Possible two-component pairings in electron-doped Bi_2Se_3 based on a tight-binding model

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(Received 11 December 2018; revised manuscript received 5 March 2019; published 17 June 2019)

Recent experiments show the spontaneous breaking of rotational symmetry in the superconducting topological insulators $M_xBi_2Se_3$ (M represents Cu, Sr, or Nd), suggesting that the pairing belongs to a two-dimensional representation of the D_{3d} symmetry group of the crystal. Motivated by this progress, we construct an exhaustive list of possible two-component pairings of the $M_xBi_2Se_3$ superconductors, both for the odd-parity E_u representation and for the even-parity E_g representation. Starting from a tight-binding model for the normal phase of Bi_2Se_3 and $M_xBi_2Se_3$, we firstly construct the pairing channels in the spin-orbital basis, up to second-nearest-neighbor pairing correlations in the basal plane. We then infer the properties of these pairings by transforming them to the band (pseudospin) basis for the conduction band. A comparison with the experiments leads to several multichannel pairings as promising pairings for $M_xBi_2Se_3$ superconductors. Besides a nematic and time-reversal symmetric pairing combination, the other pairings that we have identified are chiral and nematic at the same time, which may be nonunitary and have a spontaneous magnetization. A complementary set of experiments are proposed to identify the true pairing symmetries of these superconductors and their evolution with the doping concentration x.

DOI: 10.1103/PhysRevB.99.214507

I. INTRODUCTION

The nature of the pairing of superconducting topological insulators, to be abbreviated $M_xBi_2Se_3$, with M representing a metallic element that might be Cu, Sr, or Nd, has been mysterious since their discovery [1–6]. Various experiments made conflicting implications, alluding the pairing to be topologically nontrivial [7–11] or trivial [12,13]. Recently, a series of new experiments have shown convincingly that the pairing of this family of superconductors is unconventional (see Yonezawa [14] for a recent review). For $Cu_xBi_2Se_3$ [15,16] and $Sr_xBi_2Se_3$ [17,18], more than one experiment has revealed that the superconducting state breaks the threefold rotational symmetry of the normal phase to twofold rotational symmetry, which is possible only if the pairing belongs to a two-dimensional representation of the underlying D_{3d} point group. The pairing was thereby called nematic superconductivity [19]. For $Nd_xBi_2Se_3$, in addition to the broken threefold in-plane rotational symmetry [20,21], the time-reversal symmetry appears to be also broken [6].

Multiple theoretical analyses have been made to account for these new experimental findings [22–31], which focus mostly on the odd-parity E_u representation of the D_{3d} point group. While the studies can account for the qualitative features of various experiments, a satisfactory explanation of all crucial experimental features in terms of known pairings appears to be difficult. For example, while recent experiments deny the presence of in-gap states on the surface of superconducting $Cu_xBi_2Se_3$ [12,13], the most studied E_u pairing is shown to have robust low-energy surface states [31]. In addition, the proposed E_u pairing has not been stabilized as the leading pairing instability in any theoretical calculations based on a microscopic pairing mechanism, such as the electron-phonon interaction [32–35] or the electron-electron interaction [36]. In view of the difficulty in first-principles predictions of the pairing symmetry on one hand and the extensive experimental observations accumulated to date on the other, a promising approach is to construct an exhaustive list of possible two-component pairings and compare them with the available experimental consensuses. From this comparison, we may see to what extent the existing experiments have constrained the pairing symmetry and what further experiments are necessary to figure out definitely the genuine pairing symmetries of the $M_xBi_2Se_3$ superconductors.

Motivated by the above considerations, we construct in this work a complete list of pairing channels belonging to the two-dimensional irreducible representations of the D_{3d} point group. Starting from a tight-binding model for Bi_2Se_3 and the normal phase of $M_xBi_2Se_3$, we construct pairings belonging to the odd-parity E_u representation and pairings in the even-parity E_g representation. Consistent with the tight-binding model, which is up to second-nearest-neighbor (2NN) in-plane hoppings, the constructed pairing channels are restricted to 2NN in-plane pairing correlations. The lists of two-component pairings are constructed based purely on symmetry analyses, without referring to a specific microscopic pairing mechanism, which is unclear at the present moment. By transforming from the spin-orbital basis to the band (pseudospin) basis and retaining only the conduction band which contributes to the Fermi surface, we analyze the general properties of various interesting and typical pairing channels.

After a comprehensive review over the experimental consensuses on these superconductors, including their bulk spectrum, surface spectrum, and magnetic properties, we infer the constraints of these experiments on the pairing symmetry.

Besides a well-known E_u pairing [19,32], the comparison leads to several pairing combinations that are multichannel, in addition to having two components. A purely nematic pairing combination in the E_u representation can give a fully gapped and twofold symmetric bulk spectrum, a fully gapped surface spectrum, and a twofold symmetric electronic spin susceptibility. In addition, we find several chiral and nematic pairing combinations that can explain more than one key experimental result in both the E_g representation and the E_u representation. The chiral and nematic pairing of the E_u representation, besides breaking the time-reversal symmetry, may also be nonunitary and having a spontaneous magnetization. We finally discuss the implications of the present work to the future experiments, which are highly desirable to determine the true pairing symmetry of the $M_x\mathrm{Bi_2Se_3}$ superconductors.

II. MODEL IN THE SPIN-ORBITAL AND PSEUDOSPIN BASIS

The low-energy band structures of $\mathrm{Bi_2Se_3}$ and $M_x\mathrm{Bi_2Se_3}$ (M denotes Cu, Sr, or Nd) can be described by the following two-orbital tight-binding model, defined on a quasi-two-dimensional hexagonal lattice [31,36–39]:

$$\begin{aligned} H_0(\mathbf{k}) = \epsilon(\mathbf{k})I_4 + M(\mathbf{k})\Gamma_5 + B_0c_z(\mathbf{k})\Gamma_4 + A_0[c_y(\mathbf{k})\Gamma_1 \\ -c_x(\mathbf{k})\Gamma_2] + R_1d_1(\mathbf{k})\Gamma_3 + R_2d_2(\mathbf{k})\Gamma_4. \end{aligned} \tag{1}$$

The basis operator is taken as $\phi^\dagger_{\mathbf{k}} = [a^\dagger_{\mathbf{k}\uparrow}, a^\dagger_{\mathbf{k}\downarrow}, b^\dagger_{\mathbf{k}\uparrow}, b^\dagger_{\mathbf{k}\downarrow}]$, where the a and b orbitals separately correspond to the p_z orbitals of the top and bottom Se layers of the $\mathrm{Bi_2Se_3}$ quintuple units, with a certain amount of hybridization with the p_z orbitals of the neighboring Bi layers [37–39]. I_4 is the 4×4 unit matrix. $\Gamma_1 = \sigma_3\otimes s_1$, $\Gamma_2 = \sigma_3\otimes s_2$, $\Gamma_3 = \sigma_3\otimes s_3$, $\Gamma_4 = -\sigma_2\otimes s_0$, and $\Gamma_5 = \sigma_1\otimes s_0$ [32,36–41]. s_i and σ_i ($i = 1, 2, 3$) are Pauli matrices for the spin and orbital degrees of freedom, and s_0 and σ_0 are the corresponding unit matrices. With the parity operator $P = \sigma_1\otimes s_0$, it is easy to verify that the model has the inversion symmetry $PH_0(\mathbf{k})P^{-1} = H_0(-\mathbf{k})$.

The above model was obtained previously [36] based on symmetry analysis and comparison with a $\mathbf{k}\cdot\mathbf{p}$ model defined near $k_x = k_y = k_z = 0$ [37]. The lattice of $\mathrm{Bi_2Se_3}$ and $M_x\mathrm{Bi_2Se_3}$, which belong to the D^5_{3d} space group, is mapped to a hexagonal lattice in the tight-binding model. The in-plane (labeled as the xy plane) and out-of-plane (labeled as the z direction) lattice parameters, a and c, are taken as $a = 4.14$ Å and $3c = 28.64$ Å [42]. $\epsilon(\mathbf{k}) = C_0 + 2C_1[1-\cos(\mathbf{k}\cdot\boldsymbol{\delta}_4)] + \frac{4}{3}C_2[3-\cos(\mathbf{k}\cdot\boldsymbol{\delta}_1) - \cos(\mathbf{k}\cdot\boldsymbol{\delta}_2) - \cos(\mathbf{k}\cdot\boldsymbol{\delta}_3)]$. $M(\mathbf{k})$ is obtained from $\epsilon(\mathbf{k})$ by making the substitutions $C_i \to M_i (i = 0, 1, 2)$. $c_x(\mathbf{k}) = \frac{1}{\sqrt{3}}[\sin(\mathbf{k}\cdot\boldsymbol{\delta}_1) - \sin(\mathbf{k}\cdot\boldsymbol{\delta}_2)]$, $c_y(\mathbf{k}) = \frac{1}{3}[\sin(\mathbf{k}\cdot\boldsymbol{\delta}_1) + \sin(\mathbf{k}\cdot\boldsymbol{\delta}_2) - 2\sin(\mathbf{k}\cdot\boldsymbol{\delta}_3)]$, and $c_z(\mathbf{k}) = \sin(\mathbf{k}\cdot\boldsymbol{\delta}_4)$. Finally, $d_1(\mathbf{k}) = -\frac{8}{3\sqrt{3}}[\sin(\mathbf{k}\cdot\mathbf{a}_1) + \sin(\mathbf{k}\cdot\mathbf{a}_2) + \sin(\mathbf{k}\cdot\mathbf{a}_3)]$ and $d_2(\mathbf{k}) = -8[\sin(\mathbf{k}\cdot\boldsymbol{\delta}_1) + \sin(\mathbf{k}\cdot\boldsymbol{\delta}_2) + \sin(\mathbf{k}\cdot\boldsymbol{\delta}_3)]$. Here, the four NN bond vectors of the hexagonal lattice are $\boldsymbol{\delta}_1 = (\frac{\sqrt{3}}{2}a, \frac{1}{2}a, 0)$, $\boldsymbol{\delta}_2 = (-\frac{\sqrt{3}}{2}a, \frac{1}{2}a, 0)$, $\boldsymbol{\delta}_3 = (0, -a, 0)$, and $\boldsymbol{\delta}_4 = (0, 0, c)$. The three in-plane 2NN bond vectors in $d_1(\mathbf{k})$ are $\mathbf{a}_1 = \boldsymbol{\delta}_1 - \boldsymbol{\delta}_2$, $\mathbf{a}_2 = \boldsymbol{\delta}_2 - \boldsymbol{\delta}_3$ and $\mathbf{a}_3 = \boldsymbol{\delta}_3 - \boldsymbol{\delta}_1$. The last and second last terms of $H_0(\mathbf{k})$ induce hexagonal warping of the Fermi surface and the topological surface states [37,38]. We mention in passing that $\mathrm{Nd}_x\mathrm{Bi_2Se_3}$ was reported to have multiple Fermi surfaces, with possible contributions from the d orbitals of the Nd dopants [43]. We will neglect this complexity and work with the above model for all three superconductors [26,27].

The dopants of $M_x\mathrm{Bi_2Se_3}$ (M is Cu, Sr, or Nd) dope electrons to the system so that only the conduction band contributes to the Fermi surface. Regardless of whether the superconductivity is in the weak-coupling limit or in the strong-coupling limit, as long as the Fermi energy is much larger than the superconductivity gap, as is true for the present case [2,44,45], only the states close to the Fermi surface are involved in the low-energy behavior of the superconductivity, such as the energy-gap structure and the existence of the surface Andreev bound states. Therefore, we turn to the band (pseudospin) basis and retain only the states of the conduction band in the following analyses [46–52]. Because $M_x\mathrm{Bi_2Se_3}$ in the normal state has both inversion symmetry and time-reversal symmetry, the conduction band is twofold degenerate (the Kramers degeneracy) at each wave vector $\mathbf{k}$. The operator for the inversion symmetry is the parity operator $P = \sigma_1\otimes s_0$. The time-reversal operator is taken as $T = -i\sigma_0\otimes s_2K$, where K denotes the complex conjugation. We define the pseudospin basis for the conduction-band states on the northern hemisphere (i.e., $k_z > 0$) of the three-dimensional Brillouin zone (BZ) as

$$[|\mathbf{k},\alpha\rangle, |\mathbf{k},\beta\rangle] = [|\mathbf{k},\alpha'\rangle, |\mathbf{k},\beta'\rangle]u_{\mathbf{k}}, \tag{2}$$

where α and β are the two pseudospin degrees of freedom. The Kramers degeneracy relates the two bases via $|\mathbf{k},\beta\rangle = PT|\mathbf{k},\alpha\rangle$. The two auxiliary bases are defined as [31]

$$|\mathbf{k},\alpha'\rangle = \frac{1}{\tilde{D}_{\mathbf{k}}N_{\mathbf{k}}}\begin{pmatrix}\tilde{E}_{\mathbf{k}} \\ \tilde{M}_-(\mathbf{k})\end{pmatrix}\begin{pmatrix}A_0c_+(\mathbf{k}) \\ D_-(\mathbf{k})\end{pmatrix} \tag{3}$$

and

$$|\mathbf{k},\beta'\rangle = PT|\mathbf{k},\alpha'\rangle = \frac{1}{\tilde{D}_{\mathbf{k}}N_{\mathbf{k}}}\begin{pmatrix}\tilde{M}_+(\mathbf{k}) \\ \tilde{E}_{\mathbf{k}}\end{pmatrix}\begin{pmatrix}-D_-(\mathbf{k}) \\ A_0c_-(\mathbf{k})\end{pmatrix}, \tag{4}$$

where the first and second two-component vectors are spinors separately in the subspaces of the original orbital and spin degrees of freedom. The unitary matrix connecting the two basis sets is [31]

$$u_{\mathbf{k}} = \begin{pmatrix} ie^{i(\varphi_{\mathbf{k}}+\phi_{\mathbf{k}})}\cos\frac{\theta_{\mathbf{k}}}{2} & -e^{i\phi_{\mathbf{k}}}\sin\frac{\theta_{\mathbf{k}}}{2} \\ e^{-i\phi_{\mathbf{k}}}\sin\frac{\theta_{\mathbf{k}}}{2} & -ie^{-i(\varphi_{\mathbf{k}}+\phi_{\mathbf{k}})}\cos\frac{\theta_{\mathbf{k}}}{2}\end{pmatrix}. \tag{5}$$

