Orbital-resolved vortex core states in FeSe Superconductors: calculation based on a three-orbital model

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We study electronic structure of vortex core states of FeSe superconductors based on a $t_2g$ three-orbital model by solving the Bogoliubov-de Gennes (BdG) equation self-consistently. The orbital-resolved vortex core states of different pairing symmetries manifest themselves as distinguishable structures due to different behavior of the quasi-particle wavefunctions. The obtained vortices are classified by the invariant subgroups of the symmetry group of the mean-field Hamiltonian in the presence of magnetic field as isotropic $s$ and $s_{\pm}$ wave vortices have $G_5$ symmetry for each orbital, whereas $d_{x^2-y^2}$ wave vortices show $G_6$ symmetry for $d_{xz}$ and $d_{yz}$ orbitals and $G_5^*$ symmetry for $d_{xy}$ orbital. In the case of $d_{x^2-y^2}$ wave vortices, hybridized-pairing between $d_{sz}$ and $d_{su}$ orbitals gives rise to a relative phase difference in terms of winding structures of vortices between these two orbitals and $d_{zy}$ orbital, which is essentially caused by a transformation of co-representation of $G_5$ and $G_6$ group. Calculation of particle densities show common charging feature of vortices in the cases of $s_{\pm}$ and $d_{x^2-y^2}$ wave pairing states where the electron-like vortices are observed for $d_{sz}$ and $d_{su}$ orbitals while hole-like vortices for $d_{zy}$ orbital. The results of orbital-resolved local density of states (LDOS) show that a local charge density oscillation is induced by charged $s_{\pm}$ wave vortices, while hybridized $d_{x^2-y^2}$ wave vortices show a consistent pattern of LDOS with scanning tunneling microscopy (STM) measurement results. The phase difference of orbital-resolved $d_{x^2-y^2}$ wave vortices and their charging effects can be verified by further experiment observation.

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I. INTRODUCTION

Quantized vortices, as stable topological defects, appearing in a variety of fermionic systems such as superconductivity and superfluidity, are characterized by their nature of soliton solutions of dynamical systems with off-diagonal long range order.\footnote{2}\footnote{3} Electronic structure of vortices in cuprate superconductors have its signature as charging effects\footnote{2} and anisotropy of core states due to unconventional $d_{x^2-y^2}$ wave pairing symmetry.\footnote{3} Pioneering theoretical works have been done to investigate the vortex line states based on microscopic models.\footnote{2}\footnote{4}\footnote{5} However, band structure and multi-orbital pairing play much important role in iron-based superconductors as compared with cuprates. Therefore the vortex structures may be richer and more wonderful due to multi-orbital dependency. Vortex core states of two-fold rotational symmetry, which is proposed to be attributed to the fact that orbital-dependent reconstruction lifts the degeneracy of $d_{xz}$ and $d_{yz}$ orbitals in FeSe superconductors\footnote{6}\footnote{7}, have been reported in work done by C. L. Song et al. by STM observation.\footnote{15}

The orbital degrees of freedom, Fermiology, and symmetry of lattice give rise to a various superconducting (SC) states. Angle-resolved photoemission spectroscopy (ARPES) measurements for single layer FeSe superconductors show that the Fermi surface only consists of electron pockets around M point at the corners of the folded Brillouin zone (BZ).\footnote{12} The $s_{\pm}$ pairing symmetry in iron pnictide superconductors has been predicted by spin-fluctuation theory\footnote{13}\footnote{14} in the presence of hole pocket at Γ point, while $d_{x^2-y^2}$ wave pairing channel starts to co-exist with it when the hole pocket at Γ vanishes.\footnote{16} Additionally, isotropic $s$ wave pairing state was also argued to be more favorable against strong disorder.\footnote{17} Intuitively, one may expect that the vortex core states will behave distinctly with respect to different pairing symmetries and exhibit vivid orbital diversity. Calculation based on two-orbital model shows that the $d_{x^2-y^2}$ wave vortex states are bounded with hole pockets at Γ point for different doping level,\footnote{18} and the pinning effect in the presence of impurity has also been investigated.\footnote{19} Taking into account the orbital ordering and mixed-pairing states in order to describing FeSe superconductors, the vortex structure of two-fold rotation symmetry are obtained by numerical calculation.\footnote{20} However, the Fermi surface obtained from two-orbital model is not enough to eliminate pockets at Γ point. Furthermore, a comprehensive study of vortex states was also presented based on several band models for pnictide superconductors, but the open boundary condition may not be consistent with the situation of Abrikosov lattice.\footnote{21}

