiltonian (1), we see that the external strain u_0 plays similar to the external electric field E role: 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

$$\frac{\partial^2 u}{\partial t^2} - \left[C - \frac{be}{a}\right]\frac{\partial u}{\partial x} = \left[e + \frac{b\varepsilon}{4\pi a}\right]\frac{\partial E}{\partial x}, \qquad (7)$$

where C is the elastic modulus, connected with the considered strain, e is the piezoelectric modulus, and ε is the electric permittivity, 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 (magnetically disordered in the ground state) behavior can take place.

In summary, we have studied the effect of the external electric field and the external strain on the low-temperature behavior of the quantum spin chain. We have shown that the external electric field or the strain can cause the quantum magnetic structural phase transition between two magnetically ordered phases with different order parameters. We have also shown that such a quantum critical point can be observed in the special behavior of the low-temperature specific heat: At the critical value of the field (or the strain), the gap of low-energy eigenstates is closed, and the low-temperature specific heat manifests linear in T behavior instead of the exponentially small one. Also, at the critical value of the external electric field or strain, the ground state magnetic susceptibility is zero for the values of the magnetic field, larger than the critical one. The electric field dependence of the magnetic susceptibility at low temperatures manifests the nonmonotonic behavior, with extrema related to the critical values of the electric and magnetic fields.

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Індуковані електричним полем та деформацією квантові фазові переходи в спіновому ланцюжку

A. A. Zvyagin

Вивчається вплив зовнішнього електричного поля та/або зовнішньої деформації на низькотемпературну поведінку моделі квантового спінового ланцюжка. Зовнішнє електричне поле або деформація можуть спричинити магнітний структурний квантовий фазовий перехід між двома магнітно-впорядкованими фазами з різними параметрами порядку. Таку квантову критичну точку можна побачити в спеціальній поведінці низькотемпературної теплоємності: при критичному значенні низькотемпературна теплоємність виявляє лінійну температурну залежність замість експоненціально малої для інших значень поля. Магнітна сприйнятливість також виявляє особливу поведінку, в якій проявляються квантові фазові переходи.

Ключові слова: квантовий спіновий ланцюжок, електричне поле, зовнішня деформація.