**XY-anisotropy and magnetoelectric effect in**  
\( S = 1/2 \) **XY-spin chain**

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A magnetoelectric effect according to Katsura-Nagaosa-Balatsky mechanism in \( S = 1/2 \) **XY-chain** is considered. Configuration of the electric field is chosen in such way to provide an exact solution in term of free spinless fermions. The simplest model of quantum spin chain with magnetoelectric effect, zero temperature case of \( \gamma = 0 \) chain is described, demonstrating the simplest possible form of the magnetization, polarization and susceptibility functions with dependence on electric and magnetic field. For the case of arbitrary \( \gamma \) a non-uniform dependence of the magnetization on the **XY-anisotropy** parameter is figured out. This non-uniform behaviour is governed by the critical point, connected with possibility to drive the system gapless or gapped by the electric field. Singularities of the magnetoelectric susceptibility at the critical value of system parameters is shown.

**Keywords:** KNB-mechanism, Magnetoelectric effect, XY-chain, free spinless fermions

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### 1. Introduction

Magnetoelectrics are materials having both dielectric polarization and magnetization in a single phase and exhibiting a magnetoelectric effect (MEE), a vast class of phenomena of intercoupling of magnetization and polarization in matter [1–4]. These materials are particularly important for their application in spintronic devices [5, 6]. The MEE is a class of phenomena in solids, which can be detected as magnetic field dependence of dielectric polarization and electric field dependence of magnetization. In most interesting cases of non-trivial MEE the magnetization (dielectric polarization) can be induced by only applying an electric (magnetic) field. Nowadays, several microscopic mechanisms of the MEE is known [1–4]. One of these mechanisms is based on so-called spin-current model or inverse Dzyaloshinskii-Moriya (DM) model and have been proposed in a seminal paper by Katsura, Nagaosa and Balatsky [7]. The Katsura-Nagaosa-Balatsky (KNB) mechanism establishes a connection between the dielectric polarization of the crystal structure unit consisting of two magnetic ions chemically bounded to one or more \( p \)-elements and the spin states of the ions [7, 8]. The dielectric polarization, induces into the bond between two spins in this model is given by the following expression:

\[
P_{ij} = \mu e_{ij} \times S_i \times S_j,
\]

here \( e_{ij} \) is the unit vector pointing from site \( i \) to site \( j \) and \( \mu \) is a microscopic constant characterizing the quantum chemical features of the bond between two metallic ions and \( p \)-element(s) [7, 8]. \( S_i \) and \( S_j \) are the spin operators of the corresponding ion states. The simplest case of the KNB mechanism is the linear arrangement of magnetic ions (spins), the straight spin chain. If we suppose the chain to be directed...
toward the $x$-axis then the local polarization according to Eq. (1.1) acquires the following components:

$$
P_{j,j+1}^x = 0,\quad P_{j,j+1}^y = \mu \left( S_j^y S_{j+1}^x - S_j^x S_{j+1}^y \right),\quad P_{j,j+1}^z = \mu \left( S_j^z S_{j+1}^x - S_j^x S_{j+1}^z \right).\quad (1.2)
$$

Among a large family of magnetoelectric materials there are those which feature a one-dimensional arrangement of exchange-interaction paths between Cu$^{2+}$ ions, with ferromagnetic nearest-neighbour ($J_1 > 0$) and antiferromagnetic next-to-nearest neighbour ($J_2 > 0$) interactions. The corresponding model of one-dimensional $S = 1/2$ J$_1$ – J$_2$ spin chain is usually referred to as multiferroic spin chain. A list of magnetic materials successfully describing by this model is quite broad: LiCuO$_2$ [9–12], LiCuVO$_4$ [13–15], CuCl$_2$ [16], CuBr$_2$ [17, 18], PbCu(SO$_4$)$_2$(OH)$_2$ [19, 20], CuCrO$_4$ [21], SrCuTe$_2$O$_6$ [22] just to mention few of them.

