Nematic superconductivity in topological insulators induced by hexagonal warping

R.S. Akzyanov,1, 2 D. A. Khokhlov,1, 2, 3 and A.L. Rakmanov1, 2, 3

1Dukhov Research Institute of Electronics, Moscow, 127055 Russia
2Institute for Theoretical and Applied Electrodynamics, Russian Academy of Sciences, Moscow, 125412 Russia
3Moscow Institute of Physics and Technology, Dolgoprudny, Moscow Region, 141700 Russia

We study superconducting properties of the bulk states of a doped topological insulator. We obtain that the hexagonal warping stabilizes the nematic spin-triplet superconducting phase with $E_u$ pairing. The nematic order parameter opens a full gap in the electron spectrum. This order parameter exhibits non-BCS behavior. In particular, the order parameter scales with temperature as $\sqrt{1 - (T/T_c)^2}$. It depends on the chemical potential, that is, doping and on the value of the hexagonal warping. We discuss a relevance of the obtained results for the explanation of the experimental observations.

PACS numbers: 03.67.Lx, 74.90.+n

INTRODUCTION

Introduction. — The non-trivial band structure of topological insulators brings fascinating phenomena such as robust gapless surface states and ‘topological’ electromagnetic response [1]. The proximity-induced superconductivity in the topological insulators attracts great attention due to possible existence of Majorana fermions [2]. Upon doping, the topological insulator becomes a bulk superconductor. Along with the trivial s-wave pairing with $A_1$ symmetry, topologically non-trivial pairings with $A_{1u}$, $A_{2u}$, and $E_u$ symmetries are possible [3]. The $E_u$ symmetry corresponds to the vector nematic order parameter with the triplet pairing that breaks rotational symmetry. Such nematic phase supports the Majorana fermions [4], surface Andreev bound states [5], and vestigial order [6].

There is a lot of experimental evidence for the nematic superconductivity with the $E_u$ pairing in doped topological insulators. In particular, the data on the Knight shift support the spin-triplet nature of the superconducting order parameter in Cu-doped Bi$_2$Se$_3$ [7]. Breaking of the rotational symmetry was observed in the heat capacity, magnetotransport, magnetic and STM measurements [8]. Recently, it has been demonstrated experimentally that the strain dictates the direction of the anisotropy of the second critical field in Sr$_2$Bi$_2$Se$_3$ [9] that unambiguously confirms that the ground state in this topological insulator is the nematic superconductivity with $E_u$ symmetry [10]. The contact measurements show that the ratio of the superconducting gap to the critical temperature in doped topological insulator is much larger than in the BCS s-wave superconductors [11].

However, from the first sight, the origin of the nematic superconductivity in the doped topological insulators is a mystery. In their seminal work [3], Fu and Berg show that the triplet superconducting order parameter with $A_{1u}$ representation is always favorable in comparison with the nematic order with $E_u$ representation and competes with the usual s-wave pairing. Later, it was argued that electron-electron repulsion in Cu$_2$Bi$_2$Se$_3$ favors triplet $A_{1u}$ order parameter [12, 13]. In Ref. [14], the authors suggested that a significant Coulomb repulsion between electrons can stabilize the nematic superconductivity. However, this mechanism is a doubtful in the case of the topological insulators since the huge dielectric constant in this systems implies a weak electron-electron Coulomb interaction, which confirms, in particular, by the analysis of the ARPES data [15].