For notational simplicity, we have introduced the following abbreviations in Eqs. (3)–(5): $c_\pm(\mathbf{k}) = c_y(\mathbf{k}) \pm ic_x(\mathbf{k})$, $\tilde{M}_\pm(\mathbf{k}) = M(\mathbf{k}) \pm i[B_0c_z(\mathbf{k}) + R_2d_2(\mathbf{k})]$, $D_{\mathbf{k}} = \sqrt{A_0^2[c_x^2(\mathbf{k}) + c_y^2(\mathbf{k})] + R_1^2d_1^2(\mathbf{k})}$, $E_{\mathbf{k}} = \sqrt{|\tilde{M}_\pm(\mathbf{k})|^2 + D_{\mathbf{k}}^2}$, $\tilde{E}_{\mathbf{k}} = E_{\mathbf{k}} + D_{\mathbf{k}}$, $N_{\mathbf{k}} = \sqrt{2E_{\mathbf{k}}\tilde{E}_{\mathbf{k}}}$, $D_\pm(\mathbf{k}) = D_{\mathbf{k}} \pm R_1d_1(\mathbf{k})$, $\tilde{D}_{\mathbf{k}} = \sqrt{2D_{\mathbf{k}}D_-(\mathbf{k})}$, and

$$c_+(\mathbf{k}) = i\sqrt{c_x^2(\mathbf{k}) + c_y^2(\mathbf{k})}e^{-i\varphi_{\mathbf{k}}} = ic(\mathbf{k})e^{-i\varphi_{\mathbf{k}}}, \tag{6}$$

$$W_{\mathbf{k}} = \frac{\tilde{E}_{\mathbf{k}} + \tilde{M}_+(\mathbf{k})}{\sqrt{2}N_{\mathbf{k}}} = |W_{\mathbf{k}}|e^{i\phi_{\mathbf{k}}}, \tag{7}$$

$$R_1d_1(\mathbf{k}) + iA_0c(\mathbf{k}) = D_{\mathbf{k}}e^{i\theta_{\mathbf{k}}}. \tag{8}$$

The above formulas define the pseudospin basis for the conduction-band states on the northern hemisphere of the BZ

($k_z > 0$). For conduction-band states on the southern hemisphere (i.e., $k_z < 0$), the pseudospin basis are related to the pseudospin basis for states on the northern hemisphere by the symmetry operations: $|\mathbf{k},\alpha\rangle = P|-\mathbf{k},\alpha\rangle = -T|-\mathbf{k},\beta\rangle$ and $|\mathbf{k},\beta\rangle = P|-\mathbf{k},\beta\rangle = T|-\mathbf{k},\alpha\rangle$. We introduce the new Pauli matrices ϱ_i ($i = 1, 2, 3$) and the corresponding unit matrix ϱ_0 in the subspace of the two pseudospin bases. The reduced model containing only states of the conduction band is simply

$$h_0(\mathbf{k}) = E(\mathbf{k})\varrho_0, \tag{9}$$

where the dispersion of the conduction band is $E(\mathbf{k}) = \epsilon(\mathbf{k}) + E_{\mathbf{k}}$.

III. LISTS AND GENERAL PROPERTIES OF TWO-COMPONENT PAIRINGS

We now construct the full lists of the basis functions for the E_g and E_u representations of the D_{3d} group, up to 2NN in-plane pairing correlations, consistent with the tight-binding model, which is up to 2NN in-plane hopping terms [36]. Corresponding to the two basis of the model defined in the previous section, there are two ways of classifying the possible pairing channels in $M_x\mathrm{Bi_2Se_3}$. The first approach focuses on the low-energy states close to the Fermi surface [23,24,28]. For the $x > 0$ case of all three superconductors, the Fermi surface consists of states in the conduction band. Then we can neglect the valence band from our full model and work with a reduced model with only the states in the conduction band. In the second approach, we work with the full two-orbital model and construct the basis functions in the spin-orbital basis [26,27,32]. If we are interested only in the low-energy properties of the $M_x\mathrm{Bi_2Se_3}$ superconductor in the bulk, or if the normal phase is topologically trivial, the two approaches give essentially the same results. However, if we are also interested in the topological aspect of the system inherited from the topologically nontrivial normal phase, such as the coexistence of the topological surface states with the Fermi surface [2,44,45], then it is advantageous, if not imperative, to work with the second approach.

We will first construct in the spin-orbital basis the full lists of pairing channels in both the E_g and the E_u representations, up to 2NN in-plane pairing correlations. Basis functions for the irreducible representations of the D_{3d} symmetry group can be constructed in terms of the Γ matrices or the symmetrized Fourier functions. Here, we define the "symmetrized Fourier functions" as linear combinations of the trigonometric functions $\cos(\mathbf{k}\cdot\mathbf{l})$ and $\sin(\mathbf{k}\cdot\mathbf{l})$, where $\mathbf{k}$ is the wave vector and $\mathbf{l}$ represents a NN or 2NN bond vectors defined in Sec. II. Full lists of these basis functions exist in previous works [36,37]. To be self-contained, we include them in Tables I and II. For each representation, there are two sets of basis functions in terms of the Γ matrices. Up to a constant number of unit modules, the two basis sets differ by a factor of Γ_5. This is easy to understand from the fact that Γ_5 belongs to the A_{1g} representation, which respects the full symmetry of the crystal and maps an existing basis set to a new basis set belonging to the same representation. For the E_g and E_u representations, the two basis sets in Table I transform in the same manner under the D_{3d} group [36]. The symmetrized Fourier functions in Table II and their expansions in the limit of small in-plane wave vectors (i.e., $k_x a \simeq 0$ and $k_y a \simeq 0$) are

$$\varphi_0(\mathbf{k}) = \frac{1}{3}[\cos\mathbf{k}\cdot\boldsymbol{\delta}_1 + \cos\mathbf{k}\cdot\boldsymbol{\delta}_2 + \cos\mathbf{k}\cdot\boldsymbol{\delta}_3] \simeq 1 - \tfrac{1}{6}\left(k_x^2 + k_y^2\right)a^2, \tag{10}$$

$$\varphi_1(\mathbf{k}) = \frac{1}{2}[\cos\mathbf{k}\cdot\boldsymbol{\delta}_1 - \cos\mathbf{k}\cdot\boldsymbol{\delta}_2] \simeq -\frac{\sqrt{3}}{4}k_xk_ya^2, \tag{11}$$

$$\varphi_2(\mathbf{k}) = \frac{[\cos\mathbf{k}\cdot\boldsymbol{\delta}_1 + \cos\mathbf{k}\cdot\boldsymbol{\delta}_2 - 2\cos\mathbf{k}\cdot\boldsymbol{\delta}_3]}{2\sqrt{3}} \simeq -\frac{\sqrt{3}}{8}\left(k_x^2 - k_y^2\right)a^2, \tag{12}$$

$$\varphi_3(\mathbf{k}) = d_1(\mathbf{k}) \simeq \left(k_x^3 - 3k_xk_y^2\right)a^3 = \tfrac{1}{2}\left(k_+^3 + k_-^3\right)a^3, \tag{13}$$

$$\varphi_4(\mathbf{k}) = d_2(\mathbf{k}) \simeq \left(3k_yk_x^2 - k_y^3\right)a^3 = \frac{1}{2i}\left(k_+^3 - k_-^3\right)a^3, \tag{14}$$

$$\varphi_5(\mathbf{k}) = c_x(\mathbf{k}) \simeq k_xa, \tag{15}$$

and

$$\varphi_6(\mathbf{k}) = c_y(\mathbf{k}) \simeq k_ya. \tag{16}$$

We have introduced the abbreviation $k_\pm = k_x \pm ik_y$. If we extend this to include the inter-quintuple-layer pairings, we

TABLE I. Basis functions in terms of the Γ matrices. The symbols in the brackets of the first column are another commonly used name for the corresponding representation [36,37]. The semicolons in the second column separate different basis sets of the same representation.

Representation	Basis
$A_{1g}(\tilde{\Gamma}_1^+)$	I_4; Γ_5
$A_{2g}(\tilde{\Gamma}_2^+)$	Γ_{12}; Γ_{34}
$E_g(\tilde{\Gamma}_3^+)$	$\{\Gamma_{13}, \Gamma_{23}\}$; $\{\Gamma_{24}, \Gamma_{41}\}$
$A_{1u}(\tilde{\Gamma}_1^-)$	Γ_3; Γ_{35}
$A_{2u}(\tilde{\Gamma}_2^-)$	Γ_4; Γ_{45}
$E_u(\tilde{\Gamma}_3^-)$	$\{\Gamma_1, \Gamma_2\}$; $\{\Gamma_{15}, \Gamma_{25}\}$

TABLE II. Basis functions in terms of the symmetrized Fourier functions. The symmetrized Fourier functions are defined as linear combinations of $\cos(\mathbf{k}\cdot\mathbf{l})$ and $\sin(\mathbf{k}\cdot\mathbf{l})$, where $\mathbf{k}$ is the wave vector and $\mathbf{l}$ represents an NN or 2NN bond vectors defined below Eq. (1). The symbols in the brackets of the first column are another commonly used name for the corresponding representation [36,37]. The semicolon in the second line of the second column separates different basis sets of the A_{1g} representation.

Representation	Basis
$A_{1g}(\tilde{\Gamma}_1^+)$	1; $\varphi_0(\mathbf{k})$
$A_{2g}(\tilde{\Gamma}_2^+)$	None
$E_g(\tilde{\Gamma}_3^+)$	$\{\varphi_1(\mathbf{k}), \varphi_2(\mathbf{k})\}$
$A_{1u}(\tilde{\Gamma}_1^-)$	$\varphi_3(\mathbf{k})$
$A_{2u}(\tilde{\Gamma}_2^-)$	$\varphi_4(\mathbf{k})$
$E_u(\tilde{\Gamma}_3^-)$	$\{-\varphi_6(\mathbf{k}), \varphi_5(\mathbf{k})\}$

can replace $\varphi_0(\mathbf{k})$ with $\varphi_0'(\mathbf{k}) = \cos \mathbf{k}\cdot\boldsymbol{\delta}_4$ and replace $\varphi_4(\mathbf{k})$ with $\varphi_4'(\mathbf{k}) = \sin \mathbf{k}\cdot\boldsymbol{\delta}_4$. However, we will focus on the intra-quintuple-layer pairings in this work.

By multiplying the basis functions in Table I and those in Table II, we can get various product representations of the D_{3d} group. These product representations can be decomposed into the irreducible representations according to the group theory [53]. For example, $A_{1u}\otimes E_g = E_u$ and $E_g\otimes E_u = A_{1u} + A_{2u} + E_u$. In such a manner, we can identify all the realizations of the possible irreducible representations. When taken as a part of the model Hamiltonian, they are subject to further constraints. If a term is taken as a part of the model for the electronic structures in the normal state, this term should belong to the A_{1g} representation and has to be Hermitian [36,37]. These constraints, together with the time-reversal symmetry of the materials, eliminate many combinations.