From a theoretical point of view, vortices in mixed states of type II superconductors are ground states of fermionic system which is characterized by interaction between a homogenous magnetic field with $C_\infty$ symmetry and cooper pairs with a definite superconducting (SC) pairing symmetry. In iron-based superconductors, situation becomes complicated because of diversities of band structure, or equivalently if the pairing is defined on

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orbital basis, the pairing wavefunction with orbital degrees of freedom. Consequently, symmetry of states of band electrons, SC pairing, and magnetic field together determine the electronic structures of vortices. Among these symmetries constraints, the vortex structures are mainly dominated by magnetic translation invariance, whose generator are crystal momentum and vector potential of magnetic field. However, such conventional magnetic translation group (CMTG) defines a magnetic unit cell (MUC) containing two vortices. It is not the symmetry group of Abrikosov lattice in which only single vortex is within one MUC. Breakthrough of this difficulty was presented by M. Ozaki et al. In their work the magnetic translation group (MTG) describing single vortex was discovered to be a subgroup of direct product of CMTG and gauge transformation group U(1). Therefore, stable vortex structure can be solved numerically in one MUC taking advantages of nontrivial winding boundary conditions derived from properties of MTG.

In this work, we study electronic structures of vortices in multi-orbital FeSe superconductors. Instead of doing calculations of two vortices in one MUC, we follow the method given by M. Ozaki et al., in which only single vortex structures are calculated in one MUC, so that the calculated results can be classified by irreducible representations of MTG. The numerical calculations in previous works, as mentioned above, are mostly carried out for two vortices in one MUC. However, these vortex states can not be identified by invariant subgroups of MTG because they belong to the irreducible representations of CMTG. Additionally, two vortices in one MUC cannot be regarded as two independent sub-MUC not only because the symmetry operation is not defined for single vortex but the induction of interaction between two vortex core states. It is well-known that the topological defect in unconventional superconductors and superfluids with certain symmetry breaking behave distinguishably from the conventional singular (hard core) vortices. For instance, a continuous vortex in $^3He$ has a finite amplitude of order parameter in the soft core region whose size is larger than the coherent length, whereas the winding structure is non-trivial. Therefore in our numerical calculation, we concentrate on winding structures of vortices for each orbitals, although the vortices in iron-based superconductors are most hard core vortices, and classify the obtained vortex structures of isotropic s, $s_\pm$, and $d_{x^2-y^2}$ wave pairing symmetries in terms of invariant subgroups of MTG. Special attention will be paid to the difference of vortex states between $A_{1g}$ (isotropic s and $s_\pm$ wave) and $B_{1g}$ ($d_{x^2-y^2}$ wave) irreducible unitary representations (IUR) of $D_{4h}$ group because the latter corresponds to a point group symmetry broken SC ground state.

The paper is organized as follows. Section II presents the Hamiltonian of the three-orbital model and the self-consistent BdG approach. The classification of vortex solutions are also presented. In section III, we discuss and compare the results of the properties of the vortex core states for different pairing symmetries. Finally, a summary is given in section IV.