In this letter, we calculate the phase diagram of the doped topological insulator with attractive coupling between charge carriers. Following the approach of Ref. [3], we calculate for this purpose a superconducting susceptibility of the bulk states to determine the critical temperature of the superconducting phases with different symmetries allowed by the symmetry of the Hamiltonian. In Ref. [3] the authors used low-energy expansion of the Hamiltonian with respect to momentum taking into account only linear terms to elucidate the main features of the problem. In our calculations, we included one more term which is responsible for the hexagonal warping of the Fermi surface. This term is proportional to the third power of the momentum and arises due to the hexagonal symmetry of the real topological insulators, which, in turn, gives rise to the hexagonal warping of the Fermi surface [16, 17]. The hexagonal warping affects significantly the charge and spin transport in the topological insulators [18, 19]. It also is of importance for the characteristics of the nematic superconductivity: the presence of the hexagonal warping can give rise to opening a full superconducting gap in the spectrum [10]. We found that the hexagonal warping stabilizes superconducting phase with the nematic $E_u$ order. If the hexagonal warping is significant, the nematic phase becomes a ground state of the system. This result can explain the observations of nematic $E_u$ superconductivity in the experiments with doped topological insulators. We calculate the ratio of
the superconducting gap at zero temperature to the critical temperature and obtain that, in contrast to common s-wave BCS result, the ratio $\Delta(0)/T_c$ is non-universal and depends on the chemical potential. We also calculate the temperature dependence of the superconducting order parameter and find $\Delta(T) \sim \sqrt{1 -(T/T_c)^3}$, which also differs crucially from the BCS prediction for the s-wave pairing. The obtained results can explain the observed non-BCS behavior of $\Delta(T)$ \[11\]. Therefore, the hexagonal warping may be a key for explanation of the existence of nematic $E_u$ superconductivity in real doped topological insulators.

**Model Hamiltonian.** We use the low energy Hamiltonian of the bulk states of topological insulator in the $\mathbf{k} \cdot \mathbf{p}$ model \[17\]. The first-order momentum expansion of this Hamiltonian is written as

$$H_0(\mathbf{k}) = m\sigma_x - \mu + v(k_x\sigma_z s_y - k_y\sigma_z s_x) + v_z k_z \sigma_y,$$  

where $s_i$ and $\sigma_i$ ($i = x, y, z$) are Pauli matrices, $s_i$ acts in the spin space, $\sigma_i$ acts in the orbital space $\mathbf{p} = (P^1, P^2)$, vector $\mathbf{k} = (k_x, k_y)$ is the momentum, $2m$ is a single electron gap, $\mu$ is the chemical potential, $v$ is the Fermi velocity in the $(\Gamma K, \Gamma M)$ plane, and $v_z$ is the Fermi velocity along $\Gamma Z$ direction.

Hamiltonian Eq.\[1\] is invariant under a continuous rotation in the $(x, y)$ plane. However, crystal structure of a real 3D topological insulator (e.g., $\text{Bi}_2\text{Se}_3$) has only a discrete three fold rotational symmetry and an anisotropic term (that referred to as the hexagonal warping), $H_w(\mathbf{k}) = \lambda(k_x^3 - 3k_x k_y^2)\sigma_z s_z$, appears in the Hamiltonian \[17\]. The total single-electron Hamiltonian is

$$H(\mathbf{k}) = H_0(\mathbf{k}) + H_w(\mathbf{k}).$$ \[2\]

It obeys an inversion symmetry $PH(\mathbf{k})P = H(-\mathbf{k})$, where the inversion operator is $P = \sigma_x$.

Inelastic neutron scattering measurements on $\text{Sr}_x\text{Bi}_2\text{Se}_3$ reveal that highly anisotropic acoustic phonons along the [001] direction are mainly responsible for the electron-phonon coupling and superconductivity \[20\]. The authors of Ref. \[20\] also argue that this phonon mode enhances interorbital electron-electron coupling and we can expect that the inerorbital coupling is comparable or larger than intraorbital one. Thus, it is reasonable to apply a so-called $U - V$ model to describe the electron-electron interaction. Following Ref. \[3\], we write down corresponding term in the Hamiltonian in the short-range approximation

$$H_{\text{int}} = -U(n_1^2 + n_2^2) - 2Vn_1 n_2.$$ \[3\]

| Representation | $\Delta_1$ | $\Delta_2$ | $\Delta_3$ | $\Delta_4$ |
|---------------|----------|----------|----------|----------|
| Matrix form   | $\sigma_1$ | $\sigma_u$ | $\sigma_2$ | $(\sigma_y s_x, \sigma_y s_y)$ |

We consider here only the case of attractive interaction, that is, $U, V > 0$.

**Superconducting order parameters.** In Ref. \[3\] the model Hamiltonian $H_0 + H_{\text{int}}$ (neglecting warping term $H_w$) was treated using BCS-like mean-field approach. Four possible superconducting pairing symmetries have been classified. The addition of the term $H_w$ does not affect this classification and the results are listed in Table I.