Last few years were marked by an interest toward exact and numerical investigation of one-dimensional quantum spin models with KNB-mechanism. Exact description for the MEE are available, so far, only for simplified models, such as strictly linear integrable $XXZ$ chain [23], the same system but in both longitudinal and transverse fields [24], spin-1/2 $XY$-chain [25], the spin-1/2 $XY$ chain with three-spin interaction [24–28], generalized quantum compass model with magnetoelectric coupling [30], spin-1/2 Heisenberg-Ising ladder [31]. However, exact results are very helpful for understanding general features of the phenomena. Moreover, some of them can serve as a mean-field approximation for the more realistic models. The latter case is typical for a class of exactly solvable spin chain models, where spins interact to each other via two coplanar components (usually taken as $S^x$ and $S^y$).

In the present paper we focused on the MEE in a $XY$-chain, which was introduced in seminal paper of Lieb, Schulz and Mattis [32]. As KNB mechanism is essentially affected by the physical form of the lattice, the simplest case corresponds to the linear arrangement of spins, which features the polarization given in Eq. (1.2). Then, seeking for exactly solvable case we have to chose an electric field to be pointed in $y$-direction. This leads to a model of $XY$-chain with DM terms, when DM-vector is parallel to $z$-axis. This model is well known [33–44], however, for the last half-century quite restricted amount of papers have been devoted to it. The paper is organized as follows: in the second Section the formulation of the model and its exact solution in terms of Jordan-Wigner fermionization is given, in the next Section the zero temperature MEE for the simplest model of MEE in quantum spin chains are described, then the finite temperature MEE and effects of the $XY$-anisotropy $\gamma$ are analyzed. The paper is ended with a Conclusion.

### 2. The model and its exact solution

Let us consider $S = 1/2$ $XY$-chain which has linear form and spin dependent polarization due to KNB-mechanism. Supposing the chain to be collinear with the $x$-axis and the electric field to be pointed in $y$-direction according to Eq. (1.2) we arrive at the following Hamiltonian:

$$
\mathcal{H} = J \sum_{j=1}^{N} \left[ (1 + \gamma) S_j^x S_{j+1}^y + (1 - \gamma) S_j^y S_{j+1}^x \right] + E \sum_{j=1}^{N} \left( S_j^y S_{j+1}^x - S_j^x S_{j+1}^y \right) - B \sum_{j=1}^{N} S_j^z, \quad (2.1)
$$

where $S_j^\alpha$ are the $S = 1/2$ spin operators at lattice site $j$, $E$ is the magnitude of the electric field written in proper units (with coefficient $\mu$ absorbed in it) and $B$ is an external magnetic field pointing in $z$-direction. Various aspects of this model have been considered in a series of papers in last decades [33–44]. In the present paper we are interested in the MEE in this model, and particularly, in the effects of $XY$-anisotropy $\gamma$. The model is exactly solvable within the Jordan-Wigner fermionization. To proceed we first should perform a Jordan-Wigner transformation from spin operators to the creation and annihilation operators of lattice spinless fermions:

$$
S_j^x = e^{i \pi \sum_{j=1}^{N-1} c_j^\dagger c_j} c_j, \quad S_j^+ = (S_j^x)^*, \quad S_j^z = c_j^\dagger c_j - \frac{1}{2}, \quad (2.2)
$$
where $S^z_j = S^+_j + i S^y_j$. In terms of $c$ operators the Hamiltonian reads:

$$\mathcal{H} = \sum_{j=1}^{N} \left[ \frac{J + i E}{2} c^+_j c_{j+1} - \frac{J - i E}{2} c^+_j c_{j+1} + \frac{J_y}{2} (c^+_j c_{j+1} - c_j c_{j+1}) - B (c^+_j c_j - 1/2) \right].$$

(2.3)

Here periodic or anti-periodic boundary conditions are assumed, depending on the number of spinless fermions which is a conserved quantity. For even (odd) number particle number the anti-periodic (periodic) boundary conditions for $c_j$ operators is imposed, $c_{j+N} = -c_j$ ($c_{j+N} = c_j$). The further step toward the diagonalization of the Hamiltonian is a Fourier transformation,

$$c_j = \frac{1}{\sqrt{N}} \sum_k e^{-ijk} c_k, \quad c_k = \frac{1}{\sqrt{N}} \sum_j e^{ijk} c_j,$$

