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Effect of magnetic field orientation and disorder on Majorana polarization in wires with topological superconductivity

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Majorana polarization, previously introduced by Sticlet *et al.* [Phys. Rev. Lett. **108**, 096802 (2012)], is studied for wires in a topological superconductive state with varying orientation of the magnetic field. Numerical calculations show that in the case of a canted field, this polarization can differ in sign, as well as absolute magnitude, at the opposite ends of a wire. Since the Majorana polarization changes sign at one end when the orientation of the magnetic field is changed from perpendicular to longitudinal, there is always a range of angles for which this quantity is significantly suppressed or equals zero. Thus, the Majorana polarization does not always appear as a local order parameter for an arbitrary angle of the magnetic field in the plane perpendicular to the effective Rashba spin-orbital interaction field. It is shown that the introduction of disorder does not lead to qualitatively new effects. At the same time, additional regions with weak Majorana polarization do show up in high magnetic fields. *Published by AIP Publishing.*
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1. Introduction

Since the publication of two papers by Kitaev,[1,2] Majorana coupled states (MCC) in solid systems have been of great interest to researchers. It is known that the main problem with building a quantum computer is the sensitivity of quantum states in a cubit to perturbations which disturb the phase of the wave function of the system.[3] Since MCC are protected topologically from external interactions, a cubit consisting of a pair of MCC is stable against decoherence processes. The state of this kind of cubit can be controlled by changing the site of the MCC or by looping one MCC around another,[4,5] since Majorana fermions obey nonabelian statistics.[6] Various systems for producing MCC have been proposed in recent years.[7,8] Of these, 1D semiconducting wires[9,10] and chains of magnetic atoms[11,12] appear to be the most attractive, since it has already been shown experimentally that MCC exist in these systems.[13,14]

One way of transforming a real physical 1D system into a topologically nontrivial phase is to make an effectively spinless system with superconducting pairing. In the case of a 1D semiconducting wire examined in this article, the required conditions are achieved by combining a strong spin-orbit interaction (SOI), a magnetic field perpendicular to the effective SOI field, and an *s*-type superconductivity induced by the proximity effect.[9,10]

Various ideas have been proposed for detecting MCC in solid systems: measurement of conductivity,[15] noise,[16] and interference.[17] The behavior of the transverse spin polarization of a 1D wire, i.e., the polarization in a plane perpendicular to the magnetic field, has been studied.[18,19] In particular, the concept of Majorana polarization has been introduced and it has been shown that its magnitude is nonzero at the ends of a wire just in the topologically nontrivial case. Thus, Majorana polarization can be treated as a local order parameter and can be measured by spin-polarization scanning tunnelling microscopy. In this article, we demonstrate that in the general case, when the magnetic field is oriented at an arbitrary angle to the wire and perpendicular to the effective SOI field, the Majorana polarization at the two ends of a wire can differ in sign and in absolute magnitude. Here there must be a range of angles of the magnetic field such that the Majorana polarization at one of the ends of a wire in the topological phase is substantially suppressed or even equal to zero. Thus, in order to describe the topological phase transition in the case of a canted field, it is necessary to analyze some integral characteristic, which accounts for the absolute magnitudes of the spin polarization simultaneously at both ends of the wire.

2. The system to be studied and its Hamiltonian

We consider a 1D semiconducting wire parallel to the x axis and characterized by a strong SOI Rashba field on the surface of an s-type superconductor in an external magnetic field oriented at an arbitrary angle in the xz plane. Cooper pairing of electrons takes place in the wire because of the proximity effect, which is described by the induced potential Δ. We model noncollinearity of the magnetic field B relative to the z axis by directly introducing terms for single point spin-flip processes into the standard microscopic Hamiltonian.[20] As a result, the canted magnetic field has components $\mathbf{B} = (B_x, 0, -B_z)$ Therefore, the Hamiltonian for this system takes the form

$$\hat{H}_W = \sum_{j=1}^{N}\left[\sum_{\sigma}\xi_\sigma a^+_{j\sigma}a_{j\sigma} + \left(\Delta a_{j\uparrow}a_{j\downarrow} - V_x a^+_{j\uparrow}a_{j\downarrow} + \mathrm{H.c.}\right)\right] - \sum_{\sigma;j=1}^{N-1}\left[\frac{t}{2}a^+_{j\sigma}a_{j+1,\sigma} + \frac{\alpha}{2}\sigma a^+_{j\sigma}a_{j+1,\bar{\sigma}} + \mathrm{H.c.}\right], \quad (1)$$