The singlet order parameter $\Delta_1$ has even symmetry under time inversion, while $\Delta_2$, $\Delta_3$ and $\Delta_4$ are odd under this inversion. The nematic phase, that observed in many experiments, corresponds to the vector order parameter $\Delta_4 = (\Delta_{1x}, \Delta_{1y}) = \Delta_4(n_x, n_y)$ in $E_u$ representation. Here vector $\vec{n} = (n_x, n_y) = (\cos \theta, \sin \theta)$ shows a direction of the nematicity. The hexagonal warping affects the gap in the electron energy spectrum \[10\]: the warping opens a full gap and this gap is largest if $\vec{n} = (1, 0)$ even in the case $\lambda \neq 0$.

Following a standard approach, we use the superconducting susceptibilities $\chi_\alpha$ to calculate critical temperature $T_c$ for each possible superconducting phase. The phase with the highest $T_c$ is the ground state of the system. Formally, we can use equations for $T_c$ in a form presented in Ref. \[3\] but functions entering these equations correspond to different Hamiltonian and the results for the ground state are quite different. Thus, we can write \[3\]

$$\hat{\Delta}_1 : \text{det} \left( \begin{array}{cc} U_{\chi_0}(T_c) - 1 & U_{\chi_01}(T_c) \\ V_{\chi_0}(T_c) & V_{\chi_01}(T_c) - 1 \end{array} \right) = 0,$$ \[4\]

$$\hat{\Delta}_2,4 : V_{\chi_2,4}(T_c) = 1,$$ \[5\]

$\hat{\Delta}_3 : U_{\chi_3}(T_c) = 1,$ \[6\]

where superconducting susceptibilities are

$$\chi_{\alpha}(T) = \int \frac{d(T)}{2T} \int d\xi(\xi - \xi_0) \text{Tr}[(\hat{m}_\alpha P_{\mathbf{k}})^2] d^3 \mathbf{k}.$$ \[6\]

The integration is taken over all $\mathbf{k}$. Here $\alpha = 0, 1, 2, 3, 4x, 4y$, notation $\hat{m}_\alpha$ represents the matrix structure of the superconducting order parameter in the $\alpha$-phase that given in Table I, $\hat{m}_0 = s_0$, $\hat{m}_1 = \sigma_x$, $\hat{m}_2 = \sigma_y s_x$, $\hat{m}_3 = \sigma_z$, $\hat{m}_{4x} = \sigma_y s_x$, $\hat{m}_{4y} = \sigma_y s_y$. Operator $\text{Tr}[]$ is the trace of a matrix and $P_{\mathbf{k}} = \sum_{j=1,2} |\phi_j, \mathbf{k}\rangle \langle \phi_j, \mathbf{k}|$, $\phi_j, \mathbf{k}$ is an eigenvector of the Hamiltonian for the partially filled band, and $\xi$ is the quasiparticle spectrum in the normal state, $(H_0 + H_w)\phi_j, \mathbf{k} = \xi \phi_j, \mathbf{k}$. 

| $\Delta_1$ | $\Delta_2$ | $\Delta_3$ | $\Delta_4$ |
|-----------|-----------|-----------|-----------|
| Representation | $A_{1y}$ | $A_{1u}$ | $A_{2u}$ | $E_u$ |
| Matrix form | $1, \sigma_1$ | $\sigma_2$ | $(\sigma_y s_x, \sigma_y s_y)$ |
Since $k_z$ enters to integrands only with factor $v_z$, integrals (5) are proportional to $1/v_z$ and the phase diagram does not depend on $v_z$.

**Phase diagram.** — A numerical analysis of Eqs. (1) and (5), with Hamiltonian $H_0 + H_w + H_{in}$ shows that the phase $\Delta_3$ has always lower $T_c$ than $\Delta_1$. For the nematic phase with $\Delta_4$, the highest $T_c$ is attained when $n = (0,1)$ and the gap has no nodes. Depending on the parameters, the ground state of the system can be $\Delta_1$, either $\Delta_3$ or $\Delta_4$ in contrast to the case $\lambda = 0$, when only $\Delta_1$ and $\Delta_2$ are candidates for this role (3).

