The direction of the $d$-vector in a nematic triplet superconductor

Lin Yang$^{1,2}$ and Qiang-Hua Wang$^{1,2}$

$^1$ National Laboratory of Solid State Microstructures & School of Physics, Nanjing University, Nanjing, 210093, People’s Republic of China

$^2$ Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, People’s Republic of China

E-mail: qhwang@nju.edu.cn

Keywords: superconductor, triplet pairing, $d$-vector, nematic

Abstract

We investigate the states of triplet pairing in a candidate nematic superconductor versus typical material parameters, using the mean field theory for two- and three-dimensional tight-binding models with local triplet pairing in the $E_d$ representation of the $D_{3d}$ point group of the system. In the two-dimensional model, the system favors the fully gapped chiral state for weaker warping or lower filling level, while a nodal and nematic $\Delta_{4\alpha}$ state is favorable for stronger warping or higher filling, with the $d$-vector aligned along the principle axis. In the presence of lattice distortion, relative elongation along one of the principle axes, $a$, tends to rotate the nematic $d$-vector orthogonal to $a$, resulting in the nematic $\Delta_{4\alpha}$ state at sufficient elongation. Three-dimensionality is seen to suppress the chiral state in favor of the nematic ones. Our results may explain the variety in the probed direction of the $d$-vector in existing experiments.

1. Introduction

Time-reversal-invariant (TRI) topological superconductors (TSC) attract sustained interests due to the interesting Majorana zero modes in vortices and itinerant Majorana fermions on the boundary [1–3]. It has been established that the key requirement for TSC in inversion symmetric systems is odd-parity pairing [4, 5]. Although considerable efforts are made both theoretically and experimentally [6–10], definite evidence of a TRI-TSC is yet to be found. The earliest signature was found in Cu$_2$Bi$_2$Se$_3$ [11], which is made by intercalation of Cu into Bi$_2$Se$_3$. The parent compound is a topological insulator. While the topology of the normal state is not necessary for TSC [1], the strong spin–orbital coupling in such a material makes TSC more likely. The maximum transition temperature $T_c$ observed is 3.8 K. Early specific heat measurement [12] seems to indicate a full pairing gap. The upper critical field exceeds the Pauli limit [13], suggesting triplet pairing. Assuming odd parity triplet pairing, a candidate local pairing function is $\phi(\mathbf{k}) = \tau_3\sigma_i\mathbf{r}_1\tau_3$ [4], dubbed $\Delta_2$ pairing. Henceforth, $\tau_i$ ($\sigma_i$) is the Pauli matrix in the orbital (spin) basis. Note the local spin-triplet pairing is made possible by the orbital-singlet $\Delta_2$ pairing (through $\tau_3$). The two orbitals are derived from the $p_z$ orbitals of the Se- and Bi-atoms in a quintuple layer of Bi$_2$Se$_3$ [14]. The $\Delta_2$ pairing is a nondegenerate representation of $D_{3d}$, the point group of the system. We note that a general pairing function may be written as $(g + V \cdot \sigma) i\sigma_2$, where $g$ describes singlet pairing, and $V$ is the so-called $d$-vector describing triplet pairing. In this definition, the $d$-vector in the case of the $\Delta_2$ pairing is along $z$, and it is shown to be generically fully gapped [4]. The zero-bias conductance peak observed in the point-contact spectroscopy indicates the existence of unusual in-gap surface states [15], as would be expected for a TRI-SC. However, the scanning-tunneling-microscopy (STM) measurement reveals a full gap with no sign of in-gap surface states [16]. With the spectroscopic uncertainty in mind, recent nuclear magnetic resonance (NMR) experiment [17] makes a breakthrough in this field. The observed Knight-shift $K$ develops a two-fold oscillation as a function of the angle of the in-plane applied field $H$, with strongest (or no) suppression of $K$ below $T_c$ for $H$ along (or orthogonal to) one of the Se–Se bonds, the principle axes henceforth. This could be understood if the $d$-vector of the triplet aligns along a principle axis [18], since the spin of the triplet Cooper pair is orthogonal to the $d$-vector, and the superconductor can respond to the applied field without (or by) breaking a Cooper pair if the field is applied along (or orthogonal to) the spin of the triplet Cooper pair. Fu realized that the in-plane NMR nematicity suggests the pairing function must belong to a doublet $E_d$ representation of the underlying point
group $D_{3d}$ [19]. For local pairing, the desired pairing function is obvious, $\phi(k) = \gamma_1 V \cdot \delta i\sigma_3$, where $V$ is a linear combination of inplane vectors $(1, 0)$ and $(0, 1)$. Specifically, the case of $V \propto (1, 0)$ is dubbed $\Delta_4$-pairing, and $V \propto (0, 1)$ the $\Delta_{4f}$ pairing. The $d$-vector is along and orthogonal to the principle axis, respectively. Note that $\Delta_{4e}$-pairing leads to nodal SC gap, protected by the remaining mirror symmetry about $y$ (sending $x \rightarrow -x$), while $\Delta_{4f}$-pairing could become fully gapped in the presence of warping effect in the normal state band structure [19]. While the nematicity is observed by various probes, the identified direction of the $d$-vector varies [17, 20–25]. Theoretically [26], direct visualization of the $d$-vector is possible by quasi-particle interference (QPI) [27] and STM: the leading peak momentum in QPI at sub-gap energies should be along the $d$-vector, and the STM profile of the vortex at low energies should be elongated also along the $d$-vector. The agreement between the results in the momentum space (from QPI and real space (from vortex profile) is a stringent constraint for the nematic triplet.