where $\xi_\sigma = t + \sigma V_z - \mu$ is the single point energy of an electron with spin σ in a perpendicular magnetic field; μ is the chemical potential of the system; $V_{x(z)} = {}^1\!/\!_2\mu_B g B_{x(z)}$ are the

x- and z-components of the Zeeman energy; t is the electron jump parameter between closest neighbors; and, α is the intensity of the Rashba SOI. In the strong coupling approximation $t = \hbar^2/2m^*a^2$, where m^* is the effective electron mass and a is the distance between atoms in the wire. In the following $\alpha = \alpha_R/a$, where α_R is the Rashba parameter. For an InSb wire, $m^* = 0.015m_e$, $\alpha_R = 0.2$ eV Å, $\Delta \sim 10^{-4}$ eV, $g \approx 50$, $B_{x,z} = 0.01 - 1\,\mathrm{T}\pi$, (i.e., $V_{x,z} \sim 10^{-5} - 10^{-3}$ eV).[13] If $a \sim 1$ nm here, then $t \sim 1$ eV and $\alpha \sim 10^{-2}$ eV. Thus, $t \gg \alpha, V_{x,z}, \Delta$.

3. The Majorana number for a wire in a canted field

In order to evaluate the influence of the noncollinearity of the magnetic field in the region of the topological superconducting phase for a wire of finite length, we analyze the dependence of the Majorana number $M(H_W)$ on the system parameters for a closed wire described by the Hamiltonian H_W. This number is given[1] by

$$M(H_W) = \mathrm{sgn}\left[Pf\,\tilde{A}(k=0)\right]\mathrm{sgn}\left[pf\tilde{A}(k=\pi)\right], \qquad (2)$$

where Pf denotes the pfaffian of the antisymmetric matrix A, i.e., $(PfA)^2 = \det A{\cdot}\tilde{A}(k)$ is the Fourier transform of the antisymmetric matrix of the Hamiltonian for a closed wire in the Majorana operator representation, $\gamma_{Ak\sigma} = a^+_{n\sigma} + a_{n\sigma}$, $\gamma_{Bk\sigma} = i(a^+_{n\sigma} - a_{n\sigma})$,

$$H_W = \frac{i}{2}\sum_{k>0}\hat{\gamma}^+\tilde{A}(k)\hat{\gamma}, \qquad (3)$$

where $\hat{\gamma} = \left[\gamma_{AK\uparrow}\,\gamma_{AK\downarrow}\,\gamma_{BK\uparrow}\,\gamma_{BK\downarrow}\right]^T$. After some simple calculations, we find that

$$M(H_W) = \mathrm{sgn}\Big\{\left[\mu^2 - V_x^2 - V_z^2 + \Delta^2\right] \times \left[(2t-\mu)^2 - V_x^2 - V_z^2 + \Delta^2\right]\Big\}. \qquad (4)$$

It follows naturally from Eq. (4) that single site spin-flip processes make an additional contribution to the magnetic field acting on the wire. Then a topologically nontrivial phase $(M = -1)$ develops if the square of the resulting field lies within the range

$$\mu^2 + \Delta^2 < V_x^2 + V_z^2 < (2t-\mu)^2 + \Delta^2. \qquad (5)$$

Equation (5) shows that a topological superconducting phase can evidently also develop in the case of a longitudinal or transverse field, as well as in a canted field.

4. Electron spin polarization in MCC and Majorana polarization

To analyze the properties of the elementary excitations of a wire, in particular the MCC, we use the Bogolyubov transform

$$\beta_l = \sum_j\left[u_{lj}a_{j\uparrow} + v_{lj}a^+_{j\downarrow} + w_{lj}a_{j\downarrow} + z_{lj}a^+_{j\uparrow}\right]. \qquad (6)$$

Following Ref. 18, we introduce the x-component of the Majorana polarization at the j-th site in the wire and the