We introduce dimensionless parameters: chemical potential $\mu/m$, hexagonal warping $\lambda m^2/v^3$, and interaction $U/V$. The computed phase diagram of the system is shown in Fig. 1 in the plane $(\mu/m, U/V)$ for different $\lambda m^2/v^3$. The singlet pairing $\Delta_1$ is the only ground state of the system if $U > V$. The phase diagram becomes more reach when $V > U$. In the case of the warping, the ground state is either $\Delta_1$, or $\Delta_2$ depending on the chemical potential, Fig. 1 (a). In the case of small warping, Fig. 1 (b), the nematic phase $\Delta_4$ becomes a ground state at large chemical potential and the area with stable nematic $E_u$ paring rapidly increases with the increase of $\lambda m^2/v^3$, Fig. 1 (c) and (d).

The phase diagram in the plane $(\mu/m, \lambda m^2/v^3)$ is shown in Fig. 2 for different values $U/V$. As we can see, a moderate ratio between interorbital $V$ and intraorbital $U$ couplings is favorable for the nematic ordering. The increase of the chemical potential benefits both the singlet $\Delta_2$ and the triplet nematic $\Delta_4$ pairings. Increase of the hexagonal warping makes $\Delta_2$ phase less favorable in comparison to the both singlet $\Delta_1$ and nematic pairings. The growth of $\mu/m$ stimulates nematic phase $\Delta_4$ as compared to the single pairing $\Delta_1$, especially, at small values of intraorbital interaction $U$.

The numerical results reveal also that the increase of the hexagonal warping gives rise to a growth of the gap in the spectrum in the plane of the nematic phase $\Delta_4$ and to a decrease of the gap for $\Delta_2$ pairing. In the case of the singlet pairing $\Delta_1$, the gap is practically independent of the warping. Thus, the hexagonal warping favors the nematic phase since the energy gain due to superconducting transition is roughly proportional to the square of the gap.

**Mean field calculations for $E_u$ pairing.** — Here we calculate the absolute value $\Delta$ of the nematic order parameter $\Delta_4 = \Delta(0,1)$. We choose the Nambu basis as

$$\Psi_k = (\phi_k, -is_y\phi^+_k)^t,$$

where $\phi_k = (\phi_{t,1,k}, \phi_{1,1,k}, \phi_{t,-1,k}, \phi_{-1,k})^t$ and the superscript $t$ means transposition. In this basis the mean-field Hamiltonian of the topological insulator with the nematic superconducting order can be written as

$$H_{BdG}(k) = (H_0 + H_w)\tau_z + \Delta \sigma_y s_y \tau_x,$$

where $\tau_i$ is the Pauli matrix in the electron-hole space. Taking in mind that in terms of the creation-annihilation operators the considered nematic order corresponds to $c_{1\sigma}c_{2\sigma}$ pairing (3), we can write the mean-field free energy in the form

$$\Omega = \frac{2\Delta^2}{V} - 2T \sum \int \frac{d^3k}{(2\pi)^3} \ln \left\{ 1 + \exp \left[ -\epsilon_i(k)/T \right] \right\},$$

where $\epsilon_i(k)$ is the $i$-th eigenvalue of $H_{BdG}$. We compute $\Delta(T)$ by minimizing $\Omega$. This calculations reveal, in particular, that the ratio $\Delta(0)/T_c$ is not a constant value in contrast to the s-wave BCS superconductivity and depends on the chemical potential and the warping, see Fig. 3. The value $\Delta(0)/T_c$ decreases with $\mu$ and $\lambda$ and may be considerably larger than the BCS value 1.76. In Fig. 3 we show the dependence of $\Delta(T)/\Delta(0)$ on temperature, which also has non-BCS appearance. It can be approximated as $\Delta(T)/\Delta(0) \approx \sqrt{1 - (T/T_c)^3}$ and is almost independent of the hexagonal warping.