If a basis set is taken as the superconducting pairing term, then it has to satisfy the Fermi exchange statistics. Another important aspect of the symmetry of the pairing term is related to the peculiar transformation property of the pairing term under the time-reversal operation [54,55]. In the spin-orbital basis $\phi_{\mathbf{k}}^\dagger$, the pairing term has the following general expression:

$$\phi_{\mathbf{k}}^\dagger \underline{\Delta}(\mathbf{k})[\phi_{-\mathbf{k}}^\dagger]^{\mathrm{T}} + \text{H.c.}, \tag{17}$$

where the superscript T means taking the transpose, and H.c. means the Hermitian conjugate of the first term. According to Blount [54,55], the time-reversed creation operator transforms under the symmetry operation just like the corresponding annihilation operator. That is,

$$T[\phi_{\mathbf{k}}^\dagger]^{\mathrm{T}} = -i\sigma_0\otimes s_2[\phi_{-\mathbf{k}}^\dagger]^{\mathrm{T}} \tag{18}$$

transforms in the same manner as $\phi_{\mathbf{k}}$ under the action of the D_{3d} symmetry group and the time-reversal operation [54]. This means that, by transforming the creation operator part of the pairing term to

$$\phi_{\mathbf{k}}^\dagger \underline{\Delta}(\mathbf{k})[\phi_{-\mathbf{k}}^\dagger]^{\mathrm{T}} = \phi_{\mathbf{k}}^\dagger \underline{\Delta}(\mathbf{k}) i\sigma_0\otimes s_2(-i\sigma_0\otimes s_2)[\phi_{-\mathbf{k}}^\dagger]^{\mathrm{T}}, \tag{19}$$

the matrix

$$\underline{\Delta}(\mathbf{k}) i\sigma_0\otimes s_2 \tag{20}$$

has the same transformation property as the terms in the model for the normal-state electronic structures. As a result, we can construct the basis functions according to the general procedure for the normal state [37,53]. Since the obtained basis is of the form of Eq. (20), we multiply $-i\sigma_0\otimes s_2$ *from the right* and get the basis functions of the pairing term. Then we single out from the results those obeying the Fermi exchange statistics, namely, $\underline{\Delta}^{\mathrm{T}}(-\mathbf{k}) = -\underline{\Delta}(\mathbf{k})$. The above discussions correspond to taking the Nambu basis as $[\phi_{\mathbf{k}}^\dagger, \phi_{-\mathbf{k}}^{\mathrm{T}}]$. If we take the Nambu basis as $[\phi_{\mathbf{k}}^\dagger, \phi_{-\mathbf{k}}^{\mathrm{T}}(i\sigma_0\otimes s_2)]$ instead, then the pairing term will be in the form of Eq. (20) spontaneously [46]. Hereafter, we will stick to the first Nambu basis.

The resulting basis sets (up to 2NN in-plane pairing correlations) for the E_g and E_u representations are separately shown in Table III and Table IV. The new Γ matrices in the tables with two subindices are defined as $\Gamma_{\mu\nu} = \frac{1}{2i}[\Gamma_\mu, \Gamma_\nu]$, where both μ and ν run from 1 to 5. Explicitly, $\Gamma_{12} = \sigma_0\otimes s_3$, $\Gamma_{13} = -\sigma_0\otimes s_2$, $\Gamma_{14} = \sigma_1\otimes s_1$, $\Gamma_{15} = \sigma_2\otimes s_1$, $\Gamma_{23} = \sigma_0\otimes s_1$, $\Gamma_{24} = \sigma_1\otimes s_2$, $\Gamma_{25} = \sigma_2\otimes s_2$, $\Gamma_{34} = \sigma_1\otimes s_3$, $\Gamma_{35} = \sigma_2\otimes s_3$, and $\Gamma_{45} = \sigma_3\otimes s_0$. Note that, we have multiplied a factor of $\sigma_0\otimes is_2$ to each component of the basis sets. To get the final expressions for the pairing components, we have to multiply back a factor of $\sigma_0\otimes(-is_2)$ to each component listed in the tables [46,54–56]. Also notice that each basis set can be multiplied by a factor of an arbitrary linear combination of $\varphi_0(\mathbf{k})$ and a constant.

TABLE III. Basis functions for the even-parity two-dimensional representation E_g, expressed as linear combinations of products between the Γ matrices and the symmetrized Fourier functions. The first column is the numbering of the various pairing channels. The second and third columns are separately the two components of the corresponding basis sets.

$E_g^{(n)}$	$\psi_1^{(n)}(\mathbf{k})(\sigma_0\otimes is_2)$	$\psi_2^{(n)}(\mathbf{k})(\sigma_0\otimes is_2)$
$n=1$	$-I_4\varphi_2(\mathbf{k})$	$I_4\varphi_1(\mathbf{k})$
$n=2$	$-\Gamma_5\varphi_2(\mathbf{k})$	$\Gamma_5\varphi_1(\mathbf{k})$
$n=3$	$-\Gamma_4\varphi_6(\mathbf{k})$	$\Gamma_4\varphi_5(\mathbf{k})$
$n=4$	$\Gamma_2\varphi_3(\mathbf{k})$	$-\Gamma_1\varphi_3(\mathbf{k})$
$n=5$	$\Gamma_1\varphi_4(\mathbf{k})$	$\Gamma_2\varphi_4(\mathbf{k})$
$n=6$	$\Gamma_3\varphi_5(\mathbf{k})$	$\Gamma_3\varphi_6(\mathbf{k})$
$n=7$	$\Gamma_2\varphi_5(\mathbf{k})+\Gamma_1\varphi_6(\mathbf{k})$	$-\Gamma_2\varphi_6(\mathbf{k})+\Gamma_1\varphi_5(\mathbf{k})$

The symmetry channels listed in Tables III and IV are one central result of this work. Two features of the tables are apparent. First, only the two basis functions of $E_u^{(1)}$ are completely $\mathbf{k}$ independent. This is the pairing channel that has attracted the most attention as a promising candidate for the nematic pairing in $Cu_xBi_2Se_3$ [19,22]. Second, among the listed basis sets in the E_g channel, only the leading three channels are spin-singlet in the spin-orbital basis. Among the twelve E_u channels, only $E_u^{(3)}$ is spin-singlet in the spin-orbital basis.

According to a theorem by Yip and Garg, the most general pairing can be written as a linear combination of all inde-

TABLE IV. Basis functions for the odd-parity two-dimensional representation E_u, expressed as linear combinations of products between the Γ matrices and the symmetrized Fourier functions. The first column is the numbering of the various pairing channels. The second and third columns are separately the two components of the corresponding basis sets.

$E_u^{(n)}$	$\tilde{\psi}_1^{(n)}(\mathbf{k})(\sigma_0\otimes is_2)$	$\tilde{\psi}_2^{(n)}(\mathbf{k})(\sigma_0\otimes is_2)$
$n=1$	Γ_{15}	Γ_{25}
$n=2$	$\Gamma_{35}\varphi_1(\mathbf{k})$	$\Gamma_{35}\varphi_2(\mathbf{k})$
$n=3$	$\Gamma_{45}\varphi_2(\mathbf{k})$	$-\Gamma_{45}\varphi_1(\mathbf{k})$
$n=4$	$\Gamma_{15}\varphi_2(\mathbf{k})+\Gamma_{25}\varphi_1(\mathbf{k})$	$\Gamma_{15}\varphi_1(\mathbf{k})-\Gamma_{25}\varphi_2(\mathbf{k})$
$n=5$	$\Gamma_{12}\varphi_5(\mathbf{k})$	$\Gamma_{12}\varphi_6(\mathbf{k})$
$n=6$	$\Gamma_{34}\varphi_5(\mathbf{k})$	$\Gamma_{34}\varphi_6(\mathbf{k})$
$n=7$	$\Gamma_{13}\varphi_3(\mathbf{k})$	$\Gamma_{23}\varphi_3(\mathbf{k})$
$n=8$	$-\Gamma_{24}\varphi_3(\mathbf{k})$	$\Gamma_{14}\varphi_3(\mathbf{k})$
$n=9$	$\Gamma_{23}\varphi_4(\mathbf{k})$	$-\Gamma_{13}\varphi_4(\mathbf{k})$
$n=10$	$\Gamma_{14}\varphi_4(\mathbf{k})$	$\Gamma_{24}\varphi_4(\mathbf{k})$
$n=11$	$-\Gamma_{13}\varphi_5(\mathbf{k})+\Gamma_{23}\varphi_6(\mathbf{k})$	$\Gamma_{13}\varphi_6(\mathbf{k})+\Gamma_{23}\varphi_5(\mathbf{k})$
$n=12$	$\Gamma_{14}\varphi_6(\mathbf{k})+\Gamma_{24}\varphi_5(\mathbf{k})$	$\Gamma_{14}\varphi_5(\mathbf{k})-\Gamma_{24}\varphi_6(\mathbf{k})$

pendent basis sets of the representation [57]. We therefore write the general expression of the pairing term in the E_g representation as

$$\underline{\Delta}_g(\mathbf{k}) = \sum_{\alpha=1}^{7} \Delta_\alpha\big[\eta_1\psi_1^{(\alpha)}(\mathbf{k}) + \eta_2\psi_2^{(\alpha)}(\mathbf{k})\big]. \tag{21}$$

(η_1, η_2) is the same vector for all seven E_g pairing channels, so that the order parameter transforms as a well-defined vector in the subspace of the E_g representation. Similarly, the general pairing in the E_u representation is written as

$$\underline{\Delta}_u(\mathbf{k}) = \sum_{\alpha=1}^{12} \tilde{\Delta}_\alpha[\tilde{\eta}_1\tilde{\psi}_1^{(\alpha)}(\mathbf{k}) + \tilde{\eta}_2\tilde{\psi}_2^{(\alpha)}(\mathbf{k})]. \tag{22}$$

Again, $(\tilde{\eta}_1, \tilde{\eta}_2)$ is the same vector for all twelve E_u pairing channels. Notice that we have restricted the pairing to the same (i.e., E_u or E_g) irreducible representation of the symmetry group. The superconducting state with mixed even-parity and odd-parity components, which was found to stabilize under suitable circumstances [28,58], will not be considered in the present work.

Among the pairing combinations contained in Eqs. (21) and (22), we are particularly interested in those pairings that have been stabilized as the ground state in previous studies, based on a microscopic or phenomenological pairing mechanism, and those that are possibly consistent with more than one key experimental consensuses on the $M_x\mathrm{Bi}_2\mathrm{Se}_3$ superconductors. The theoretical studies motivated by the recent experiments focus on pairings in the odd-parity E_u channel. Besides $E_u^{(1)}$ [19,31], other E_u pairings have been studied in previous works. Direct comparison shows that $E_u^{(6)}$ and $E_u^{(11)}$ were studied by Yuan *et al.* [26], $E_u^{(6)}$ and $E_u^{(9)}$ (if we replace $\varphi_4(\mathbf{k})$ with $\varphi_4'(\mathbf{k}) = \sin\mathbf{k}\cdot\boldsymbol{\delta}_4$) were studied by Chirolli *et al.* [27]. These pairing channels exhaust the three kinds of pairings in Tables III and IV, with regard to the difference between the two pairing components: For $E_u^{(1)}$ and $E_u^{(9)}$ the difference comes from the two different Γ matrices, Γ_{15} versus Γ_{25} for $E_u^{(1)}$ and Γ_{13} versus Γ_{23} for $E_u^{(9)}$; for $E_u^{(6)}$ the difference between the two components comes from the $\varphi_5(\mathbf{k})$ and $\varphi_6(\mathbf{k})$ symmetry factors; for $E_u^{(11)}$ the distinction comes from a combination of the difference between Γ_{13} and Γ_{23} and the difference between $\varphi_5(\mathbf{k})$ and $\varphi_6(\mathbf{k})$.

The even-parity E_g channels have attracted much less attention. The only theoretical paper focusing on the even-parity pairings studied the leading pairing instabilities resulting from the purely repulsive short-range electron-electron interactions [36,56]. The six pairings found in that paper could be identified as the six pairing components of $E_g^{(1)}$, $E_g^{(2)}$, and $E_g^{(3)}$. In all these three E_g channels, the difference between the two basis components comes completely from the $\mathbf{k}$-dependent symmetry factors.

The nature of the pairing defined by Eq. (21) [Eq. (22)] depends both on the pairing strengths Δ_α ($\tilde{\Delta}_\alpha$) and on the two-component vector (η_1, η_2) [$(\tilde{\eta}_1, \tilde{\eta}_2)$]. For simplicity, we will assume in the following analysis that Δ_α ($\alpha = 1, \ldots, 6$) and $\tilde{\Delta}_\alpha$ ($\alpha = 1, \ldots, 12$) are all real numbers. By this convention, we neglect pairings analogous to the single-component chiral pairings, like the $s + is'$, $d + id'$, and $p + ip'$ pairings [59–61]. The nonzero Δ_α or $\tilde{\Delta}_\alpha$ indicate the pairing channels that contribute to the superconducting order parameter. The relative magnitudes of the Δ_α or $\tilde{\Delta}_\alpha$ parameters characterize the contributions of different pairing channels. Then, depending on the (η_1, η_2) or the $(\tilde{\eta}_1, \tilde{\eta}_2)$ vector, we may define the chirality and nematicity of the two-component superconducting order parameters [19,23,24]: The pairing is nematic if at least one of $|\eta_1|^2 - |\eta_2|^2$ ($|\tilde{\eta}_1|^2 - |\tilde{\eta}_2|^2$) and $\eta_1\eta_2^* + \eta_1^*\eta_2$ ($\tilde{\eta}_1\tilde{\eta}_2^* + \tilde{\eta}_1^*\tilde{\eta}_2$) is nonzero. The pairing is chiral if $\eta_1\eta_2^* - \eta_1^*\eta_2 \neq 0$ ($\tilde{\eta}_1\tilde{\eta}_2^* - \tilde{\eta}_1^*\tilde{\eta}_2 \neq 0$), or equivalently, η_1/η_2 ($\tilde{\eta}_1/\tilde{\eta}_2$) is a nonzero and finite complex number.