In real samples, there may be lattice distortions [28], e.g. in-plane one-axis elongation and c-axis inclination. The effect of such distortions on the direction of the $d$-vector is not explored so far. On the other hand, the extent of warping, the filling level, the thickness of the sample, as well as the strength of inter-layer hybridization, may vary from sample to sample, and their roles for the $d$-vector are to be unravelled. Here we study how the nematic pairing, and the direction of the $d$-vector in particular, depends on the above typical material parameters, in order to understand the variety in the probed $d$-vector direction in existing experiments. We use a mean field theory (MFT) based on a tight-binding model, assuming local triplet pairing in the $E_u$ representation of the $D_{3d}$ group.

Our main results are as follows. In the two-dimensional (2D) model, the system favors the fully gapped chiral state for weaker warping or lower filling level, while a nodal and nematic $\Delta_{4u}$ state is favorable for stronger warping or higher filling. In the presence of lattice distortion, relative elongation along one of the principle axes, tends to rotate the nematic $d$-vector in favor of the nematic $\Delta_{4f}$ state. In the 3D model, increasing inter-layer hybridization suppresses the chiral state in favor of the nematic ones.

The rest of the paper is organized as follows. The model is described in section 2, the effect of warping in the 2D model is described in section 3, the effect of lattice distortion in section 4, and the effect of inter-layer hybridization in section 5. Finally, section 6 is a summary of this work.

## 2. Model and methods

According to the first-principles calculations [14], the conduction and valence bands of Bi$_2$Se$_3$ are superpositions of Se $p_z$ orbitals on the top and bottom layers of the unit cell, each of which mixed with its neighboring Bi $p_z$ orbital. The angle-resolved photoemission spectroscopy (ARPES) experiment [29] shows that the band structure of Cu$_x$Bi$_2$Se$_3$ is quite similar to Bi$_2$Se$_3$. In the spirit of $k \cdot p$ theory, a two-orbital continuum model [19] has been proposed to describe the low energy physics of Cu$_x$Bi$_2$Se$_3$. Here we compactify it on the layered triangular lattice to make the discussion more directly related to the material. The free part of the Hamiltonian can be written as, in the momentum space, $H_0 = \sum_{\mathbf{k}} \psi^\dagger_{\mathbf{k}} h_{\mathbf{k}} \psi_{\mathbf{k}}$, where $\psi_{\mathbf{k}}$ is a four-component spinor describing two orbitals and two spins, with $\psi_{\mathbf{k}} = (\psi_{\mathbf{k}1\uparrow}, \psi_{\mathbf{k}2\uparrow}, \psi_{\mathbf{k}1\downarrow}, \psi_{\mathbf{k}2\downarrow})$, and