**Discussion.** — The presented results show that the existence of the hexagonal warping can explain the experimental observations of the $E_u$ superconducting pairing in the doped topological insulators if the dimensionless parameters $\lambda m^2/v^3$ and $\mu/m$ are not small. In the undoped Bi$_2$Se$_3$ the chemical potential lies near the band edge $\mu/m = 1.3$ and the strength of the warping is estimated as $\lambda m^2/v^3 = 0.11$ [17]. These values are too small for the existence of the nematic phase. However, the doping by Cu or Sc can significantly increase the chemical potential and the value $\mu/m = 2$ or larger looks realistic [21,22]. The Fermi velocity also significantly affects the warping parameter $\lambda m^2/v^3$. The reported Fermi velocities for the surface states in the topological insulators lie in a wide range from $v = 5 \times 10^7$ cm/s in Ref. [23] to $v = 10^7$ cm/s in Ref. [24] and even down to $v = 3 \times 10^5$ cm/s in Ref. [25].

Thus, the necessary large value of the effective hexagonal warping are experimentally possible. For example, if the Fermi velocity for the bulk states $v$ decreases by half in comparison with DFT calculations for the undoped Bi$_2$Se$_3$, then, the warping parameter increases by eight, $\lambda m^2/v^3 \approx 0.9$, and the nematic phase is favorable. It is hard to estimate the ratio of the interorbital to interorbital attraction $U/V$. In Ref. [13] the electron-phonon couplings have been calculated for Cu$_{0.16}$Bi$_2$Se$_3$ using DFT approach under an assumption of a weak effect of the Cu doping on the structural properties. It has been obtained that the triplet pairing $A_{2g}$ has lower free energy than $A_{1g}$. In our terms, it means that $V > U$, which is necessary for the nematic $E_u$ pairing. However, the X-ray experiments show that even small doping has a considerable effect on the structural properties of the topological insulators [9,26], so values of the Fermi velocity $v$ and hexagonal warping $\lambda$ can be also affected by doping.

The gap in the energy spectrum $2\Delta$ relates to the order
FIG. 1. The phase diagram of the system in the plane \((\mu/m, U/V)\). Blue area corresponds to the ground state with the order parameter \(\Delta_1\) (or \(A_{1g}\) representation), grey area corresponds to \(\Delta_2\) (\(A_{2g}\) representation), and red area corresponds to the nematic order parameter \(\Delta_4\) (\(E_u\) representation). Panels (a), (b), (c), and (d) show phase diagrams for different values of the hexagonal warping, \(\lambda m^2/v^3 = 0, 0.3, 0.5, \) and 1, respectively.

FIG. 2. The phase diagram in the plane \((\mu/m, \lambda m^2/v^3)\) for different values of the interaction parameter \(U/V\). The notations for the ground state are the same as in Fig. 1. Panels (a), (b), and (c) show the phase diagrams at \(U/V = 0.3, 0.5, \) and 0.7 respectively.

Conclusion. — In this letter we suggest a possible mechanism of the ground-state nematic superconductivity with the spin-triplet \(E_u\) pairing which observed in doped topological insulators. We show that the hexagonal warping is an essential feature for the realization of the nematic superconductivity. The nematic superconductivity has a non-BCS behavior of the energy gap. In particular, the ratio of the gap at \(T = 0\) to the critical temperature is non-universal and depends on the value of the chemical potential and the warping. The order parameter scales with temperature as \(\sqrt{1 - (T/T_c)^3}\).

Acknowledgement. — ALR acknowledge the support by JSPS-RFBR Grant No. 19-52-50015 and RFBR Grant No. 19-02-00421. RSA and DAK were supported by the Foundation for the Advancement of Theoretical Physics and Mathematics BASIS.

[1] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. 83, 1057 (2011)
[2] L. Fu and C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008)
[3] L. Fu and E. Berg, Phys. Rev. Lett. 105, 097001 (2010)
[4] F. Wu and I. Martin, Phys. Rev. B 95, 224503 (2017)
[5] L. Hao and C. S. Ting, Phys. Rev. B 96, 144512 (2017)
[6] M. Hecker and J. Schmalian, npj Quantum Materials 3.
FIG. 3. Ratio of the order parameter at zero temperature and the critical temperature, Δ(0)/T_c, as a function of the chemical potential for different values of the hexagonal warping. Blue line corresponds to zero warping λ = 0, red dashed line to λm^2/v^3 = 0.5, and green dot dashed line to λm^2/v^3 = 1.