To understand the properties of various pairings, we turn from the spin-orbital basis to the band (pseudospin) basis [46–52], defining $U_\mathbf{k} = [|\mathbf{k}, \alpha\rangle, |\mathbf{k}, \beta\rangle]$ and $U_{-\mathbf{k}} = [|-\mathbf{k}, \alpha\rangle, |-\mathbf{k}, \beta\rangle]$ for $k_z > 0$. A pairing wave function (i.e., superconducting order parameter) expressed as $\underline{\Delta}(\mathbf{k})$ in the original spin-orbital basis transforms to

$$\tilde{\underline{\Delta}}(\mathbf{k}) = U_\mathbf{k}^\dagger \underline{\Delta}(\mathbf{k}) U_{-\mathbf{k}}^* \tag{23}$$

in the pseudospin basis [31]. As the properties of the six symmetry factors $\varphi_i(\mathbf{k})$ ($i = 1, \ldots, 6$) are known from Eqs. (11)–(16), the remaining task is to calculate the basis transformations for the sixteen 4×4 matrices in Tables III and IV.

A. The E_g pairings

First consider the E_g representation. Define $I_4' = I_4(-\sigma_0 \otimes is_2)$ and $\Gamma_i' = \Gamma_i(-\sigma_0 \otimes is_2)$ ($i = 1, \ldots, 5$), and define the Pauli matrices in the pseudospin basis as ϱ_i ($i = 0, 1, 2, 3$). In terms of Eq. (23), the relevant transformations are found to be

$$\tilde{I}_4'(\mathbf{k}) = -i\varrho_2, \tag{24}$$

$$\tilde{\Gamma}_1'(\mathbf{k}) = -\frac{A_0 c_y(\mathbf{k})}{E_\mathbf{k}} i\varrho_2, \tag{25}$$

$$\tilde{\Gamma}_2'(\mathbf{k}) = \frac{A_0 c_x(\mathbf{k})}{E_\mathbf{k}} i\varrho_2, \tag{26}$$

$$\tilde{\Gamma}_3'(\mathbf{k}) = -\frac{R_1 d_1(\mathbf{k})}{E_\mathbf{k}} i\varrho_2, \tag{27}$$

$$\tilde{\Gamma}_4'(\mathbf{k}) = -\frac{B_0 c_z(\mathbf{k}) + R_2 d_2(\mathbf{k})}{E_\mathbf{k}} i\varrho_2, \tag{28}$$

$$\tilde{\Gamma}_5'(\mathbf{k}) = -\frac{M(\mathbf{k})}{E_\mathbf{k}} i\varrho_2. \tag{29}$$

While only three (i.e., $E_g^{(1)}$, $E_g^{(2)}$, and $E_g^{(3)}$) out of the seven channels listed in Table III are spin singlet in the original spin-orbital basis, all seven E_g channels are pseudospin singlets in the pseudospin basis. In particular, although $E_g^{(7)}$ is very different from $E_g^{(1)}$ and $E_g^{(2)}$ in the spin-orbital basis, the symmetry factors of the two basis components of $E_g^{(7)}$ behave like $k_x^2 - k_y^2$ and $-2k_xk_y$ in the band (pseudospin) basis, qualitatively the same as the corresponding basis components of $E_g^{(1)}$ and $E_g^{(2)}$, if the slight anisotropy introduced by $E_\mathbf{k}$ and $M(\mathbf{k})$ is neglected. In addition, $E_g^{(4)}$ is identical to $E_g^{(6)}$ in the pseudospin basis, up to a $\mathbf{k}$-independent constant factor. Finally, we point out that the seemingly different $E_g^{(3)}$ and $E_g^{(5)}$ are closely related. In fact, if we replace $\varphi_4(\mathbf{k}) = d_2(\mathbf{k})$ in $E_g^{(5)}$ by $\varphi_4(\mathbf{k}) + \frac{B_0}{R_2}\varphi_4'(\mathbf{k}) = d_2(\mathbf{k}) + \frac{B_0}{R_2}c_z(\mathbf{k})$, which have the same symmetry as that of $\varphi_4(\mathbf{k})$ under D_{3d}, then $E_g^{(3)}$ and

$E_g^{(5)}$ are identical in the pseudospin basis up to a constant factor.

Notice that the six spin-singlet pairings identified in a previous study combine to $E_g^{(1)}$, $E_g^{(2)}$, and $E_g^{(3)}$ [36,56]. The two components of $E_g^{(3)}$ were incorrectly identified as belonging to the E_u representation [36,56] because of neglecting the different transformation properties of the pairing term compared to the model for the normal-state electronic structures, as we explained in Eqs. (17)–(20).

To understand the qualitative properties of the various pairing channels, we consider each pairing channel separately. That is, we assume that only one among the seven Δ_α parameters in Eq. (21) is nonzero. From the transformations in Eqs. (24)–(29) and the expansions in Eqs. (11)–(16), it is easy to see that all 14 pairing components, $\psi_m^{(n)}$ ($n = 1, \dots, 7$ and $m = 1, 2$), included in Table III have line nodes for both spheroidal and corrugated cylindrical Fermi surfaces. If the Fermi surface is corrugated cylindrical, a chiral combination of $\psi_1^{(1)}$ and $\psi_2^{(1)}$ can give a fully gapped bulk spectrum. The same is true for the two components of $E_g^{(2)}$ and the two components of $E_g^{(7)}$. If the Fermi surface is spheroidal, the chiral combination of the two components of $E_g^{(1,2,7)}$ give a bulk spectrum with two point nodes at $k_x = k_y = 0$ of the Fermi surface. The remaining four pairing channels, $E_g^{(3)}$–$E_g^{(6)}$, have line nodes for arbitrary (η_1, η_2), for both spheroidal and corrugated cylindrical Fermi surfaces. One common set of line nodes for $E_g^{(3)}$ comes by setting the $B_0 c_z(\mathbf{k}) + R_2 d_2(\mathbf{k})$ factor of Eq. (28) to zero. Six line nodes persist for $E_g^{(4)}$ and $E_g^{(6)}$, which both come from $\varphi_3(\mathbf{k}) = d_1(\mathbf{k}) = 0$. $E_g^{(5)}$ also has six prevalent line nodes, which come from $\varphi_4(\mathbf{k}) = d_2(\mathbf{k}) = 0$. For a spheroidal Fermi surface, the six line nodes from $d_1(\mathbf{k}) = 0$ or $d_2(\mathbf{k}) = 0$ connect at the two points of the Fermi surface with $k_x = k_y = 0$.

We can also estimate the magnitude of the superconducting gaps. For $M_x\mathrm{Bi_2Se_3}$ (M is Cu, Sr, or Nd), the chemical potential $\mu > 0$ lies in the conduction band. According to experiments [2,44] and first-principles calculations [37,39], $k_x a$ and $k_y a$ are all very small for wave vectors on the Fermi surface. The superconducting gap of a certain pairing channel can therefore be characterized in terms of its power in $ka = \sqrt{k_x^2 + k_y^2}a$. For states lying on the Fermi surface, we have $E_\mathbf{k} + \epsilon(\mathbf{k}) = \mu$. $\epsilon(\mathbf{k})$ and $M(\mathbf{k})$ vary only slightly over states on the Fermi surface, and so does $E_\mathbf{k}$ [31]. As an approximation, we treat $E_\mathbf{k} = \mu - \epsilon(\mathbf{k})$ and $M(\mathbf{k})$ as constants. Under these conditions, we see that the gap of $E_g^{(1)}$ is of the order $(ka)^2$. $E_g^{(2)}$ and $E_g^{(7)}$ also open superconducting gaps in the order of $(ka)^2$ but reduced by a factor of $M(\mathbf{k})/E_\mathbf{k}$ and $A_0/E_\mathbf{k}$ compared to $E_g^{(1)}$. The superconducting gaps of $E_g^{(4,5,6)}$ are all in the order of $(ka)^4$ and are two powers smaller than $(ka)^2$. For $c_z(\mathbf{k}) = 0$, the superconducting gap for $E_g^{(3)}$ is also in the order of $(ka)^4$. However, the two components of $E_g^{(3)}$ behave more like $(k_x a)(k_z c)$ and $(k_y a)(k_z c)$, and are more efficient than $E_g^{(4,5,6)}$ in opening the superconducting gap. The angular dependence of the pairing amplitudes on the $k_x k_y$ plane, which was neglected in the above analysis in terms of the ka factor, can be obtained from Eqs. (11)–(16). The above estimations are summarized in Table V.

TABLE V. Order-of-magnitude estimations of the superconducting gaps for the E_g pairing channels defined in Table III, on the $k_z = 0$ slice of the Fermi surface. The first column is the numbering of the various pairing channels. The second column contains the order-of-magnitude estimation of the corresponding pairing channel in terms of the magnitude of the wave vector on the $k_z = 0$ slice of the Fermi surface. $k = \sqrt{k_x^2 + k_y^2}$ is the magnitude of the Fermi wave vector. $a = 4.14$ Å is the in-plane lattice parameter. Notice that, as is explained in the text, $E_g^{(3)}$ is more effective in opening an energy gap away from the $k_z = 0$ plane.

$E_g^{(n)}$	Order of magnitude of the pairing
$n = 1$	$(ka)^2$
$n = 2$	$\frac{\lvert M(\mathbf{k})\rvert}{E_\mathbf{k}}(ka)^2$
$n = 3$	$\frac{\lvert R_2\rvert}{E_\mathbf{k}}(ka)^4$
$n = 4$	$\frac{\lvert A_0\rvert}{E_\mathbf{k}}(ka)^4$
$n = 5$	$\frac{\lvert A_0\rvert}{E_\mathbf{k}}(ka)^4$
$n = 6$	$\frac{\lvert R_1\rvert}{E_\mathbf{k}}(ka)^4$
$n = 7$	$\frac{\lvert A_0\rvert}{E_\mathbf{k}}(ka)^2$

Among the seven pairing channels in Table III, only the two components of $E_g^{(3)}$ can have a sign change in the pseudospin basis, when we substitute $-k_z$ for k_z. This implies that only $E_g^{(3)}$ can give surface Andreev bound states on the natural xy surface of the $M_x\mathrm{Bi_2Se_3}$ superconductors. As regards the topological surface states of the normal phase, according to a previous theoretical study [62], all the pairing channels in Table III except for $E_g^{(3)}$ can open a gap in the topological surface states. Therefore, among all seven E_g pairings, $E_g^{(3)}$ is special with regard to the surface properties. The surface states for the $E_g^{(3)}$ pairings were studied in a previous work [36]. On the other hand, since all seven E_g pairings are pseudospin singlets, they are expected to have trivial isotropic electronic spin susceptibility in the xy plane.

B. The E_u pairings

We next study the pairings belonging to the E_u representation. We define $\Gamma'_{\mu\nu} = \Gamma_{\mu\nu}(-i\sigma_0 \otimes s_2)$ for $\mu, \nu = 1, \dots, 5$ and $\mu < \nu$. As noticed in previous studies, the $E_u^{(1)}$ channel, which is $\mathbf{k}$ independent in the spin-orbital basis, has a complicated $\mathbf{k}$ dependence in the band (pseudospin) basis [19,31,46]. This is generally true for all the 12 E_u channels listed in Table IV. Besides the $E_u^{(1)}$ channel, only the symmetry factors of $E_u^{(2)}$, $E_u^{(3)}$, and $E_u^{(4)}$ are even functions of $\mathbf{k}$. In addition, $E_u^{(2)}$ (multiplied by $\sigma_0 \otimes is_2$ from right) is a direct product of Γ_{35} which belongs to the A_{1u} representation (Table I) and $\{\varphi_1(\mathbf{k}), \varphi_2(\mathbf{k})\}$ which belongs to the E_g representation (Table II). Γ'_{35} was a chief candidate of the pairing for $\mathrm{Cu}_x\mathrm{Bi_2Se_3}$ in early theoretical discussions [32,40,46,63]. The relevant basis transformations for these four channels are

$$\tilde{\Gamma}'_{15}(\mathbf{k}) = [(B_0 c_z + R_2 d_2)\varrho_1 - R_1 d_1 \varrho_2 - A_0 c_x \varrho_3]\frac{i\varrho_2}{E_\mathbf{k}}, \quad (30)$$

$$\tilde{\Gamma}'_{25}(\mathbf{k}) = [R_1 d_1 \varrho_1 + (B_0 c_z + R_2 d_2)\varrho_2 - A_0 c_y \varrho_3]\frac{i\varrho_2}{E_\mathbf{k}}, \quad (31)$$

$$\tilde{\Gamma}'_{35}(\mathbf{k}) = [A_0c_x\varrho_1 + A_0c_y\varrho_2 + (B_0c_z + R_2d_2)\varrho_3]\frac{i\varrho_2}{E_{\mathbf{k}}}, \quad (32)$$

$$\tilde{\Gamma}'_{45}(\mathbf{k}) = [-A_0c_y\varrho_1 + A_0c_x\varrho_2 - R_1d_1\varrho_3]\frac{i\varrho_2}{E_{\mathbf{k}}}. \quad (33)$$

The **k** dependence of the terms in the results are suppressed to simplify the notations. In contrast to the salient twofold anisotropy in the spin structure factors in the two bases for $E_u^{(1)}$, the spin structure factors for $E_u^{(2)}$, $E_u^{(3)}$, and $E_u^{(4)}$ are fairly symmetric in the xy plane.