\[
h_{\mathbf{k}} = \sum_{i} t'_{i}(\mathbf{b}_{i} \times \sigma)_{\mathbf{k}_{\mathbf{2}}} \sin k_{i} + \sum_{i} t''_{i} \sigma_{\mathbf{k}_{\mathbf{2}}} f_{i} \sin k_{i} + [m + \sum_{i} t(1 - \cos k_{i}) + t_{c}(1 - \cos k_{z})] \gamma_{1}
+ t_{z} \sin k_{z} \gamma_{2} - \mu. \tag{1}\]

Here $t'$ and $t''$ are inplane spin-orbital-coupled hopping integrals, the summation is over the three inplane translation vectors $\mathbf{b}_{1} = (1, 0)$, $\mathbf{b}_{2} = (1/2, \sqrt{3}/2)$ and $\mathbf{b}_{3} = (-1/2, \sqrt{3}/2)$, with $k_{i} = \mathbf{k} \cdot \mathbf{b}_{i}$. The form factor $f_{1,2,3} = (1, -1, 1)$ is compatible with the $D_{3d}$ symmetry, causing a warping effect on the band structure. For this reason, $t_{c}$ is taken as a hexagonal warping parameter. In addition, $\mu$ is the chemical potential that controls the filling level, $t_{c}$ is the interlayer hopping, and $m$ is a parameter that decides the topology of the normal state band structure. For the parent lattice, we take $t' = t$ and $t'' = t_{c}$ to be isotropic in bond direction, but they will depend on direction in distorted lattices. Throughout this work we take $t = 1$ as the unit of energy for qualitative purposes, and we fix $m = -0.5$ for concreteness. The Hamiltonian is invariant under time-reversal, $h_{\mathbf{k}} = TH_{\mathbf{k}} T^{-1}$ with $T = i\sigma_{y} K$ (with $K$ the complex conjugation), and invariant under inversion, $h_{\mathbf{k}} = \tau_{1} h_{-\mathbf{k}} \tau_{1}$. In the continuum limit, the above lattice model reduces to the form of the effective model in [4, 19].

As an example, we show the band structure (near the Fermi level) in the 2D limit in figure 1(a) for $\mu = 3.4$ and $t_{c} = 0.1$, which is consistent with the ARPES measurement [29]. Note the band is two-fold degenerate because of the time-reversal and inversion symmetries. The corresponding density of states (DOS) is shown in figure 1(b). The DOS is particle–hole asymmetric and has a Van Hove singularity near the Fermi level, and this makes the system sensitive to perturbations that we will be addressing.

The NMR nematicity in the SC state strongly implies triplet pairing in a doublet $E_u$ representation of the point group. While the underlying pairing mechanism is not yet clear, for our purpose it is sufficient and
reasonable to start with an effective MF Hamiltonian with attractive pairing interaction in the $E_u$ channel,

$$H_{MF} = H_0 + \sum_{k} (\psi^+_k \tau_3 V \cdot \sigma \psi_{-k} + \text{h.c.}),$$

where $t$ means transpose, and $V = (\Delta_{4\xi}, \Delta_{4\eta})$ is the $d$-vector order parameter. The local triplet is made possible by the antisymmetric pairing between the two orbitals (or orbital singlet through $\tau_3$). The property of the pairing function in the above form has been discussed in quite details in [19]. For example, if $V \times V^* = 0$, or if $V$ is real up to a global factor (which can be gauged away), the pairing function is time-reversal invariant. This is the analog of $\delta k_x$ or $\delta k_y$ pairing in the single-orbital case [30, 31]. The resulting pairing gap is anisotropic in momentum space, hence nematic. On the other hand, when $V \times V^* \neq 0$, the relative phase between $\Delta_{4\xi}$ and $\Delta_{4\eta}$ cannot be gauged away, in analogy to the $(\delta + i\gamma)(k_x + ik_y)$ pairing (or the A1 phase) in the single-orbital case [30, 31]. This breaks time-reversal symmetry hence is chiral.