FIG. 4. Dependence of the order parameter Δ on temperature for different values of the hexagonal warping. Blue line corresponds to zero warping, red line to λm^2/v^3 = 1, both curves are plotted at µ/m = 2. Green dot-dashed line is a fit Δ(T)/Δ(0) = √1 – (T/T_c)^3.

[7] K. Matano, M. Kriener, K. Segawa, Y. Ando, and G.-q. Zheng, Nature Physics 12, 852 (2016).
[8] M. Chen, X. Chen, H. Yang, Z. Du, and H.-H. Wen, Science Advances 4 (2018).
[9] A. Y. Kuntsevich, M. A. Bryzgalov, R. S. Akzyanov, V. P. Martovitskii, A. L. Rakmanov, and Y. G. Selivanov, Phys. Rev. B 100, 224509 (2019).
[10] L. Fu, Phys. Rev. B 90, L00509 (2014).
[11] T. Kirzhner, E. Lahoud, K. B. Chaska, Z. Salman, and A. Kanigel, Phys. Rev. B 86, 064517 (2012).
[12] P. M. R. Brydon, S. Das Sarma, H.-Y. Hui, and J. D. Sau, Phys. Rev. B 90, 184512 (2014).
[13] X. Wan and S. Y. Savrasov, Nature Communications 5, 4144 (2014).
[14] F. Wu and I. Martin, Phys. Rev. B 96, 144504 (2017).
[15] C. Chen, Z. Xie, Y. Feng, H. Yi, A. Liang, S. He, D. Mou, J. He, Y. Peng, X. Liu, Y. Liu, L. Zhao, G. Liu, X. Dong, J. Zhang, L. Yu, X. Wang, Q. Peng, Z. Wang, S. Zhang, F. Yang, C. Chen, Z. Xu, and X. J. Zhou, Scientific Reports 3, 2411 (2013).
[16] L. Fu, Phys. Rev. Lett. 103, 266801 (2009).
[17] C.-X. Liu, X.-L. Qi, H. Zhang, X. Dai, Z. Fang, and S.-C. Zhang, Phys. Rev. B 82, 045122 (2010).
[18] R. S. Akzyanov and A. L. Rakmanov, Phys. Rev. B 97, 075421 (2018).
[19] R. S. Akzyanov and A. L. Rakmanov, Phys. Rev. B 99, 045436 (2019).
[20] J. Wang, K. Kan, S. Li, Z. Ma, S. Bao, Z. Cai, Y. Zhang, K. Nakajima, S. Ohira-Kawamura, P. ernk, A. Schneidewind, S. Y. Savrasov, X. Wan, and J. Wen, Nature Communications 10, 2802 (2019).
[21] E. Lahoud, E. Maniv, M. S. Petrushevsky, M. Naamneh, A. Ribak, S. Wiedmann, L. Petaccia, Z. Salman, K. B. Chashka, Y. Dagan, and A. Kanigel, Phys. Rev. B 88, 195107 (2013).
[22] M. Neupane, Y. Ishida, R. Sankar, J.-X. Zhu, D. S. Sanchez, I. Belopolski, S.-Y. Xu, N. Alidoust, M. M. Hoson, S. Shin, F. Chou, M. Z. Hasan, and T. Durakiewicz, Scientific Reports 6, 22557 (2016).
[23] H. Zhang, C.-X. Liu, X.-L. Qi, X. Dai, Z. Fang, and S.-C. Zhang, Nature Physics 5, 438 (2009).
[24] M. Veldhorst, M. Snelder, M. Hoek, T. Gang, V. K. Guduru, X. L. Wang, U. Zeitler, W. G. van der Wiel, A. A. Golubov, H. Hilgenkamp, and A. Brinkman, Nature Materials 11, 417 (2012).
[25] A. Wolos, S. Szyzsko, A. Drabinska, M. Kaminska, S. G. Strzelecka, A. Hruban, A. Materna, and M. Piersa, Phys. Rev. Lett. 109, 247604 (2012).
[26] A. Y. Kuntsevich, M. A. Bryzgalov, V. A. Prudkoglyad, V. P. Martovitskii, Y. G. Selivanov, and E. G. Chizhevskii, New Journal of Physics, 20, 103022 (2018).