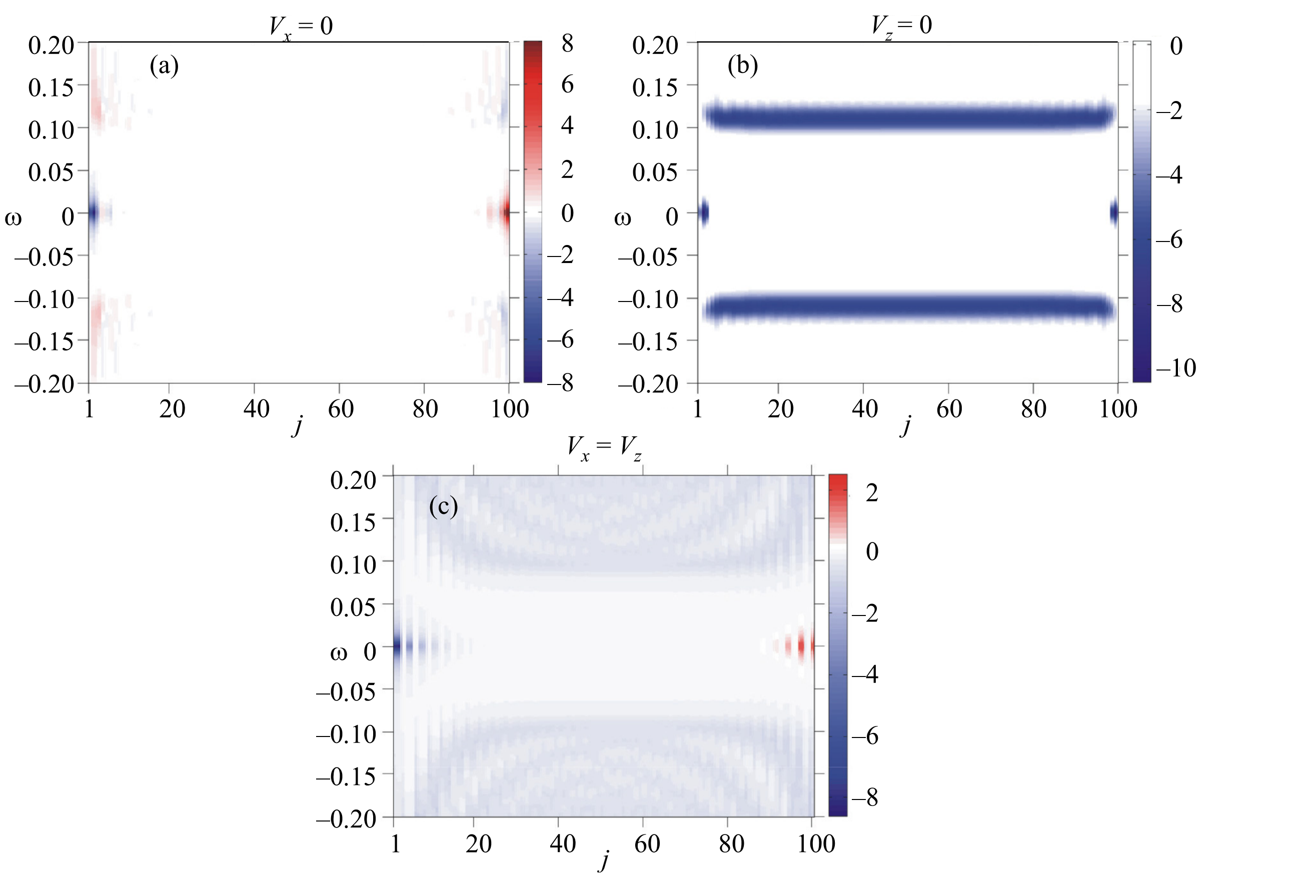

Fig. 1. The Majorana polarization as a function of the energy ω of single-electron excitation and the number j of a site in the wire; $N = 100$: $V_x = 0$ (a); $V_z = 0$ (b), and $V_x = V_z$ (c).