The MF hamiltonian can be written compactly as $H_{MF} = \frac{1}{2} \sum_{k} \psi^+_k M_k \psi_{-k} \cdot \text{up to MF constants}$, where $\Psi^+_k = (\psi^+_k, \psi^*_{-k})$ is the Nambu spinor, and

$$M_k = \begin{pmatrix} h_k & i \tau_3 V \cdot \sigma \psi_{-k} \\ -i \tau_3 V^* \cdot \sigma & -h_{-k}^* \end{pmatrix}.$$  

The Bogoliubov-de Gennes (BdG) eigenenergy $E_{k,n}$ ($n = 1, 2, \ldots, 8$) is the eigenvalue of the matrix $M_k$. In the following we define the BdG gap $\Delta_{BdG}$ along a radial direction as the minimum of all $|E_{k,n}|$ for $k$ along the radial path in the Brillouin zone. Usually this minimum is on the normal state Fermi surface (FS), but in the present model the unusual pairing may cause the minimum to deviate from the FS [19]. The pairing order parameters are determined self-consistently by

$$\begin{align*} 
\Delta_{4\xi,4\eta} &= \frac{V_c}{N} \sum_{k} (\psi^+_k (-i \sigma_2) \tau_2 \psi_{-k}) \\
&= \frac{V_c}{N} \sum_{k,n} (\gamma_{k,n} (-i \sigma_2) \tau_2 \mu_{k,n}) f(E_{k,n}),
\end{align*}$$

where $V_c < 0$ is the pairing interaction, $N$ is the number of lattice sites, $|\mu_{k,n}|$ and $|\gamma_{k,n}|$ are, respectively, the particle and hole part of the $n$th eigenvector $|k, n\rangle$ of $M_k$, and $f$ is the Fermi function.

### 3. Two dimensional limit

First, we consider the 2D limit, $t_z = 0$. We fix $(\mu, V_c) = (3.4, 1.5)$ and perform the MF calculation at the temperature $T = 10^{-5}$, the zero temperature limit. The solid (dotted) lines in figure 2(a) show the MF evolution of the real (imaginary) part of the ratio $r = \Delta_{4\eta}/\Delta_{4\xi}$ for $t_w = 0.1$ (blue) and $t_w = 0.4$ (red). Clearly, a chiral state with $V \propto (1, i)/\sqrt{2}$ is obtained for $t_w = 0.1$. An equivalent state is $V \propto (1, -i)/\sqrt{2}$. On the other hand, a nematic state with $V \propto (1, \sqrt{3})/2$ is obtained for $t_w = 0.4$. There is a discrete six-fold degeneracy in the nematic states, with

$$\Delta_{4\eta}/\Delta_{4\xi} = \tan(n\pi/3), \quad n = 1, 2, \ldots, 6.$$  

The value of $n$ in the converged MF solution depends on the initial condition. We note that up to the forth order in a phenomenological Landau theory for the continuum model (in the absence of warping), [32] it is possible to distinguish the chiral versus the nematic phase, but the nematic phase would be degenerate with respect to continuous rotation about the $z$ axis. Since our result indicates only six-fold degeneracy of the nematic vector, it
are the \( i \) component increases rapidly for positive \( b \) versus \( i \).

The evolution of the real part \( (\gamma', \text{solid lines}) \) and imaginary part \( (\gamma'', \text{dashed lines}) \) of the ratio \( r = \Delta_{4y}/\Delta_{4x} \) versus MF iteration steps for \( t_{0} = 0.1 \) (blue) and \( t_{0} = 0.4 \) (red). Here \( \mu = 3.4, V_{t} = -1.5, \) and \( T = 10^{-2} \). (b) The phase diagram obtained by MF calculations in the \((\mu, t_{0})\) space with \( V_{t} = -1.5 \). The insets illustrate the characteristic BdG gap versus the polar angle in the respective phases.