II. METHODOLOGY AND BAND MODEL

The Hamiltonian of the SC system in the presence of a homogeneous magnetic field along $\hat{z}$ direction is obtained from its zero-field form by modifying the hopping and pairing terms with Peierls phase, respectively, which is of the following form

$$H = H_0 + H_{pair}$$

$$H_0 = \sum_{i,j,\alpha,\beta,\sigma} [\tilde{t}_{\sigma\sigma}(i\alpha, j\beta) - \mu \delta_{ij}\delta_{\alpha\beta}]a_{i\alpha\sigma}^\dagger a_{j\beta\sigma}$$

$$H_{pair} = \sum_{i,j,\alpha,\beta} [\tilde{\Delta}_{\alpha\beta}(i\alpha, j\beta)a_{i\alpha\sigma}^\dagger a_{j\beta\sigma}^\dagger + h.c.]$$

in which

$$\tilde{t}_{\sigma\sigma}(i\alpha, j\beta) = t_{\sigma\sigma}(i\alpha, j\beta) \exp\left[\frac{i\epsilon}{\hbar c} \int_\mathbf{R}^{\alpha} \cdot d\mathbf{\vec{r}} \right]$$

$$\tilde{\Delta}_{\alpha\beta}(i\alpha, j\beta) = \Delta_{\alpha\beta}(i\alpha, j\beta) \exp[i\phi(i, j)]$$

where $a_{i\alpha\sigma}^\dagger(a_{i\alpha\sigma})$ denotes the creation (annihilation) operator of electrons with spin $\sigma = \uparrow, \downarrow$ and orbital $\alpha$ at site $i$. $t_{\sigma\sigma}(i\alpha, j\beta)$ are hopping integrals and $\mu$ is the chemical potential. We assume that the screening magnetic field inside the superconductor can be neglected except for the magnetic field extremely close to the upper critical field. The SC gap function stemming from the mean-field decoupling of the paired scattering term in extended attractive Hubbard model is expressed as $\Delta_{\alpha\beta}(i\alpha, j\beta) = V_{\alpha\beta}(i\alpha, j\beta)a_{i\alpha\sigma}^\dagger a_{j\beta\sigma}$ for singlet pairing state.

The Peierls phase in hopping terms comes from the fact that the Lagrangian of electron in a magnetic field contains a dynamical term $\vec{\mathbf{\omega}} \cdot \vec{A}$, which gives rise to the phase accumulation in the propagator of electron describing the hopping process between two lattice sites. The modification of pairing order parameters (OPs) accounts for eliminating the mixing of different pairing states under the action of MTG, the mathematical interpretation of which is essentially searching for gauge transformed order parameters (GTOPs), which span a representation of MTG. The gauge transformation, carried out by phase $\phi(i, j)$, has different definition with respect to $s_\pm$ and $d_{x^2-y^2}$ wave pairing states, whereas in the case of isotropic s wave pairing it is trivial. The GTOPs for $d_{x^2-y^2}$ wave pairing has been derived by means of group theoretical analysis. The magnetic translation operator takes following form in symmetric gauge $\vec{A} = -\frac{\mathbf{\omega}}{2} \times \hat{B}$, when it acts on creation operator $a_{i\alpha\sigma}^\dagger$.

$$L^z(\mathbf{R}_\lambda) a_{i\alpha\sigma}^\dagger = e^{\frac{i\pi}{2}[\mathbf{\omega}(\lambda_z \lambda_y)]^T(\mathbf{R}_\lambda)} a_{i\alpha\sigma}^\dagger$$

$$= e^{i\frac{\pi}{2} \mathbf{\omega}(\lambda_z \lambda_y + \frac{1}{2} (\lambda_x \lambda_y - \lambda_y \lambda_x))} a_{i\lambda + \lambda, \alpha\sigma}^\dagger$$
and the resultant transformation of OPs is

$$\langle a_{i+\lambda\beta\gamma} a_{i+\lambda\alpha\gamma} \rangle = e^{i\pi N_c}\lambda_x \lambda_y \frac{1}{\Delta} \lambda_z (i_y + j_y) - e^{i\pi \lambda_y (i_z + j_z)} \langle a_{i+\lambda\beta\gamma} a_{i+\lambda\alpha\gamma} \rangle$$