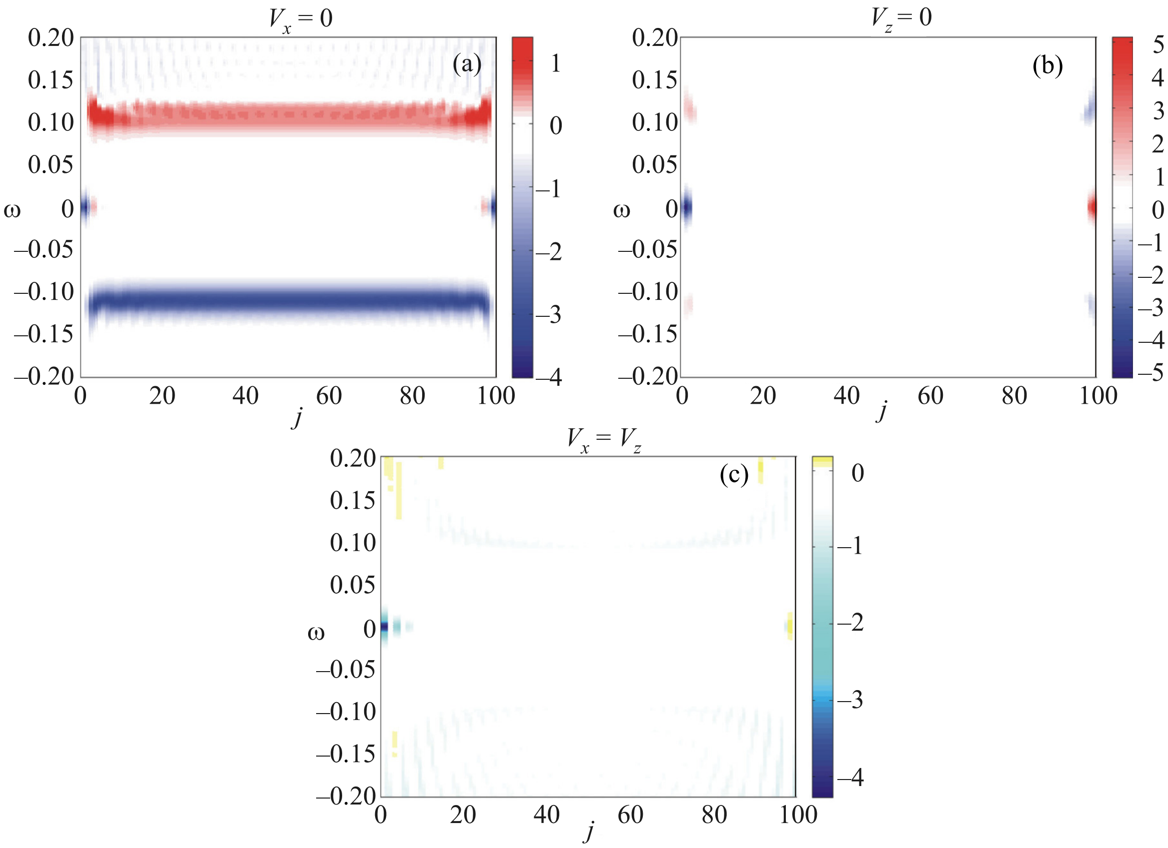

Fig. 2. Spin polarization along the z axis as a function of the energy ω of single-electron excitation and the number j of a site in the wire; $N = 100$: $V_x = 0$ (a); $V_z = 0$ (b), and $V_x = V_z$ (c).

z-component of the electron spin polarization at the j-th site in terms of the transform coefficients of Eq. (6) as follows:

$$P_{M_x}(j,\omega) = 2\sum_{l=1}^{4N} \mathrm{Re}\left[v_{lj}w_{lj}^* - z_{lj}u_{lj}^*\right]\delta(\omega - E_l), \qquad (7)$$

$$P_z(j,\omega) = \sum_{l=1}^{4N}\left\langle \Psi_{ij}\middle|\sigma_z\frac{\tau_0+\tau_z}{2}\middle|\Psi_{ij}\right\rangle \delta(\omega - E_l), \qquad (8)$$

where E_l is the eigenenergy of $\hat{H}_W$ for state l; of the wire; $|\Psi_{lj}\rangle = (u_{lj}, v_{ij}, w_{lj}, z_{lj})$ is the σ_z, τ_0, τ_z-th eigenvector; and, are the Pauli matrices acting in spin and electron-hole subspaces. The main parameters of the system for the numerical calculations will be taken from the above estimates and are quantitatively the same as in Ref. 18: $t = 1$, $\Delta = 0.3$, $\mu = 0$, $\alpha = 0.2$, $V_{x,z} = 0.4$.