Figure 2. (a) The evolution of the real part \( (\gamma', \text{solid lines}) \) and imaginary part \( (\gamma'', \text{dashed lines}) \) of the ratio \( r = \Delta_{4y}/\Delta_{4x} \) versus MF iteration steps for \( t_{0} = 0.1 \) (blue) and \( t_{0} = 0.4 \) (red). Here \( \mu = 3.4, V_{t} = -1.5, \) and \( T = 10^{-2} \). (b) The phase diagram obtained by MF calculations in the \((\mu, t_{0})\) space with \( V_{t} = -1.5 \). The insets illustrate the characteristic BdG gap versus the polar angle in the respective phases.

By systematic MF calculations with \( V_{t} = -1.5 \) and in the zero temperature limit, we obtain a phase diagram, figure 2(b), for the pairing state in the \((\mu, t_{0})\) parameter space. Note a higher value of \( \mu \) corresponds to a higher electron filling. (In the weak coupling limit, the small pairing gap hardly changes the filling level determined by \( \mu \) in the normal state). We see that the chiral state is favorable for lower warping or filling, and the nematic state is favored otherwise. We stress that the nematic state is of \( \Delta_{4x} \)-type. The \( \Delta_{4y} \)-type pairing is not obtained in the MF calculations here. The characteristic BdG gap versus the polar angle is shown as insets in the respective phase, which is nodeless/nodal in the chiral/nematic phase.

4. Lattice distortion

In the previous section, we find the \( \Delta_{4y} \) pairing is not stabilized in the ideal 2D lattice model. However, this type of pairing state was reported in experiments. We then ask how it could be realized by perturbations away from the ideal limit. One possible perturbation is the lattice distortion, which is indeed observed in Sr\(_{2}\)Bi\(_{2}\)Se\(_{3}\) by x-ray diffraction [28]. By symmetry, the effect of the inplane lattice distortion on the hopping coefficients can be expressed as \( \gamma = \alpha_{t} t^{i} + \alpha_{t^{'}} t^{i} \). (Recall that \( t = 1 \) is set as the unit of energy.) The coefficient \( \alpha_{t} = 1 + \Delta \alpha_{t} \) can be decomposed into two symmetry channels, \( \Delta \alpha_{t} \propto \gamma^{2} - y^{2} \) and \( \Delta \alpha_{t} \propto 2x_{c}y \). Here \( (x_{c}, y) = b_{i} \) are the two components of the first-neighbor bond \( b_{i} \). We concentrate on the \( d_{x^{2} - y^{2}} \) channel. (The other channel can be discussed similarly.) Although all of \( \alpha_{1,2,3} \) would be changed, we can perform rescaling so that \( \alpha_{2} = \alpha_{3} = 1, \) and \( \alpha_{1} = 1 - \gamma \), to represent the qualitative effect of the strain. A positive \( \gamma \) corresponds to relative elongation of \( b_{i} \) versus \( b_{2,3} \), and vice versa. (The rescaling may also change \( m \) and \( \mu_{i} \), but for a small distortion such changes could be ignored in the leading order approximation.)

Figure 3(a) shows the MF solution versus \( \gamma \) in the parent nematic case with \((\mu, t_{0}) = (3.4, 0.4)\). The \( \Delta_{4y} \) component increases rapidly for positive \( \gamma \), and the \( \Delta_{4x} \) component decreases to zero already for \( \mu = 0.008 \). We checked that \( \Delta_{4y}/\Delta_{4x} \) remains real, so the pairing is still nematic. We see that the relative elongation along \( x \) can rotate the \( d \)-vector to the orthogonal direction, in favor of the \( \Delta_{4y} \)-pairing. For small positive \( \gamma \), the \( d \)-vector interpolates between \( x \)- and \( y \)-directions. Such an intermediate state may have been observed in [25]. Note for a
negative $\gamma$, or relative compression of the lattice along $x$, the $\Delta_{4t}$ state is the only stable one. This is reasonable since the system favors $\Delta_{4t}$ already in the parent undistorted lattice for $(\mu, t_w) = (3.4, 0.4)$.