(2.4)

here $k$ takes $N$ values in the first Brillouin zone, $-\pi \leq k < \pi$, and is equal to $\frac{2\pi}{N} n$ for periodic boundary conditions or $\frac{2\pi}{N} (n + 1/2)$ for the antiperiodic ones ($n = -N, -N + 1, ... N - 1, N$). Then, the Hamiltonian takes the appropriate matrix-form, which is straightforward for diagonalization:

$$\mathcal{H} = \frac{1}{2} \sum_{-\pi \leq k < \pi} \begin{pmatrix} c_k & c^+_k \end{pmatrix} \begin{pmatrix} \varepsilon(k) & -iJy \sin k \\ iJy \sin k & -\varepsilon(-k) \end{pmatrix} \begin{pmatrix} c_k \\ c^+_k \end{pmatrix}.$$

(2.5)

where $\varepsilon(k) = J \cos k + E \sin k - B$. Performing Bogoliubov transformation to new Fermi creation and annihilation operators,

$$\begin{pmatrix} c_k \\ c^+_k \end{pmatrix} = \begin{pmatrix} -i u_k & v_k \\ -v_k & -i u_k \end{pmatrix} \begin{pmatrix} \beta_k \\ \beta^+_k \end{pmatrix}, \quad \begin{pmatrix} \beta_k \\ \beta^+_k \end{pmatrix} = \begin{pmatrix} -i u_k & -v_k \\ v_k & i u_k \end{pmatrix} \begin{pmatrix} c_k \\ c^+_k \end{pmatrix},$$

(2.6)

where $u_k^2 + v_k^2 = 1$. Then, putting

$$u_k = \frac{1}{\sqrt{2}} \sqrt{1 + \frac{J \cos k - B}{\lambda_k}}, \quad v_k = \text{sgn}(Jy \sin k) \frac{1}{\sqrt{2}} \sqrt{1 - \frac{J \cos k - B}{\lambda_k}},$$

$$\lambda_k = \sqrt{(J \cos k - B)^2 + J^2 y^2 \sin^2 k},$$

we finally obtain the Hamiltonian in terms of free spinless fermions:

$$\mathcal{H} = \sum_{-\pi \leq k < \pi} E_y(k) (\beta^* k \beta_k - 1/2),$$

(2.7)

$$E_y(k) = E \sin k + \text{sgn}(J \cos k - B) \lambda_k.$$ 

For the isotropic $XX$-chain with DM-terms ($\gamma = 0$) one can easily see that the Hamiltonian (2.5) is already diagonal in $c_k$ operators:

$$\mathcal{H}_{XX} = \sum_{-\pi \leq k < \pi} E_0(k) (c^*_k c_k - 1/2),$$

(2.8)

$$E_0(k) = \sqrt{J^2 + E^2 \cos (k - \phi) - B}, \quad \phi = \text{arcsin} \frac{E}{\sqrt{J^2 + E^2}}.$$

3. Zero-temperature properties and MEE

Let us first describe zero-temperature properties of the system under consideration and MEE features in it. The simplest quantum chain model exhibiting MEE via KNB mechanism is the system describing by the Hamiltonian (2.8). The free-fermion picture here is quite simple. The DM-terms broke a time-reversal
symmetry, $E_0(-k) \neq E_0(k)$, and the two Fermi point are not symmetric with respect to $k = 0$. They are given by

$$k_{1,2} = \phi \mp \arccos \frac{B}{B_c}, \quad B_c = \sqrt{J^2 + E^2}, \quad (3.1)$$

when $-B_c < B < B_c$. For $B \leq B_c$ and $B \geq B_c$ all $N$ free fermion states in the system are occupies and empty respectively. The ground state energy per one site, thus, is given by

$$e_0 = \begin{cases} \frac{B}{2}, & B \geq B_c \\ -\frac{B}{2} + \frac{1}{\pi} \left( B \arccos \frac{B}{B_c} - \sqrt{B_c^2 - B^2} \right), & -B_c \leq B \leq B_c \\ B \leq -B_c. \end{cases} \quad (3.2)$$