The symmetrized Fourier functions for the remaining E_u channels are all odd functions of **k**. The properties of these pairing channels can also be understood by combining the symmetry factors and the expressions of the remaining six Γ matrices in the pseudospin basis. By straightforward applications of Eq. (23), we get the following results:

$$\begin{aligned}\tilde{\Gamma}'_{12}(\mathbf{k}) = \big\{ &- [A_0c_x(B_0c_z + R_2d_2) + A_0c_yR_1d_1]\varrho_1 - [A_0c_y(B_0c_z + R_2d_2) - A_0c_xR_1d_1]\varrho_2 \\ &- \big[E_{\mathbf{k}}(E_{\mathbf{k}} + M) - A_0^2c^2\big]\varrho_3\big\}\frac{i\varrho_2}{E_{\mathbf{k}}(E_{\mathbf{k}} + M)},\end{aligned} \quad (34)$$

$$\begin{aligned}\tilde{\Gamma}'_{34}(\mathbf{k}) = \big\{&[A_0c_x(B_0c_z + R_2d_2) + A_0c_yR_1d_1]\varrho_1 + [A_0c_y(B_0c_z + R_2d_2) - A_0c_xR_1d_1]\varrho_2 \\ &- \big[M(E_{\mathbf{k}} + M) + A_0^2c^2\big]\varrho_3\big\}\frac{i\varrho_2}{E_{\mathbf{k}}(E_{\mathbf{k}} + M)},\end{aligned} \quad (35)$$

$$\begin{aligned}\tilde{\Gamma}'_{13}(\mathbf{k}) = \big\{&\big[R_1d_1(B_0c_z + R_2d_2) - A_0^2c_xc_y\big]\varrho_1 + \big[E_{\mathbf{k}}(E_{\mathbf{k}} + M) - A_0^2c_y^2 - R_1^2d_1^2\big]\varrho_2 \\ &-[A_0c_xR_1d_1 + A_0c_y(B_0c_z + R_2d_2)]\varrho_3\big\}\frac{i\varrho_2}{E_{\mathbf{k}}(E_{\mathbf{k}} + M)},\end{aligned} \quad (36)$$

$$\begin{aligned}\tilde{\Gamma}'_{23}(\mathbf{k}) = \big\{ &- \big[E_{\mathbf{k}}(E_{\mathbf{k}} + M) - A_0^2c_x^2 - R_1^2d_1^2\big]\varrho_1 + \big[A_0^2c_xc_y + R_1d_1(B_0c_z + R_2d_2)\big]\varrho_2 + [A_0c_x(B_0c_z + R_2d_2) \\ &- A_0c_yR_1d_1]\varrho_3\big\}\frac{i\varrho_2}{E_{\mathbf{k}}(E_{\mathbf{k}} + M)},\end{aligned} \quad (37)$$

$$\begin{aligned}\tilde{\Gamma}'_{14}(\mathbf{k}) = \big\{ &- \big[E_{\mathbf{k}}(E_{\mathbf{k}} + M) - A_0^2c_y^2 - (B_0c_z + R_2d_2)^2\big]\varrho_1 - \big[A_0^2c_xc_y + R_1d_1(B_0c_z + R_2d_2)\big]\varrho_2 \\ &- [A_0c_x(B_0c_z + R_2d_2) - A_0c_yR_1d_1]\varrho_3\big\}\frac{i\varrho_2}{E_{\mathbf{k}}(E_{\mathbf{k}} + M)},\end{aligned} \quad (38)$$

$$\begin{aligned}\tilde{\Gamma}'_{24}(\mathbf{k}) = \big\{ &- \big[A_0^2c_xc_y - R_1d_1(B_0c_z + R_2d_2)\big]\varrho_1 + \big[A_0^2c_x^2 + (B_0c_z + R_2d_2)^2 - E_{\mathbf{k}}(E_{\mathbf{k}} + M)\big]\varrho_2 \\ &- [A_0c_xR_1d_1 + A_0c_y(B_0c_z + R_2d_2)]\varrho_3\big\}\frac{i\varrho_2}{E_{\mathbf{k}}(E_{\mathbf{k}} + M)}.\end{aligned} \quad (39)$$

Again, the **k** dependence of the terms in the results are suppressed. The expression multiplying ϱ_3 in the second line of Eq. (35) can be rewritten as

$$M(E_{\mathbf{k}} + M) + A_0^2c^2 = E_{\mathbf{k}}(E_{\mathbf{k}} + M) - R_1^2d_1^2 - (B_0c_z + R_2d_2)^2.$$

The transformations in Eqs. (30)–(39) and those in Eqs. (24)–(29) are another central result of the present work.

There is an interesting relation among the six basis transformations in Eqs. (34)–(39). According to Table I, the six primed Γ matrices separate into three pairs: Γ'_{12} and $\Gamma'_{34} = \Gamma'_{12}\Gamma_5$, Γ'_{13} and $\Gamma'_{42} = \Gamma'_{13}\Gamma_5$, Γ'_{23} and $\Gamma'_{14} = \Gamma'_{23}\Gamma_5$. The connection between the two components of each pair is revealed by summing over the corresponding expressions in the pseudospin basis, which gives

$$\tilde{\Gamma}'_{12}(\mathbf{k}) + \tilde{\Gamma}'_{34}(\mathbf{k}) = -\frac{E_{\mathbf{k}} + M}{E_{\mathbf{k}}}\varrho_3(i\varrho_2), \quad (40)$$

$$\tilde{\Gamma}'_{23}(\mathbf{k}) + \tilde{\Gamma}'_{14}(\mathbf{k}) = -\frac{E_{\mathbf{k}} + M}{E_{\mathbf{k}}}\varrho_1(i\varrho_2), \quad (41)$$

$$\tilde{\Gamma}'_{31}(\mathbf{k}) + \tilde{\Gamma}'_{24}(\mathbf{k}) = -\frac{E_{\mathbf{k}} + M}{E_{\mathbf{k}}}\varrho_2(i\varrho_2). \quad (42)$$

Note that $I_4 + \Gamma_5 = I_4 + P$, which underlies the above combinations, is the projection operator to the even-parity subspace in the spin-orbital basis. Equations (40)–(42) have a clear cyclical structure. This should be related to the definition of the pseudospin basis, which was chosen to make the even-parity component of the magnetic moment operator to transform like a proper axial vector [31]. The combinations corresponding to the projection operator $I_4 - \Gamma_5 = I_4 - P$, which projects to the odd-parity subspace, are

$$\tilde{\Gamma}'_{12}(\mathbf{k})-\tilde{\Gamma}'_{34}(\mathbf{k})=\big\{-2[A_0c_x(B_0c_z+R_2d_2)+A_0c_yR_1d_1]\varrho_1-2[A_0c_y(B_0c_z+R_2d_2)-A_0c_xR_1d_1]\varrho_2 + \big[A_0^2c^2-R_1^2d_1^2-(B_0c_z+R_2d_2)^2\big]\varrho_3\big\}\frac{i\varrho_2}{E_{\mathbf{k}}(E_{\mathbf{k}}+M)}, \tag{43}$$

$$\tilde{\Gamma}'_{23}(\mathbf{k})-\tilde{\Gamma}'_{14}(\mathbf{k})=\big\{\big[A_0^2(c_x^2-c_y^2)+R_1^2d_1^2-(B_0c_z+R_2d_2)^2\big]\varrho_1+2\big[A_0^2c_xc_y+R_1d_1(B_0c_z+R_2d_2)\big]\varrho_2 + 2[A_0c_x(B_0c_z+R_2d_2)-A_0c_yR_1d_1]\varrho_3\big\}\frac{i\varrho_2}{E_{\mathbf{k}}(E_{\mathbf{k}}+M)}, \tag{44}$$

$$\tilde{\Gamma}'_{31}(\mathbf{k})-\tilde{\Gamma}'_{24}(\mathbf{k})=\big\{2\big[A_0^2c_xc_y-R_1d_1(B_0c_z+R_2d_2)\big]\varrho_1+\big[A_0^2\big(c_y^2-c_x^2\big)+R_1^2d_1^2-\big(B_0c_z+R_2d_2\big)^2\big]\varrho_2 + 2[A_0c_xR_1d_1+A_0c_y(B_0c_z+R_2d_2)]\varrho_3\big\}\frac{i\varrho_2}{E_{\mathbf{k}}(E_{\mathbf{k}}+M)}. \tag{45}$$

Although more complex than Eqs. (40)–(42), Eqs. (43)–(45) are simpler than Eqs. (34)–(39), because the $E_{\mathbf{k}}(E_{\mathbf{k}}+M)$ factors are eliminated from the numerators.

An implication of Eqs. (40)–(45) is that we can rehybridize four pairs of the E_u channels in Table IV to simplify the discussions on the properties of those pairing channels. Explicitly, the four pairs include $\{E_u^{(5)}, E_u^{(6)}\}$, $\{E_u^{(7)}, E_u^{(8)}\}$, $\{E_u^{(9)}, E_u^{(10)}\}$, and $\{E_u^{(11)}, E_u^{(12)}\}$. The eight new pairing combinations are defined in Table VI. The expressions in the pseudospin basis of the eight pairing channels in Table VI follow directly from the definitions in Table IV and Eqs. (40)–(45), and will not be written out explicitly. In shifting from Table IV to Table VI, Eq. (22) is also changed in a straightforward manner. For example, the pairing components corresponding to $E_u^{(5)}$ and $E_u^{(6)}$ are changed to $E_u^{(1p)}$ and $E_u^{(1m)}$ by

$$\sum_{\alpha=5}^{6}\tilde{\Delta}_\alpha\big[\tilde{\eta}_1\tilde{\psi}_1^{(\alpha)}(\mathbf{k})+\tilde{\eta}_2\tilde{\psi}_2^{(\alpha)}(\mathbf{k})\big] = \sum_{\alpha'=1p}^{1m}\tilde{\Delta}_{\alpha'}\big[\tilde{\eta}_1\tilde{\psi}_1^{(\alpha')}(\mathbf{k})+\tilde{\eta}_2\tilde{\psi}_2^{(\alpha')}(\mathbf{k})\big], \tag{46}$$

where the $(\tilde{\eta}_1,\tilde{\eta}_2)$ vector does not change, $\tilde{\Delta}_{1p}=(\tilde{\Delta}_5+\tilde{\Delta}_6)/2$ and $\tilde{\Delta}_{1m}=(\tilde{\Delta}_5-\tilde{\Delta}_6)/2$. Hereafter, we consider $E_u^{(1)}$ to $E_u^{(4)}$ in Table IV and the eight pairings in Table VI as the 12 independent E_u pairing channels.

TABLE VI. Redefinitions of the basis functions for the eight channels of the E_u representation in Table IV, from $E_u^{(5)}$ to $E_u^{(12)}$.