5. Numerical calculations

Figure 1(a) shows the distribution of the Majorana polarization over the sites in the wire and the energy, when the magnetic field is directed along the z axis. This plot exactly reproduces the result of Ref. 18, where it was proved that Majorana polarizations are opposite at the ends of the wire using analytic calculations of the wave function of MCC. It can be seen that P_{M_x} is determined precisely by the states

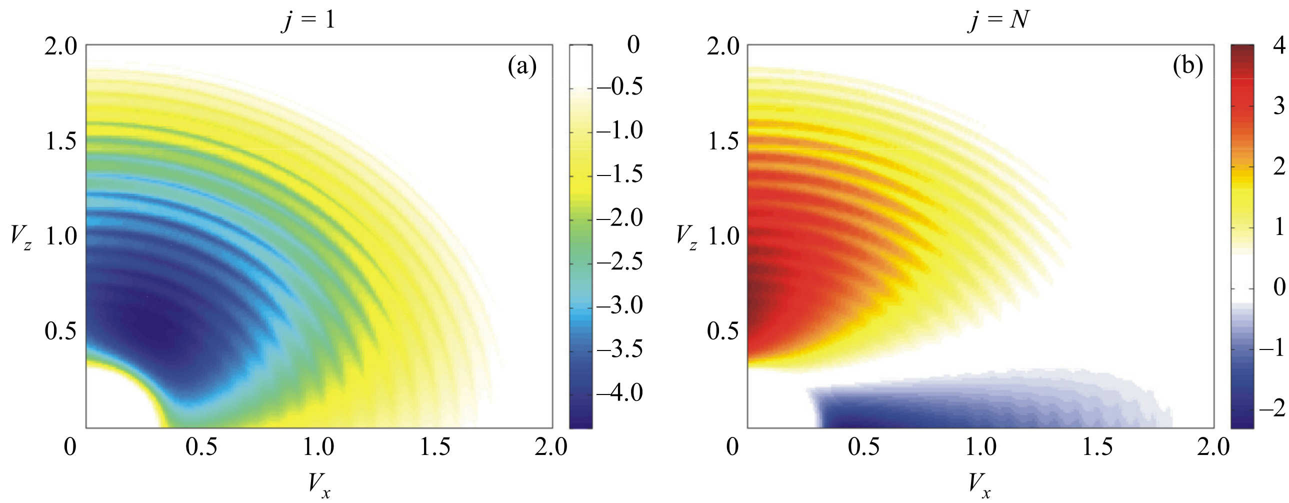

Fig. 3. The dependence of the Majorana polarization at the first (a) and last (b) sites of the wire on the direction of the magnetic field in the xz plane; $N = 30$.

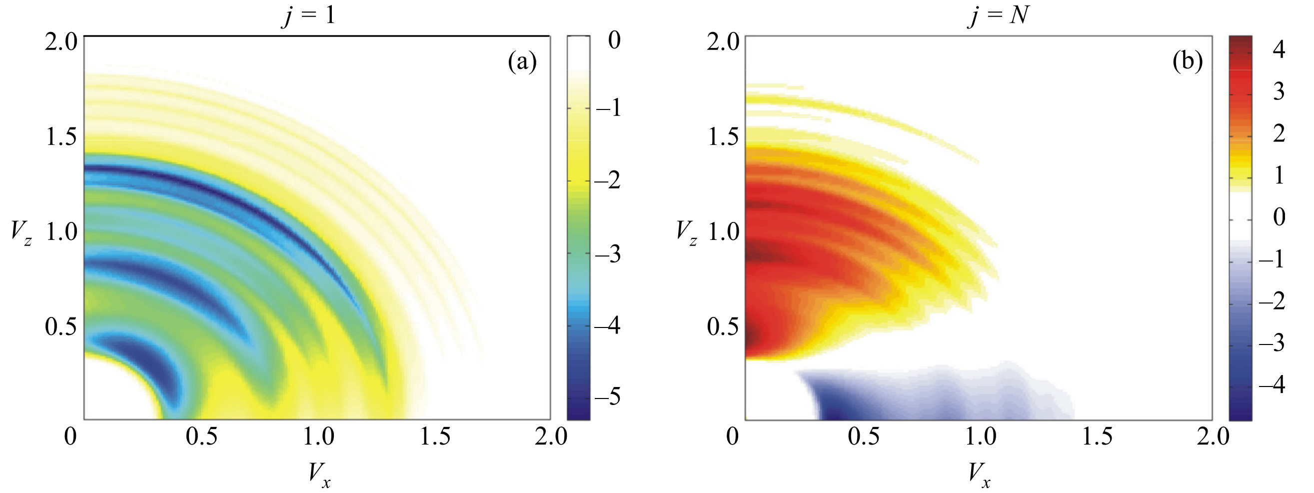

Fig. 4. The effect of disorder on the variation in the Majorana polarization at the first (a) and last (b) sites of the wire with the magnetic field direction in the *xz* plane; $N = 30$, $W = 1/2$.