In the parent chiral case with $(\mu, t_w) = (3.4, 0.1)$, the effect of $\gamma$ on the $\Delta_{4t}$ components of $V$ is shown in figure 3(b). The two components coexist within $|\gamma| \leq 0.05$, and we checked that $\Delta_{4t}/\Delta_{4\ell}$ remains imaginary. So in this regime the pairing is still chiral. However, only $\Delta_{4t} (X_{4\ell})$ is left for $\gamma > 0.05 (\gamma < -0.05)$, hence the pairing becomes nematic. Although the critical value of $\gamma$ for the transition between chiral and nematic states is relatively large, we again see that the relative elongation of the $x$-bonds in the 2D lattice tends to favor $\Delta_{4t}$ pairing, and vice versa. By symmetry, the conclusion can be generalized to the relative elongation of any one of the principle axes of the triangle lattice.

5. Dimension crossover

It is known that at low doping, Cu$_2$Bi$_2$Se$_3$ has an ellipsoidal Fermi pocket centered at the origin $G$, while at high doping the FS is open and cylinder-like along $k_x$, as observed in the photoemission [33] and de Haas–van Alphen measurements [34, 35]. In our tight-binding model, the shape of the 3D FS is controlled by the inter-layer hybridization $t_z$. For small $t_z$, the FS is open and cylinder-like. For $t_z > 2$, the FS becomes closed around the $G$ point. We should remark that in the case of an open cylinder-like FS, both types of nematic pairing are topologically trivial, irrespectively of whether they are nodal or nodeless, since the FS encloses two time-reversal invariant momenta, $(0, 0, 0)$ and $(0, 0, \pi)$. With this in mind, we continue to investigate the pairing state in the 3D limit. We model the 3D lattice by $N_z = 10$ layers of triangle lattices and periodic boundary condition along all translation directions.

As an example of the 3D model, we consider $\mu = 3.4, t_z = 1.0$ and $V_s = -2.5$. (In the 3D model, the DOS is lower. To get a sizable $T_c$, a stronger pairing strength is used.) Figure 4(a) shows the FS in the inset, and the evolution of the MF solutions in the main panel, for the real (solid line) and imaginary (dotted line) parts of the ratio $\tau = \Delta_{4t}/\Delta_{4\ell}$. We find in both cases of $t_w = 0$ (blue lines) and $t_w = 0.1$ (red lines), the solution converges to $V = (\Delta_{4t}, \Delta_{4\ell}) \propto (1, \sqrt{3})/2$, namely the $\Delta_{4t}$ state up to a $C_6$ rotation.

By systematic calculations, we obtain the phase diagram in the $(t_z, t_w)$ parameter space, see figure 4(b). The chiral state is limited to smaller $t_z$ or $t_w$, while the nematic $\Delta_{4t}$ phase prevails for larger $t_z$ or $t_w$. In reality, the hopping along $z$ is between quintuple layers, and should be weak. In this case, the result at large $t_w$, e.g. $t_w = 0.4$, is qualitatively similar to the 2D case discussed in section 3. In the artificial case of large $t_z$, e.g. $t_z = 1$, the nematic state is preferred. To understand this result, we checked the chiral state to find that in the 3D limit, although it is still fully gapped in the $x$–$y$ plane, it becomes nodal in the $x$–$z$ and $y$–$z$ planes, as already pointed out elsewhere.

![Figure 3. The amplitude of $\Delta_{4t}$ and $\Delta_{4\ell}$ versus the distortion parameter $\gamma$, for (a) $(\mu, t_w) = (3.4, 0.4)$, and (b) $(\mu, t_w) = (3.4, 0.1)$.](image-url)
This makes it energetically even less favorable than in the 2D limit, consistent with the missing of the chiral phase in the 3D limit in figure 4(b).