Using standard relations, $m_0 = -\frac{\partial e_0}{\partial B}$ and $p_0 = -\frac{\partial e_0}{\partial E}$, one can find magnetization and polarization of the ground state:

$$m_0 = \begin{cases} \frac{1}{2}, & B \geq B_c \\ -\frac{1}{2} \arccos \frac{B}{B_c}, & -B_c \leq B \leq B_c \\ -\frac{1}{2}, & B \leq -B_c. \end{cases}, \quad p_0 = \begin{cases} 0, & B \geq B_c \\ \frac{E \sqrt{J^2 + E^2} - B^2}{\pi (J^2 + E^2)}, & -B_c \leq B \leq B_c \\ 0, & B \leq -B_c. \end{cases} \quad (3.3)$$

This is a common property of the free-fermion models with KNB-mechanism that for both empty and fully filled system the dielectric polarization is zero. Besides the magnetic and dielectric susceptibilities, $\chi = \frac{\partial m}{\partial B}$ and $\chi_p = \frac{\partial p}{\partial B}$, the magnetoelectric systems have one more important quantities to describe the response, a magnetoelectric or mixed susceptibility, which in general case is defined by the following relation:

$$\alpha_{ij} = \left( \frac{\partial M_i}{\partial E_j} \right)_{T,B} = \left( \frac{\partial P_j}{\partial B_i} \right)_{T,E} \quad (3.4)$$

where, $M_i(P_j)$ and $B_i(E_j)$ are components of the magnetization (polarization) vector of the sample and external magnetic (electric) fields respectively. For our case all susceptibilities are non-zero only within $-B_c \leq B \leq B_c$ and are given by

$$\chi = \frac{1}{\pi \sqrt{B_c^2 - B^2}}, \quad \chi_p = \frac{J^2 (B_c^2 - B^2) + E^2 B^2}{\pi B_c^4 \sqrt{B_c^2 - B^2}^3}, \quad \alpha = -\frac{E B}{\pi B_c^2 \sqrt{B_c^2 - B^2}^3} \quad (3.5)$$

respectively. Important feature this simplest model of MEE in spin chains is vanishing $\alpha$ when any of two field, electric or magnetic is vanished. This is an example of trivial MEE, when magnetic (electric) field affects polarization (magnetization) but can not induce it unless the other field is non zero. It can be easily seen that at critical field, $B = B_c$, all susceptibilities have square-root singularities, which is the universal properties of $XY$-type chains. The zero temperature magnetization curve around critical field, $B = \pm B_c$, has square-root behavior. Although, finite-temperature MEE in $XX$-chain was briefly described in Ref. [23], as a limiting case of $XXZ$-chain, the zero-temperature MEE is also worth studying, as this is the simplest example of the MEE, describing by simple analytic expressions. In Fig. [1] zero-temperature polarization and magnetization of the systems are presented as functions of electric field. The polarization curves, $p_0(E)$, demonstrates three different regime of polarization processes close to $E = 0$: linear, square-root and plateau with further quadratic behavior of the polarization. The regime of polarization curve depends on the value of the magnetic field. It is very simple to see form the Eq. (3.3) that polarization curve has linear behavior for $B < J$, which becomes quadratic at $B = J$ and then changed to plateau with square-root for $B > J$. Interestingly, the simplest model of KNB magnetoelectric to great extent reproduces three of four qualitative shapes of polarization curves for more complicated $S = 1/2$ $XXZ$ chain with KNB mechanism [23]. The plots of zero-temperature magnetization and polarization magnetic field dependence are presented in Fig. [2] Here the magnetization curves, $m_0(B)$, for different values of the electric field have the same standard form. Also the polarization dependence on magnetic
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here $T$ is the temperature. Using standard relations one can easily obtain expressions for magnetization and polarization of the system:

$$m = \frac{1}{4\pi} \int_{-\pi}^{\pi} \tanh \left( \frac{E_\gamma(k)}{2T} \right) \frac{B - J \cos k}{\lambda_k} dk, \quad p = \frac{1}{4\pi} \int_{-\pi}^{\pi} \tanh \left( \frac{E_\gamma(k)}{2T} \right) \sin k dk. \quad (4.2)$$