$E_u^{(n')}$	$\tilde{\psi}_1^{(n')}(\mathbf{k})$	$\tilde{\psi}_2^{(n')}(\mathbf{k})$
$n'=1p$	$\tilde{\psi}_1^{(5)}(\mathbf{k})+\tilde{\psi}_1^{(6)}(\mathbf{k})$	$\tilde{\psi}_2^{(5)}(\mathbf{k})+\tilde{\psi}_2^{(6)}(\mathbf{k})$
$n'=1m$	$\tilde{\psi}_1^{(5)}(\mathbf{k})-\tilde{\psi}_1^{(6)}(\mathbf{k})$	$\tilde{\psi}_2^{(5)}(\mathbf{k})-\tilde{\psi}_2^{(6)}(\mathbf{k})$
$n'=2p$	$\tilde{\psi}_1^{(7)}(\mathbf{k})+\tilde{\psi}_1^{(8)}(\mathbf{k})$	$\tilde{\psi}_2^{(7)}(\mathbf{k})+\tilde{\psi}_2^{(8)}(\mathbf{k})$
$n'=2m$	$\tilde{\psi}_1^{(7)}(\mathbf{k})-\tilde{\psi}_1^{(8)}(\mathbf{k})$	$\tilde{\psi}_2^{(7)}(\mathbf{k})-\tilde{\psi}_2^{(8)}(\mathbf{k})$
$n'=3p$	$\tilde{\psi}_1^{(9)}(\mathbf{k})+\tilde{\psi}_1^{(10)}(\mathbf{k})$	$\tilde{\psi}_2^{(9)}(\mathbf{k})+\tilde{\psi}_2^{(10)}(\mathbf{k})$
$n'=3m$	$\tilde{\psi}_1^{(9)}(\mathbf{k})-\tilde{\psi}_1^{(10)}(\mathbf{k})$	$\tilde{\psi}_2^{(9)}(\mathbf{k})-\tilde{\psi}_2^{(10)}(\mathbf{k})$
$n'=4p$	$\tilde{\psi}_1^{(11)}(\mathbf{k})+\tilde{\psi}_1^{(12)}(\mathbf{k})$	$\tilde{\psi}_2^{(11)}(\mathbf{k})+\tilde{\psi}_2^{(12)}(\mathbf{k})$
$n'=4m$	$\tilde{\psi}_1^{(11)}(\mathbf{k})-\tilde{\psi}_1^{(12)}(\mathbf{k})$	$\tilde{\psi}_2^{(11)}(\mathbf{k})-\tilde{\psi}_2^{(12)}(\mathbf{k})$

Now we make an order-of-magnitude estimation over the superconducting gap amplitudes of the various pairing channels in Tables IV and VI by taking advantage of the basis transformations of the Γ matrices in Eqs. (30)–(45) and the expansions of the symmetry factors in Eqs. (11)–(16). As we have explained in the previous section, k_xa and k_ya are all very small for wave vectors on the Fermi surface. The pairing amplitude of a pairing channel can be characterized in terms of its power in $ka=\sqrt{k_x^2+k_y^2}a$. Also, as an approximation, we may treat $E_{\mathbf{k}}=\mu-\epsilon(\mathbf{k})$ and $E_{\mathbf{k}}+M(\mathbf{k})$ as constants. Under the above conditions, the gap of $E_u^{(1)}$ is in the order of ka, and the gaps of $E_u^{(2,3,4)}$ are in the order of $(ka)^3$. While $E_u^{(1p)}$ and $E_u^{(4p)}$ open gaps in the order of ka, $E_u^{(1m)}$ and $E_u^{(4m)}$ open gaps in the order of $(ka)^3$. $E_u^{(2p)}$ and $E_u^{(3p)}$ also open gaps in the order of $(ka)^3$. The gaps opened by $E_u^{(2m)}$ and $E_u^{(3m)}$ are of the order $(ka)^5$. The dependence of the superconducting gap amplitudes on the directions of the wave vectors on the k_xk_y plane can be read from the expansions in Eqs. (11)–(16). Notice that if the Fermi surface is corrugated cylindrical, the $c_z(\mathbf{k})$ factor undergoes drastic variations in scanning over the Fermi surface and may dominate the variation of the pairing amplitude [31]. The above analysis is then an estimate of the bulk pairing magnitudes on the $k_z=0$ and $k_z=\pm\pi$ planes of the BZ. From the above analysis, $E_u^{(1)}$, $E_u^{(1p)}$, and $E_u^{(4p)}$ are the most efficient in opening a large superconducting gap. In contrast, the $E_u^{(2m)}$ and $E_u^{(3m)}$ channels are least effective in producing a superconducting gap and are unlikely to be the leading pairing channels. The remaining seven E_u pairing channels have the intermediate ability in opening a bulk superconducting gap. The above analyses are summarized in Table VII.

The surface states on the natural xy surface of superconducting $M_x\mathrm{Bi}_2\mathrm{Se}_3$ may include the surface Andreev bound states and the topological surface states. The surface Andreev bound states are directly related to the superconducting order parameter and exist (do not exist) if the superconducting pairing wave function undergoes (does not undergo) a sign reversal upon the reflection changing k_z to $-k_z$. By this rule, it is easy to see that only five pairing channels *do not* support surface Andreev bound states on the xy surface, including $E_u^{(3)}$, $E_u^{(1p)}$, $E_u^{(2p)}$, $E_u^{(3p)}$, and $E_u^{(4p)}$. The topological surface states inherited from the normal state may or may not open a gap at the Fermi level in the superconducting phase, de-

TABLE VII. Order-of-magnitude estimations of the superconducting gaps for the E_u pairing channels defined in Tables IV and VI on the $k_z = 0$ slice of the Fermi surface. The first column is the numbering of the various pairing channels. The second column contains the order-of-magnitude estimations of the corresponding pairing channel. $k = \sqrt{k_x^2 + k_y^2}$ is the magnitude of the wave vector on the $k_z = 0$ slice of the Fermi surface, and $a = 4.14$ Å is the in-plane lattice parameter.

$E_u^{(n)}$	Order of magnitude of the pairing
$n = 1$	$\frac{\lvert A_0\rvert}{E_{\mathbf{k}}} ka$
$n = 2$	$\frac{\lvert A_0\rvert}{E_{\mathbf{k}}} (ka)^3$
$n = 3$	$\frac{\lvert A_0\rvert}{E_{\mathbf{k}}} (ka)^3$
$n = 4$	$\frac{\lvert A_0\rvert}{E_{\mathbf{k}}} (ka)^3$
$n = 1p$	$\frac{E_{\mathbf{k}}+M}{E_{\mathbf{k}}} ka$
$n = 1m$	$\frac{A_0^2}{E_{\mathbf{k}}(E_{\mathbf{k}}+M)} (ka)^3$
$n = 2p$	$\frac{E_{\mathbf{k}}+M}{E_{\mathbf{k}}} (ka)^3$
$n = 2m$	$\frac{A_0^2}{E_{\mathbf{k}}(E_{\mathbf{k}}+M)} (ka)^5$
$n = 3p$	$\frac{E_{\mathbf{k}}+M}{E_{\mathbf{k}}} (ka)^3$
$n = 3m$	$\frac{A_0^2}{E_{\mathbf{k}}(E_{\mathbf{k}}+M)} (ka)^5$
$n = 4p$	$\frac{E_{\mathbf{k}}+M}{E_{\mathbf{k}}} ka$
$n = 4m$	$\frac{A_0^2}{E_{\mathbf{k}}(E_{\mathbf{k}}+M)} (ka)^3$

pending both on the nature of the bulk pairing and on the nature of the topological surface states. A full list of the pairings that open a gap in the topological surface states of Bi_2Se_3 was constructed previously [40,62]. According to that list, $E_u^{(1)}$, $E_u^{(2)}$, and $E_u^{(4)}$ cannot gap the topological surface states. On the other hand, all the remaining pairings can at least partially gap the topological surface states. For example, $\tilde{\psi}_1^{(3)}$ can gap all the topological surface states at the Fermi level, except for the crossing points between the topological surface states at the Fermi level and the lines determined by $\varphi_2(\mathbf{k}) = 0$.

To infer the qualitative behaviors of the electronic spin susceptibility relevant to the Knight shift experiment, we reformulate the pairing defined by Eq. (23) in the standard expression as

$$\underline{\tilde{\Delta}}(\mathbf{k}) = [d_0(\mathbf{k})\varrho_0 + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\varrho}] i\varrho_2, \tag{47}$$

where $d_0(\mathbf{k})$ is the pseudospin-singlet component of the pairing, $\mathbf{d}(\mathbf{k}) = [d_1(\mathbf{k}), d_2(\mathbf{k}), d_3(\mathbf{k})]$ is a three-component vector for the pseudospin-triplet part of the pairing, and $\boldsymbol{\varrho} = (\varrho_1, \varrho_2, \varrho_3)$. From the above results, we have $\mathbf{d}(\mathbf{k}) = (0, 0, 0)$ for the even-parity E_g pairings and $d_0(\mathbf{k}) = 0$ for the odd-parity E_u pairings. Note that Eqs. (24)–(45) have already been written in the above standard form, from which the corresponding expressions of $d_0(\mathbf{k})$ and $\mathbf{d}(\mathbf{k})$ can be read directly. The superconducting gap for a wave vector $\mathbf{k}$ on the Fermi surface is determined by the $d_0(\mathbf{k})$ function for the E_g pairings as $\Delta_g(\mathbf{k}) = 2|d_0(\mathbf{k})|$ or determined by the $\mathbf{d}(\mathbf{k})$ vector for the E_u pairings as

$$\Delta_u(\mathbf{k}) = 2\sqrt{\mathbf{d}(\mathbf{k}) \cdot \mathbf{d}^*(\mathbf{k}) \pm i\mathbf{d}(\mathbf{k}) \times \mathbf{d}^*(\mathbf{k})}. \tag{48}$$

The $\mathbf{d}(\mathbf{k})$ vector of an E_u pairing is perpendicular to the spin direction of the corresponding Cooper pair [64–67]. The spin susceptibilities show distinct behaviors depending on the relative orientation between the external magnetic field $\mathbf{H}$ and the $\mathbf{d}(\mathbf{k})$ vector [15,49,64–67]: for $\mathbf{H} \perp \mathbf{d}(\mathbf{k})$, the spin susceptibility barely changes across the superconducting transition temperature T_c; for $\mathbf{H} \parallel \mathbf{d}(\mathbf{k})$, the spin susceptibility decreases below T_c similar to a spin-singlet superconductor. In this manner, we can understand the qualitative behaviors of the electronic spin susceptibilities for the E_u pairing channels in Tables IV and VI in terms of Eqs. (30)–(45). For simplicity and without losing much rigor, we can first set $R_1 = R_2 = 0$ and work with the effective pairing in the simplified model. It is easy to see that both of the two components of the $E_u^{(1)}$ channel break the spin rotational symmetry in the xy plane to twofold symmetry. It is also clear that both $E_u^{(2)}$ and $E_u^{(3)}$ respect the spin rotational symmetry in the xy plane. For $E_u^{(4)}$, while the two Γ matrices that are contained in each channel break the spin rotational symmetry in the xy plane, the linear combination restores this symmetry. $E_u^{(1p)}$ and $E_u^{(1m)}$ respect the spin rotational symmetry in the xy plane. The two components of $E_u^{(2p)}$ and $E_u^{(3p)}$ both break the threefold in-plane spin rotational symmetry in the xy plane to twofold symmetry. The two components of $E_u^{(2m)}$ and $E_u^{(3m)}$ only slightly break the threefold in-plane spin rotational symmetry in the xy plane. The components of $E_u^{(4p)}$ and $E_u^{(4m)}$ respect the spin rotational symmetry in the xy plane.

IV. COMPARISON TO EXPERIMENTAL RESULTS

A. Survey of experimental consensuses

In this section, we first make a survey over the main experimental consensuses on the three superconductors. Then we combine the results in the previous section to infer the most probable pairings for the three superconductors. To be clear, we categorize the relevant experiments on the $M_xBi_2Se_3$ (M is Cu, Sr, or Nd) superconductors into three broad classes, which separately probe the bulk spectrum, the surface spectrum (along the natural xy surface parallel to the basal plane), and the magnetic properties. Since both the bulk spectrum and the surface spectrum influence the magnetic properties, this division is by no means absolute.

For the bulk spectrum, both $Cu_xBi_2Se_3$ [12,68] and $Sr_xBi_2Se_3$ [69] were reported to be fully gapped. However, there is no solid consensus on the momentum dependence of the band gap. For $Cu_xBi_2Se_3$, while a scanning tunneling microscopy (STM) experiment by Levy *et al.* gives a tunneling spectrum consistent with isotropic s-wave pairing [12], a later field-angle-dependent specific heat experiment by Yonezawa *et al.* suggests an energy-gap structure with salient twofold symmetry in the k_xk_y plane [16]. In addition, the experiment of Yonezawa *et al.* seems to suggest the possible existence of (approximate) point nodes in the bulk spectrum of $Cu_xBi_2Se_3$ [16]. For $Sr_xBi_2Se_3$, an STM experiment implies an anisotropic s-wave pairing [69]. Later, an experiment shows with resistivity and Laue diffraction measurements that the energy-gap structure of $Sr_xBi_2Se_3$ also has twofold symmetry in the k_xk_y plane [17]. For $Nd_xBi_2Se_3$, an experiment finds evidence for point nodes in its bulk spectrum [70].

For the surface spectrum, the situation is rather confusing for all three superconductors. While several early experiments, in particular those based on point-contact spectroscopy, claim to have found evidence of surface Andreev bound states for $Cu_xBi_2Se_3$ [7–9], later experiments denied the existence of surface Andreev bound states [12,13]. Similar confusion exists for $Sr_xBi_2Se_3$. An experiment infers the existence of surface states in $Sr_xBi_2Se_3$ through the Shubnikov–de Haas oscillations [3]. However, an STM/scanning tunneling spectroscopy (STS) experiment does not report any in-gap states [69]. For superconducting $Nd_xBi_2Se_3$, an angle-resolved photoemission spectroscopy experiment shows that the topological surface states in the normal state are preserved in the superconducting state [6]. But it is unclear whether or not the topological surface states are gapped at the Fermi level and whether or not there are surface Andreev bound states on the xy surface of superconducting $Nd_xBi_2Se_3$.