We note that the phenomenological Landau theory analysis\[32, 37\] reaches a similar conclusion that reduced 3D dispersion would favor the chiral state, however, it does not include the effect of warping, hence is unable to capture the nematic phase in the 2D limit. On the other hand, we have further checked the effect of lattice distortion in the 3D model. The qualitative effect is the same as in figure 3(a), namely, a relative elongation along $x$ would favor the $\Delta_x$ pairing.

6. Summary

To conclude, we studied the pairing states in a model for doped Bi$_2$Se$_3$ superconductor with triplet pairing in the $E_u$ representation of the $D_{3d}$ group. In the 2D model, the fully gapped chiral state is favored if the warping parameter is small, while the nodal nematic triplet with the $d$-vector $= \Delta_{xy}$ is favored otherwise. Under lattice distortion, a relative elongation along $x$ would favor a $d$-vector $= (0, \Delta_{xy})$. In the 3D model, the chiral state disappears for large interlayer hopping, in favor of the nematic $\Delta_x$, state, and the effect of lattice distortion is similar to the case of the 2D model.

We note that the NMR experiment\[17\] suggests the $d$-vector is along $x$ (or the Cooper pair spin is orthogonal to $x$) and hence $\Delta_x$ pairing. However, the specific heat measurement\[20\] suggests the pairing gap is maximal along $y$ in the momentum space, hence is consistent with the $\Delta_{xy}$ pairing instead. More experimental results are summarized nicely in\[38\], showing almost equal popularities of $\Delta_x$ and $\Delta_{xy}$ pairing. Such a variety of the probed $d$-vectors implies the $d$-vector may be fragile and therefore dependent on material details, as demonstrated by our results. However, a close comparison between theory and experiment would require the material parameters, that are unfortunately difficult to extract. But it should be easier to interchange $\Delta_x$ and $\Delta_{xy}$ in the same sample by applying a uniaxial strain, a prediction to be explored by future experiments. On the other hand, no chiral phase has been observed yet.

Finally, we should remark that there are quantum as well as thermal fluctuation effects beyond the MFT, and especially so in 2D. However, in the limits of zero temperature and weak-coupling, such effects are not expected to change the MF results qualitatively, as in conventional superconductors. We also remark that the triplet pairing function in the $E_u$ representation is an assumption based on experiments\[17, 19\]. As a future topic, it will be interesting to ask what microscopic mechanism could drive such an unusual Cooper pairing.

Figure 4. MF results for the 3D model with $\mu = 3.4$ and $V_s = -2.5$. (a) The evolution of the real part ($r'$, solid lines) and imaginary part ($r''$, dashed lines) of the ratio $r = \Delta_{xy}/\Delta_{xx}$ versus MF iteration steps for $t_w = 0$ (blue) and $t_w = 0.1$ (red). Here $t_z = 1.0$. The inset shows the FS. (b) The phase diagram in the ($t_x, t_w$) space.
Acknowledgments

The project was supported by the National Key Research and Development Program of China (under grant No. 2016YFA0300401) and the National Natural Science Foundation of China (under Grant No. 11574134).