Also, the mixed magnetoelectric susceptibility is useful for figuring out important properties of the MEE:

$$\alpha = \frac{1}{8\pi T} \int_{-\pi}^{\pi} \frac{(B - J \cos k) \sin k}{\lambda_k \cosh^2 \left( \frac{E_\gamma(k)}{2T} \right)} dk. \quad (4.3)$$

Particularly, we are going to figure out an effect of $XY$-anisotropy parameter $\gamma$ on the MEE. In case of vanishing electric field, the spectrum of the model is always non-negative, thus, the system is always empty (in terms of Bogoliubov quasi-particles), and increasing $\gamma$ always decreases the magnetization. Polarization in this case is zero. In virtue of DM-terms and electric field the model with KNB mechanism features non-monotonic behavior of magnetization as a function of $\gamma$. In the Fig. 3 the magnetization and polarization dependence on $\gamma$ are exhibited. As in the case of finite $\gamma$ the system can have gapless spectrum as well as gapped one depending on the mutual relation between electric field, magnetic field and $XY$-anisotropy. Therefore, the behavior of local observables is also non-monotonous. In contrast with the $E = 0$ case one can see magnetization growing with $\gamma$ (Fig. 3 (left panel)) within the gapless phase. Once the value of $\gamma$ crosses the value,

$$|\gamma_c| = \frac{1}{|J|} \sqrt{1 + E^2 - B^2}, \quad (4.4)$$

a gap opens and magnetization begins to decrease (Fig. 3, left panel, red solid and blue dashed lines). If the value of magnetic field is greater that $\sqrt{E^2 + J^2}$ (Fig. 3, left panel, black dot-dashed line) there are no gapless phase and magnetization exhibits monotonous decrease with decreasing $\gamma$. Behavior of the polarization with respect to $\gamma$ (Fig. 3 right panel) shares much in common with the effect of magnetic field, the monotonous decrease in gapless phase with plateau at zero for gapped phase. Red solid and blue dashed lines go to zero at the same value of $\gamma$, as for $B^2 \leq J^2$ the value of $\gamma$ at which the free fermion states start to fill up is the same, $J^2 \gamma^2 = E^2$. In Fig. 4 polarization (left panel) and magnetization (right panel) dependence on the magnetic field are illustrated. Though, the behaviour of magnetization of the $XY$-chain is well known and understood, here an additional feature can be pointed out. For $E = 0$ and non zero $\gamma$ besides the absence of the saturation field there is only one phase without any features on
the magnetization curve. In case of finite \( E \) it is possible to have both smooth magnetization curve for \( E^2 < J^2\gamma^2 \) (Fig. 4 right panel, red solid line) as well as curve with a cusp, corresponding to transition form gapless regime to gapped one (Fig. 4 right panel, blue dashed and black dot-dashed lines). Interestingly, for all values of \( E^2 < J^2\gamma^2 \) the magnetization curves are exactly the same, as in all these cases the spectrum touches zero at one single point. For the values of electric field \( E^2 \geq J^2\gamma^2 \) the magnetization curves has a cusp at \( B_c = \sqrt{E^2 + J^2(1 - \gamma^2)} \) separating gapless regime from gapped one (Fig. 4 right panel, blue dashed and black dot-dashed lines). The left panel of the Fig. 4 demonstrates magnetic field effect on the polarization. Three curves are presented for three different constant values of the electric field. All three curves share the same regular pattern, monotonous decrease from maximal values at \( E=0 \) to zero at \( B=0 \) to zero at \( B_0 = \sqrt{E^2 + J^2(1 - \gamma^2)} \). Electric field dependence of polarization and magnetization is presented in the Fig. 5. Here again one can distinguish two part of the curve, corresponding to gapless and gapped regimes respectively. The transition takes place at \( E_c = \sqrt{B^2 - J^2(1 - \gamma^2)} \). Appearance of the critical point brings to the thermal singularity in the behavior of susceptibilities. Considering magnetoelectric susceptibility given by Eqs. (3.4) and (4.3) one can see well pronounced peaks at the corresponding values of \( \gamma \) given by Eq. (4.4). Left panel shows the \( \gamma \) dependence of the magnetoelectric susceptibility for \( E=2, B=1.5 \) and three different temperatures, \( T=0.5, 0.1 \) and 0.015. As the magnetization and polarization are strongly competing, \( \alpha \) is always negative (for positive fields). The development of peaks (negative) corresponding to the critical value of \( \gamma \) is well pronounced here. The peaks are gradually smearing out with increasing temperature. Thus, one can see, that within the gapless phase the absolute value of the magnetoelectric susceptibility is growing with increasing \( \gamma \) reaching a peak at the transition from gapless regime to gapped one. The peak shows a tendency to singularity at \( T \rightarrow 0 \). The same pattern can be seen in the magnetic field dependence (right panel), according to aforementioned property the peak for negative value of the magnetic field is positive.