with zero or near-zero energies and falls off rapidly toward the center. When the magnetic field is collinear with the wire, P_{M_x} has the same sign at the ends [Fig. 1(b)]. Here the polarization differs significantly from zero for the high-energy excitations as well. In the intermediate situation of a canted field, the distribution of P_{M_x} relative to the center of the wire is no longer symmetric. In particular, for a field oriented at an angle of $\pi/4$, the Majorana polarization has different signs and amplitudes at the opposite ends [Fig. 1(c)].

The behavior of P_{M_x} described above also shows up in the variation of the spin polarization P_z along the z axis in Fig. 2. The difference is that here it follows naturally from the proposed model that $P_z(j = 1) = P_z(j = N)$ in a perpendicular field [Fig. 2(a)] and $P_z(j = 1) = -P_z(j = N)$ in a longitudinal field [Fig. 1(b)]. Furthermore, $|P_z(j = 1)| \neq |P_z(j = N)|$ in a canted field. As opposed to the case of Fig. 1(c), however, here the z-component of the spin polarization approaches zero for $V_x = V_z$ [Fig. 2(c)]. Since the characteristics P_{M_x} and P_z behave similarly as the direction of the magnetic field is changed, in the following we analyze only the x-component of the Majorana polarization, P_{M_x}.

Since the Majorana polarization at the last site has a different sign in the two limiting cases of $V_x = 0$ and $V_z = 0$, it is obvious that this characteristic should equal zero for some angle of the magnetic field in the *xz* plane. This is confirmed by the numerical calculations of Fig. 3(b). It can be seen that for components of the magnetic field that satisfy the inequality (5) (the colored region), there is a range within which P_{M_x} is close to zero (the white region separating the yellow and blue sections). At the same time, other properties of the MCC, such as the low energy of this state, the gap in the spectrum of the elementary excitations, and the localization at the edges, remain unchanged. In Fig. 3(a), P_{M_x} at the first site in the topologically nontrivial region is everywhere negative. Note that the white segments in Figs. 3(a) and 3(b), correspond to low and high magnetic fields for which the inequality (5) is not satisfied. This results in a topologically trivial phase where the Majorana polarization is also close to zero.[18] We can, therefore, see that in a canted field the characteristic P_{M_x} cannot always be regarded as a local order parameter. Instead, it is more convenient to use the resultant parameter $|P_{M_x}(j = 1)| + |P_{M_x}(j = N)|$.

6. The effect of disorder on the Majorana polarization

We now examine the effect of disorder on the Majorana polarization in a canted field. For this, we introduce a random single-site potential W_j with a uniform distribution within the interval $[-W/2, W/2]$. The plots of Fig. 4 illustrate the role of disorder in forming the features of the Majorana polarization. These graphs show that there are no qualitative changes in the behavior of P_{M_x} owing to the introduction of random additions to the single-site energy. A certain nonuniformity does show up. However, the regions with different signs, and, therefore, the region of weak and zero Majorana polarization at one of the ends of the wire, are retained. A comparison of Figs. 3 and 4 shows that the disorder also suppresses the polarization at high fields.

7. Conclusion

In this paper we have shown the results of a numerical analysis of the behavior of the x-component of the Majorana polarization P_{M_x} at the ends of a wire with strong Rashba SOI and induced superconducting pairing for different directions of the magnetic field in the plane perpendicular to the effective Rashba field vector. We have shown that in the topological superconductivity phase this characteristic changes sign at one of the ends of the wire. As a consequence, within some range of orientation angles for the magnetic field in the *xz* plane, the Majorana polarization is characterized by zero or small absolute magnitudes. Thus, as opposed to the case of longitudinal and perpendicular magnetic fields, in a canted field this quantity will not always serve as a local order parameter describing the transition into a topologically nontrivial phase. Introducing a diagonal disorder into the system does not lead to qualitative changes in the behavior of the Majorana polarization. At the same time, for high magnetic fields an additional region appears with a weak Majorana polarization.

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