For the magnetic properties, $Nd_xBi_2Se_3$ was reported to have spontaneous magnetization in the superconducting phase [6], which seems to be related to the magnetism of the Nd dopants. The $Cu_xBi_2Se_3$ and $Sr_xBi_2Se_3$ superconductors are usually considered as nonmagnetic in the absence of external magnetic fields [6]. On the other hand, for all three superconductors, there are magnetism-related experiments indicating that the threefold rotational symmetry in the normal phase is broken down to twofold rotational symmetry in the superconducting phase. The Knight shift experiment by Matano *et al.* shows that the electronic spin susceptibilities of $Cu_xBi_2Se_3$ is twofold symmetric in the basal plane and is invariant for an out-of-plane magnetic field [15]. Another magnetic measurement is the upper critical field B_{c2}. By varying the direction of the magnetic field in the basal plane of the superconductors, a twofold symmetry in the upper critical field is observed for $Cu_xBi_2Se_3$ [16], $Sr_xBi_2Se_3$ [18], and also for $Nd_xBi_2Se_3$ [21]. For $Nd_xBi_2Se_3$, the twofold rotational symmetry in the basal plane is also confirmed in a torque magnetometry measurement [20].

B. Promising two-component pairings inferred from comparison with experiments

In light of the above survey, the most well-established experimental feature is the twofold rotational symmetry in the basal plane for all three superconductors. This twofold symmetry has two incarnations: (1) in the electronic spin susceptibility and (2) in the momentum dependence of the superconducting gap amplitude. As we explain below, these two aspects of the twofold symmetry are independent of each other.

The nematic combination of two components of $E_u^{(1)}$ is the most well-known candidate for the twofold symmetry in the electronic spin susceptibility [15,19,22]. $E_u^{(2p)}$ and $E_u^{(3p)}$ can also lead to twofold symmetry in the spin susceptibility in the xy plane. Because for $E_u^{(2p)}$ and $E_u^{(3p)}$ the $\mathbf{d}(\mathbf{k})$ vectors in the pseudospin basis do not have the third component, as shown in Eqs. (41) and (42), the corresponding spin susceptibility will stay invariant for an out-of-plane magnetic field. On the other hand, the $\mathbf{d}(\mathbf{k})$ vectors for the two $E_u^{(1)}$ pairing components, as shown in Eqs. (30) and (31), have finite third components. The spin susceptibility for a pairing in the $E_u^{(1)}$ channel should therefore decrease slightly for an out-of-plane magnetic field [49]. In this respect, $E_u^{(2p)}$ and $E_u^{(3p)}$ fit the Knight shift experiment better than the $E_u^{(1)}$ pairing [15].

The twofold symmetry in the $\mathbf{k}$ dependence of the superconducting gap amplitudes could be explained by the nematic realization of $E_u^{(1)}$ or $E_g^{(3)}$. $E_u^{(2m)}$ and $E_u^{(3m)}$ also result in twofold symmetry in the k_xk_y plane. But the $(ka)^5$ dependence of their pairing amplitude implies that they are unlikely the leading pairing instability. The remaining channels in Tables III and Table IV do not give clear twofold symmetry in the superconducting gap amplitude in the k_xk_y plane to account for the experiments. Therefore, with regard to the twofold symmetry in the basal plane, the $E_u^{(1)}$ channel is the only channel that naturally accounts for both of the two aspects of the twofold rotational symmetry. On the other hand, each incarnation of the twofold symmetry has alternative realizations other than $E_u^{(1)}$.

Now we consider further constraints imposed by the bulk spectra of the superconducting state. For both $Cu_xBi_2Se_3$ [12,68] and $Sr_xBi_2Se_3$ [69], the bulk spectra were reported to be fully gapped, without true or approximate nodes in the bulk spectrum. However, the recent experiment of Yonezawa *et al.* seems to imply the possible presence of true or approximate nodes in the bulk spectrum of superconducting $Cu_xBi_2Se_3$ [16]. Here, we define an approximate node as a very tiny energy gap in the bulk quasiparticle spectrum that is easily overcome by the relevant experimental temperature or smeared by scatterings due to nonmagnetic or magnetic impurities (e.g., the Cu, Sr, or Nd dopants). In the light of a previous work [31], the gap minima for the $\tilde{\psi}_2^{(1)}(\mathbf{k})$ pairing component of $E_u^{(1)}$ is 2–3 orders of magnitude smaller than the gap maxima. According to the experimental estimation, the magnitude of the gap maxima is in the order of 1 meV [2]. The gap minima of $\tilde{\psi}_2^{(1)}(\mathbf{k})$ would thus be in the range of 0.001–0.01 meV. This tiny gap is easily smeared by a temperature of 0.1 K, which is small compared to the superconducting critical temperature (usually above 3 K). Therefore, the approximate nodes of $\tilde{\psi}_2^{(1)}(\mathbf{k})$ in a practical sense appear to be true nodes in the quasiparticle spectrum [71,72]. The two components of $E_u^{(4p)}$ individually open a full gap on the Fermi surface if we have a corrugated cylindrical Fermi surface, with the size of the gap scaling as ka for wave vectors on the Fermi surface. For spheroidal Fermi surfaces, both of the two components of $E_u^{(4p)}$ give two point nodes at $k_x = k_y = 0$. All the remaining individual pairing components in Tables III, IV, and VI [including $\tilde{\psi}_1^{(1)}(\mathbf{k})$ of $E_u^{(1)}$] give true nodes to the bulk spectrum, for both spheroidal and corrugated cylindrical Fermi surfaces.

For several of the pairing channels other than $E_u^{(4p)}$, we can also get a fully gapped bulk spectrum by forming chiral combinations of the two pairing components for suitable Fermi surface topology. These channels include $E_g^{(1,2,7)}$ of the E_g representation and $E_u^{(2,3,1p)}$ of the E_u representation. When the Fermi surface is a corrugated cylinder, the chiral combinations (e.g., $\eta_1 = 1$ and $\eta_2 = i$, or $\tilde{\eta}_1 = 1$ and $\tilde{\eta}_2 = i$)

TABLE VIII. Single pairing channels which are separately compatible with one of the following four types of properties of the superconducting state: (1) twofold symmetry of the electronic spin susceptibility in the xy plane; (2) twofold symmetry of the pairing amplitude in the xy plane; (3) a fully gapped bulk spectrum, in terms of time-reversal symmetric combinations of the two components, and for a corrugated cylindrical Fermi surface; (4) a fully gapped bulk spectrum, in terms of chiral combinations of the two components which break the time-reversal symmetry, and for a corrugated cylindrical Fermi surface. The first column is the numbering of the various properties. The second column contains the pairing channels (separated by semicolons) that are compatible with the corresponding property.

Property	Compatible pairing channels
(1)	$E_u^{(1)};E_u^{(2p)};E_u^{(3p)}$
(2)	$E_g^{(3)};E_u^{(1)};E_u^{(2m)};E_u^{(3m)}$
(3)	$E_u^{(4p)}$
(4)	$E_g^{(1)};E_g^{(2)};E_g^{(7)};E_u^{(1)};E_u^{(2)};E_u^{(3)};E_u^{(1p)}$

of the two components of $E_g^{(1,2,7)}$ or $E_u^{(2,3,1p)}$ all lead to a fully gapped bulk quasiparticle spectrum. For a chiral *and* nematic combination (e.g., $\eta_1 = 0.5$ and $\eta_2 = i$, or $\tilde{\eta}_1 = 0.5$ and $\tilde{\eta}_2 = i$) of the two components of $E_g^{(1,2,7)}$ or $E_u^{(2,3,1p)}$, the bulk quasiparticle spectrum is also fully gapped, if we have a corrugated cylindrical Fermi surface. When the Fermi surface is a spheroid, these chiral or chiral and nematic pairings have two point nodes at the $k_x = k_y = 0$ points of the Fermi surface. None of the above pairing channels, including $E_g^{(1,2,7)}$ and $E_u^{(2,3,1p,4p)}$, can account for the twofold symmetries observed in the experiments.

The time-reversal symmetry breaking combinations of the two components of $E_u^{(1)}$ have more complicated behaviors. For a spheroidal Fermi surface, the purely chiral combinations of the two components of $E_u^{(1)}$ have two point nodes at the $k_x = k_y = 0$ points of the Fermi surface [24,26]. These point nodes disappear both when we consider a chiral and nematic combination of the two components, and when the Fermi surface turns to a corrugated cylinder. On the other hand, all these various time-reversal symmetry-breaking pairing combinations within the $E_u^{(1)}$ channel support surface Andreev bound states on the xy surface and keep the topological surface states at the Fermi level ungapped.

Summing up the above discussions into Table VIII, it is clear that for $Cu_xBi_2Se_3$ and $Sr_xBi_2Se_3$, there is not a time-reversal symmetric pairing combination of a single pairing channel that can simultaneously explain the twofold in-plane symmetries and the fully gapped bulk spectrum. For $Nd_xBi_2Se_3$, while the $E_u^{(1)}$ channel can explain the twofold symmetry and bulk spectrum with (true or approximate) point nodes, the complexity of the Fermi surface of this compound complicates the comparison [43]. If the (true or approximate) point nodes in superconducting $Cu_xBi_2Se_3$ implied by the experiment of Yonezawa *et al.* [16] can be confirmed, then $E_u^{(1)}$ is the ideal candidate for the pairing, and the remaining task is to look for the theoretically predicted robust surface Andreev bound states [31]. If, on the other hand, we consider the bulk spectrum of $Cu_xBi_2Se_3$ and $Sr_xBi_2Se_3$ as fully gapped, then an implication of the above comparison is that we have to consider more than one pairing channel. In other words, the pairing has to be *multichannel*, in addition to having two components. Leaving alone the well-studied $E_u^{(1)}$ pairings [19,31,32], in what follows we focus on the superconductors with a fully gapped bulk spectrum and explore various possible multichannel pairing combinations. We will relax the constraint of time-reversal symmetry and explore all the possible pairing combinations that give both the twofold symmetry in the basal plane and the fully gapped bulk quasiparticle spectrum. The obtained pairing combinations are listed in Table IX, together with the chiral and nematic pairing combination in the $E_u^{(1)}$ channel.

TABLE IX. Pairing combinations identified from the comparison with the experiments. The first column lists the various combinations. In each pairing combination, the numberings of the two major pairing channels are indicated in the bracket of the superscript, with the pairing amplitude of the first pairing channel much larger than the pairing amplitude of the second pairing channel. Pairing combinations with similar properties are listed in the same row and are separated by semicolons. The second column specifies the important properties of the corresponding pairing combination. The properties are specified by the numbers defined in the caption of Table VIII. The third column indicates the presence (Y) or absence (N) of surface states on the xy surface of the superconductor. The surface states include the surface Andreev bound states *and* the topological surface states inherited from the normal phase. Note that all pairing combinations are nematic. The combination is time-reversal symmetric if it has property (3) and has broken time-reversal symmetry (i.e., chiral) if it has property (4).

Pairing combinations	Properties	Surface states
$E_g^{(1,3)}$; $E_g^{(2,3)}$; $E_g^{(7,3)}$	(1);(2);(4)	N
$E_u^{(4p,1)}$	(1);(2);(3)	N
$E_u^{(3,1)}$	(1);(2);(4)	N
$E_u^{(2,1)}$	(1);(2);(4)	Y
$E_u^{(1)}$	(1);(2);(4)	Y

To get a fully gapped bulk spectrum with twofold symmetry in the superconducting gap amplitude, in terms of a multichannel pairing in the E_g representation, the (η_1, η_2) vector in Eq. (21) must be simultaneously chiral and nematic. The chirality and nematicity of the pairing are separately responsible for the fully gapped bulk spectrum and the twofold symmetry in the k_xk_y plane. The full gap may be achieved by a chiral combination of $E_g^{(1)}$, or $E_g^{(2)}$, or $E_g^{(7)}$, under the premise that the Fermi surface is a corrugated cylinder. Including a finite contribution of $E_g^{(3)}$, the nematicity of the pairing can account for the twofold symmetry in the gap amplitude. The fully gapped bulk spectrum requires the strength of the $E_g^{(1)}$ (or $E_g^{(2)}$, or $E_g^{(7)}$) channel to be larger than the strength of the $E_g^{(3)}$ channel, namely, that Δ_1 (or Δ_2, or Δ_7) is sufficiently large compared to Δ_3. In this case, the superconducting order parameter (the wave function of the Cooper pairs) does not undergo a sign reversal upon scattering off the xy surface, implying the absence of surface Andreev bound states. In addition, the chiral combination of the dominant $E_g^{(1)}$ (or $E_g^{(2)}$, or $E_g^{(7)}$) pairing component fully gaps the topological surface states. Therefore, there are no low-energy in-gap states on the *xy* surface for this chiral and nematic pairing in the E_g representation.