5. Conclusion

In the present paper we considered MEE in the exactly solvable \( S = 1/2 \) \( XY \)-chain with KNB mechanism. Our main goals was to figure out the interplay between \( XY \)-anisotropy \( \gamma \) and MEE. In turned out that the main difference from the properties of underlying \( XY \)-chain stems out from the fact that appearance of DM-terms in the Hamiltonian makes possible gapless structure of the spectrum in some region of system parameters, which in their turn are electric field, magnetic field and \( XY \)-anisotropy. Thus, even for the ordinary magnetization curve interplay between \( XY \)-anisotropy and electric field (DM-terms) bring to essential modifications. In is well known that in case of \( E = 0 \) the magnetization curve is always smooth, and there is no saturation phenomena. For the chain with KNB-mechanism this is still the case for weak electric field, but when \( E^2 > J^2\gamma^2 \) situation changes drastically and transition
Figure 5. Low-temperature polarization (left panel) and magnetization (right panel) dependance on electric field for the $S = 1/2$ $XX$-chain with KNB-mechanism at $J = 1$ in appropriate units. $T = 0.0001$, $\gamma = 0.5$. For both panels, $B = 0.5$ (red solid line), $B = 1$ (blue dashed line) and $B = 2$ (black dot-dashed line).

Figure 6. Magnetoelectric susceptibility dependance on $\gamma$ (left panel) and magnetic field (right panel) for $J = 1$ and $E = 2$ in appropriate units. For the left panel $B = 1.5, T = 0.5$ (red solid line), $T = 0.1$ (blue dashed line) and $T = 0.015$ (black dot-dashed line). For the right panel $\gamma = 0.5, T = 0.5$ (red solid line), $T = 0.1$ (blue dashed line) and $T = 0.015$ (black dot-dashed line).

point (cusp) appears on the magnetization curve. This point corresponds to the transition from gapless to gapped form of the spectrum. This point is characterized by the following relations between system parameters: $B^2 = E^2 + J^2(1 - \gamma^2)$ and $E^2 > J^2\gamma^2$. Furthermore, influence of the $XY$-anisotropy on the behaviour of the magnetization curve is essentially different for gapless and gapped phases. As far as the spectrum is gapless magnetization is growing with increasing $\gamma$. For the gapped phase $XY$-anisotropy makes opposite contribution to magnetization. As polarization is always zero for gapped situation in our model, $\gamma$ can affect polarization only within the gapless phase, where it is decreasing with increasing $\gamma$. Magnetoelectric susceptibility is shown to have a characteristic peaks at critical point, when gap appears in the spectrum. We also presented a zero-temperature description of the MEE for the $\gamma = 0$ case. This is the simplest possible model of magnetoelectric spin chain, describing by a very simple relations.

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