References

[1] Snyder A P, Ryu S, Furusaki A and Ludwig A W 2008 Phys. Rev. B 78 195125
[2] Qi X-L, Hughes T L, Raghu S and Zhang S-C 2009 Phys. Rev. Lett. 102 147001
[3] Roy R 2008 arXiv:0803.2866
[4] Fu L and Berg E 2010 Phys. Rev. Lett. 105 097001
[5] Sato M 2010 Phys. Rev. B 81 220504(R)
[6] Qi X-L, Hughes T L and Zhang S-C 2010 Phys. Rev. B 81 134508
[7] Nakosai S, Tanaka Y and Nagaosa N 2012 Phys. Rev. Lett. 108 147003
[8] Scheurer M S and Schmalian J 2015 Nat. Commun. 6 6005
[9] Wang J, Xu Y and Zhang S-C 2014 Phys. Rev. B 90 054503
[10] Hosur P, Dai X, Fang Z and Qi X-L 2014 Phys. Rev. B 90 045130
[11] Hor Y S, Williams A J, Checkelsky J G, Roushan P, Seo J, Xu Q, Zandbergen H W, Yazdani A, Ong N P and Cava R J 2010 Phys. Rev. Lett. 104 037001
[12] Kriener M, Segawa K, Ren Z, Sasaki S and Ando Y 2011 Phys. Rev. Lett. 106 127004
[13] Bay T V, Naka T, Huang Y-K, Luigjes H, Golden M S and de Visser A 2012 Phys. Rev. Lett. 108 057001
[14] Zhang H-J, Liu C-X, Qi X-L, Dai X, Fang Z and Zhang S-C 2009 Nat. Phys. 5 438
[15] Sasaki S, Kriener M, Segawa K, Yada K, Tanaka Y, Sato M and Ando Y 2011 Phys. Rev. Lett. 107 217001
[16] Levy N, Zhang T, Ha J, Sharifi F, Talin A A, Kuk Y and Stroscio J A 2013 Phys. Rev. Lett. 110 117001
[17] Matano K, Kriener M, Segawa K, Ando Y and Zheng G-Q 2016 Nat. Phys. 12 852–4
[18] Hashimoto T, Yada K, Yamakage A, Sato M and Tanaka Y 2013 J. Phys. Soc. Japan 82 044704
[19] Fu L 2014 Phys. Rev. B 90 100509
[20] Yonezawa S, Tajiri K, Nakata S, Nagai Y, Wang Z, Segawa K, Ando Y and Maeno Y 2017 Nat. Phys. 13 123
[21] Pan Y, Nikitin A M, Arai G K, Huang Y-K, Matsushita Y, Naka T and Visser A de 2016 Sci. Rep. 6 28632
[22] Smolyk M P et al 2018 Sci. Rep. 8 7666
[23] Asaba T, Lawson B J, Tinsman C, Chen L, Corbape L, Li G, Qiu Y, Hor Y S, Fu L and Li L 2017 Phys. Rev. X 7 011009
[24] Chen M-Y, Chen X-Y, Yang H, Du Z-Y and Wen H-H 2018 Sci. Adv. 4 eaat1084
[25] Tao R, Yan J-L, Liu X, Wang Z-W, Ando Y, Wang Q-H, Zhang T and Feng D-L 2018 Phys. Rev. X 8 041024
[26] Bao W-C, Tang Q-K, Liu D-C and Wang Q-H 2018 Phys. Rev. B 98 054502
[27] Wang Q-H and Lee D-H 2003 Phys. Rev. B 67 020511(R)
[28] Kuntsevich A Y, Bryzgalov M A, Prudkofigiadi V A, Martovitskii V P, Selivanov Y G and Chizhovskii E G 2018 New J. Phys. 20 103022
[29] Wray L, Xu S, Xiong J, Xia Y, Qian D, Lin H, Bansil A, Hor Y, Cava R J and Hasan M Z 2010 Nat. Phys. 6 855
[30] Leggett A J 1975 Rev. Mod. Phys. 47 2
[31] Mackenzie A P and Maeno Y 2003 Rev. Mod. Phys. 75 657
[32] Chirolli L 2018 Phys. Rev. B 98 014505
[33] Lahoud E et al 2013 Phys. Rev. B 88 195107
[34] Lawson B J, Hor Y S and Li L 2012 Phys. Rev. Lett. 109 226406
[35] Lawson B J, Li G, Yu F, Asaba T, Tinsman C, Gao T, Wang W, Hor Y S and Li L 2014 Phys. Rev. B 90 159414
[36] Venderbos J W F, Kozii V and Fu L 2016 Phys. Rev. B 94 180504(R)
[37] Zyzun A A, Garaud J and Babaei E 2017 Phys. Rev. Lett. 119 167001
[38] Yonezawa S 2019 Condens. Matter 4 2