If we further impose the constraint of twofold symmetry in the electronic spin susceptibility [15], we have to consider the E_u channels. A combination of $E_u^{(1)}$ (or $E_u^{(2p)}$, or $E_u^{(3p)}$) and $E_u^{(4p)}$ is possible to give a purely nematic pairing that has a fully gapped bulk spectrum, if $\tilde{\Delta}_{4p}$ is large compared to $\tilde{\Delta}_1$ (or $\tilde{\Delta}_{2p}$, or $\tilde{\Delta}_{3p}$). Let us define (I) the combination of $E_u^{(1)}$ with $E_u^{(4p)}$, (II) the combination of $E_u^{(2p)}$ with $E_u^{(4p)}$, and (III) the combination of $E_u^{(3p)}$ with $E_u^{(4p)}$. For the Knight shift experiment, combinations II and III explain the invariant *c*-axis spin susceptibility better than combination I. In addition, they can also more naturally explain the absence of surface Andreev bound states and the gapped topological surface states on the *xy* surfaces of the superconductor. For these experimental features, combinations II and III are better alternatives to combination I. On the other hand, if we consider the twofold symmetry in the superconducting gap amplitude, combination I explains it naturally, whereas combinations II and III do not lead to salient twofold symmetry in the gap amplitude. Overall, to explain at least qualitatively the key experimental features of $Cu_xBi_2Se_3$ with a nematic and time-reversal symmetric pairing, we have to consider a pairing consisting mainly of $E_u^{(1)}$ and $E_u^{(4p)}$, and possibly supplemented by $E_u^{(2p)}$ and (or) $E_u^{(3p)}$. Finally, following the same analysis as that for the above chiral and nematic E_g pairing, there are no low-energy in-gap states on the *xy* surface. Explicitly, because $\tilde{\Delta}_{4p}$ is assumed to be large compared to $\tilde{\Delta}_1$ (or $\tilde{\Delta}_{2p}$, or $\tilde{\Delta}_{3p}$), the superconducting order parameter does not undergo sign change upon the substitution of $-k_z$ for k_z, so that there are no surface Andreev bound states on the *xy* surface. In addition, since $\tilde{\Delta}_{4p}$ gaps the topological surface states at the Fermi level, there are no topological surface states that may contribute to the low-energy in-gap states.

For other E_u combinations, we again have to consider a chiral and nematic combination to account for the fully gapped bulk spectrum and the twofold in-plane rotational symmetry at the same time, similar to the E_g case. If both the superconducting gap amplitudes and the electronic spin susceptibilities are required to be twofold symmetric in the basal plane, we can choose the chiral and nematic combinations of $E_u^{(1)}$ with $E_u^{(2,3)}$. If only the electronic spin susceptibilities are required to be twofold symmetric, the chiral and nematic combinations of $E_u^{(2p,3p)}$ with $E_u^{(2,3)}$ are eligible. Again, the pairing amplitudes for $E_u^{(2,3)}$, which give the fully gapped bulk spectrum, should be larger than the pairing amplitudes for $E_u^{(1)}$. Because the dominant third component of the $\mathbf{d}(\mathbf{k})$ vector for $E_u^{(2)}$ is proportional to $B_0c_z + R_2d_2 \simeq B_0c_z$, and both $E_u^{(1)}$ and $E_u^{(2)}$ do not gap the topological surface states at the Fermi level, the chiral and nematic combination of $E_u^{(1)}$ and $E_u^{(2)}$ have surface Andreev bound states and ungapped topological surface states on the *xy* surface. The chiral and nematic combination of $E_u^{(1)}$ and $E_u^{(3)}$, with the magnitude of $\tilde{\Delta}_3$ much larger than the magnitude of $\tilde{\Delta}_1$ to ensure a fully gapped bulk spectrum, does not have surface Andreev bound states and ungapped topological surface states on the *xy* surface.

C. More discussions on the properties of the identified two-component pairings

A salient feature of the above multichannel pairings is the ubiquity of the chiral and nematic pairing combinations in both the E_g and the E_u representations. Besides the broken in-plane rotational symmetry, the chiral character of the pairing implies that it can show typical signatures in experiments such as muon spin relaxation and optical Kerr effect, which probe the broken time-reversal symmetry [73–75]. The chiral and nematic E_u pairings are also nonunitary, which can be verified by proving the nonvanishing of the vector product $\mathbf{d}(\mathbf{k}) \times \mathbf{d}^*(\mathbf{k}) \neq 0$ for general $\mathbf{k}$ [76,77]. Nonunitary pairings, as a special case of pairings with broken time-reversal symmetry, are known to have a spontaneous moment from the Cooper pairs [76,77]. Also note that the chiral or chiral and nematic pairing combinations of the two components of $E_u^{(1)}$ are all nonunitary.

Another common character of the above pairing combinations is the requirement of a corrugated cylindrical Fermi surface to have a fully gapped bulk spectrum. The undoped Bi_2Se_3 is known to have a spheroidal Fermi surface. As the concentration of the dopants increases, it is natural to expect a continuous evolution of the Fermi surface from spheroidal to corrugated cylindrical. Alongside, the nodal structure of the pairing may also change. While the experiment of Lahoud *et al.* shows that the superconducting $Cu_xBi_2Se_3$ has a corrugated cylindrical Fermi surface in the normal phase [44], there are presently no systematic studies on the evolution of the Fermi surface for any of the three superconductors.

It is also interesting to notice that several pairing channels in Tables III, IV, and VI exhibit prominent fourfold rotational symmetry, including the $E_g^{(1,2,7)}$ channels of the E_g representation and the $E_u^{(2,3,4)}$ channels of the E_u representation, through the $\mathbf{k}$ dependence of the $\varphi_1(\mathbf{k})$ and $\varphi_2(\mathbf{k})$ symmetry factors. The fourfold symmetry also breaks the threefold rotational symmetry of the underlying crystal lattice in the normal phase. Several of the chiral and nematic pairing combinations proposed above contain these pairing channels. They are therefore expected to exhibit some characteristics of the fourfold symmetry. On the experimental side, a fourfold symmetric component in the superconducting gap amplitude was indeed observed by Du *et al.* for $Sr_xBi_2Se_3$ [69]. These chiral and nematic pairings are, however, inconsistent with the general belief that the superconducting state of $Sr_xBi_2Se_3$ preserves the time-reversal symmetry.

Finally, from previous theoretical studies [78–80], the two-component pairings for electron-doped Bi_2Se_3 might be robust against nonmagnetic impurities. It has been shown that the large intrinsic spin-orbit coupling in this compound protects the odd-parity pairings against nonmagnetic impurities [78–80]. The mechanism was illustrated for both single-component [78,79] and two-component [80] odd-parity pairings. Since for single-component pairings, the conventional even-parity pairing is more robust than the odd-parity pairing [78], it is reasonable to expect that the even-parity E_g pairings are also robust against nonmagnetic impurities. It is highly desirable to carry out explicit theoretical studies to clarify the impact of impurities on the two-component pairings of electron-doped Bi_2Se_3.

V. IMPLICATIONS FOR FUTURE EXPERIMENTS

From the analysis of the previous section, the available experiments have imposed stringent constraints on the true pairing symmetries of the $M_x\mathrm{Bi_2Se_3}$ (M is Cu, Sr, or Nd) superconductors. These experiments, on the other hand, do not provide sufficient and consistent information to unambiguously identify the true pairing symmetry of these superconductors. In particular, for each of the three superconductors, the parameter x defines a series of superconductors which might have qualitatively different Fermi surface topology in the normal state and different pairing symmetries in the superconducting state. This doping dependence has not been systematically investigated for any of the three superconductors, although the phase diagram of $\mathrm{Cu}_x\mathrm{Bi_2Se_3}$ exists [81]. It is therefore highly desirable to make a systematic experimental study on each member of the series with a complementary set of experimental tools.

Based on the survey over the experimental consensuses and the comparison with the possible pairing channels, the relevant properties and the experiments that may be performed to probe them include the following: (1) The evolution of the Fermi surface with the doping concentration x. The magnetic oscillation experiments, including the Shubnikov–de Haas oscillation and the de Haas–van Alphen effect, can probe the Fermi surface contour in the normal phase [43,44,82]. From the discussions of the above section, the geometry of the Fermi surface significantly influences the bulk quasiparticle spectrum of the superconducting state. It is highly desirable to determine the systematic evolution of the Fermi surface as the doping concentration x increases. In addition, the angle-resolved photoemission spectroscopy (ARPES), which may probe the continuous evolution of the topological surface states with x [2,44,45], supplements the magnetic oscillation experiment, which gives the bulk Fermi surface. (2) The bulk quasiparticle spectrum of the superconducting state, fully gapped or not. For each doping concentration that turns the material to a superconductor, we may determine whether the superconducting state is fully gapped or not by combining the STS measurements [12] and the measurements of the zero-field bulk specific heat [68]. The STS experiment, besides probing the bulk quasiparticle spectrum, probes also the in-gap states on the surface of the superconductors [12,69]. The spin-lattice relaxation rates [83] and penetration depth [70] can also be used to probe the nodal structures of the bulk superconducting spectrum. (3) The momentum dependence of the superconducting gap amplitude. This property on one hand refines the understanding obtained from the above step and on the other hand shows the presence or not of the anisotropy in the superconducting gap amplitudes. The relevant experiments include the field-angle-dependent specific heat experiments [16,72,84], the field-angle-dependent upper critical magnetic field experiments [16,18,21], the field-angle-dependent resistivity experiments [17], the field-angle-dependent thermal conductivity experiments [71,72,85,86], and the field-angle-dependent STS [87]. Besides the above experiments for the magnitude of the superconducting gap, the phase of the superconducting gap can be probed with the orientation-dependent Josephson junctions [88]. (4) The electronic spin susceptibility, which is the most direct diagnostic tool for the structure of the **d** vectors of the pseudospin-triplet pairings. The major relevant experiment is the Knight shift measurement [15]. (5) The persistence or not of the time-reversal symmetry in the superconducting state. The time-reversal symmetry breaking of the superconductors can be probed by several techniques, such as the muon spin resonance [73], optical Kerr effect [74,75], and the Josephson effect [67]. The zero-field Hall effect was also used by Qiu *et al.* to probe the broken time-reversal symmetry in $\mathrm{Nd}_x\mathrm{Bi_2Se_3}$ [6]. (6) The presence or not of spontaneous magnetization. The above chiral and nematic E_u pairings are mostly nonunitary and should lead to spontaneous magnetization. The experiment of Qiu *et al.* reporting the spontaneous magnetization of $\mathrm{Nd}_x\mathrm{Bi_2Se_3}$ was based on the field-dependent dc magnetization, which is a measurement of the global magnetization [6]. It is desirable to study the spontaneous magnetization with a local measurement, such as the polarized neutron diffraction experiments [67].

For each member of the three series of superconductors, a systematic study of the above experiments should be able to identify the genuine pairing symmetry. From the breadth of the experimental tools involved, extensive experimental collaborations by sharing the same high-quality samples are highly desirable.

Besides the experiments listed above, other experiments which may probe further implications of the candidate pairings would also be of great potential interest. For example, as a natural consequence of the two-component nature of the pairing, the domain structure should exist in the superconducting state. Although most of the multichannel two-component pairings inferred from the analysis of the previous section do not support surface Andreev bound states on the xy surface, all the E_u pairings should give Andreev bound states as domain wall states for domain walls parallel to the z axis, because the superconducting order parameters are odd functions of k_x and k_y in the pseudospin basis. Evidence of domains was reported in the experiment of Yonezawa *et al.* [16]. However, it is unclear whether or not there are nontrivial domain wall states. Further experiments like those performed for $\mathrm{Sr_2RuO_4}$ [89] and superfluid ^{3}He-A [90] are highly desirable. As another example, for nonunitary pairings in the E_u representation, there should be collective modes associated with the oscillation of the magnetization of the Cooper pairs [76]. It would be interesting to detect this collective mode via experiments like electron-spin resonance or ultrasound attenuation [76].

VI. SUMMARY

Starting from a tight-binding model for the normal-state electronic structures, we have constructed the full lists of two-component pairings for $M_x\mathrm{Bi_2Se_3}$ (M is Cu, Sr, or Nd). We then transform the pairings to the pseudospin basis, based on which we study their qualitative properties. In addition to a well-known odd-parity pairing channel [i.e., $E_u^{(1)}$], we have identified through comparison with existing experiments several multichannel two-component pairings that can explain more than one key experiment. Besides a time-reversal symmetric nematic pairing belonging to the E_u representation, we identify chiral and nematic pairings in both the E_g and the E_u

representations. However, for all three superconductors, the existing experiments are insufficient to unambiguously determine the nature of the superconducting state. In particular, the studies on the dependence of the Fermi surface and the superconducting properties on the doping concentration x are inadequate for all three superconductors. A complementary set of experiments are suggested to identify unambiguously the genuine pairing symmetries of the three superconducting electron-doped Bi_2Se_3.

ACKNOWLEDGMENTS

L.H. thanks Ting-Kuo Lee, Sungkit Yip, and Jun Wang for helpful discussions. L.H. was supported by the National Natural Science Foundation of China under Grant No. 11204035 and the Fundamental Research Funds for the Central Universities under Grant No. 2242018K40080. C.S.T. was supported by the Robert A. Welch Foundation under Grant No. E-1146 and the Texas Center for Superconductivity at the University of Houston.

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