(7)

where $\vec{R}_\lambda = \lambda_x \vec{x} + \lambda_y \vec{y}$ is the basis vector of MUC containing N lattice sites and $N_c$ is the number of vortexes within one MUC. We have restricted ourselves to the cases of square vortex lattice with lattice constant set to unity. Eq. (6) defines actions of MTG $\{L^x(\vec{R}_\lambda)\}$ on field operators, and all the operations of it form a group in representation space spanned by GTOPs, provided that certain group condition must be satisfied. Note that the gauge transformation, as an internal symmetry transformation, takes its complex conjugate form when acts on annihilation operators. Different from the situation for annihilation operators, the re-defined SC GTOPs for $s_+ \sim \cos(k_x) \cos(k_y)$ wave OPs will mix with extended $s_\pm \sim \cos(k_x) + \cos(k_y)$, $p_x \sim i \sin(k_x)$, and $p_y \sim i \sin(k_y)$ wave OPs under operation of MTG. Such a mixing originates from the fact the symmetry group of normal state Hamiltonian contains a local gauge transformation generated by the vector potential of a magnetic field of $C_{\infty}$ symmetry. The re-defined SC GTOPs, which manifests as transforming according to invariant subgroups of $D_{4h}$ group without any gauge component, as OPs do in the absence of magnetic field, are obtained by generating all of them with the action of a conjugate rotation subgroup (CRSG) $\{C_{4z}(i_x, j_y), k = 1, 2, 3, 4\}$ on one of the pairing bonds of every local OPs accompanied by a Peierls phase factor. The generator of CRSG is defined as

$$C_{4z}(i_x, j_y) = T(i_x, j_y)C_{4z}T^{-1}(i_x, j_y)$$

(8)

where $C_{4z}$ is 4-fold rotation around the origin of the coordinate system. Therefore the mixing of OPs under magnetic translation is eliminated by redefining rotations of all local OPs at different sites back to origin. The $d_{x^2-y^2}$ wave GTOPs is consequently redefined as

$$\hat{\Delta}_{\pm}^{d_{x^2-y^2}}(i\alpha, j\beta) = \frac{V_{11}(j\beta, i\alpha)}{2} \langle a_{i\alpha} a_{j\beta} \rangle (e^{iK(i_x-i_y)}\delta_{i+\hat{z}+\hat{y}, j} - e^{iK(i_x+i_y)}\delta_{i+\hat{z}-\hat{y}, j})$$

(9)

where $K = \frac{\pi}{2\alpha}$ and $\hat{x}(\hat{y})$ denote the unit vectors along $x(y)$ directions. Note that for singlet pairing the OPs are symmetric under exchange of site-orbital quantum number.

Here we follow method given by M. Ozaki et al. to derive the GTOPs for $s_\pm \sim \cos(k_x) \cos(k_y)$ pairing symmetry. The results of action of CRSG on pairing bond along $\hat{x} + \hat{y}$ direction of are

$$C_{4z}(i_x, j_y) \langle a_{i\alpha x} a_{i\beta x} a_{i\gamma} a_{i\beta} \rangle$$

$$= e^{-i2K(i_x-i_y)} \langle a_{i\alpha x} a_{i\beta x} a_{i\gamma} a_{i\beta} \rangle$$

$$= e^{2iK(i_x+i_y)} \langle a_{i\alpha x} a_{i\beta x} a_{i\gamma} a_{i\beta} \rangle$$

from which the resultant transformation of OPs is

$$\hat{\Delta}_{\pm}^{d_{x^2-y^2}}(i\alpha, j\beta) = \frac{V_{11}(j\beta, i\alpha)}{2} \langle a_{i\alpha} a_{j\beta} \rangle (e^{iK(i_x-i_y)}\delta_{i+\hat{z}+\hat{y}, j} - e^{iK(i_x+i_y)}\delta_{i+\hat{z}-\hat{y}, j})$$

The magnetic translation property of GTOPs for $s_\pm$ wave pairing state, which is consistent with $d_{x^2-y^2}$ wave, is

$$\hat{\Delta}_{\pm}^{s_\pm}(i\alpha, j\beta)$$

$$= e^{i\pi N_c}\lambda_x \lambda_y \frac{1}{\Delta} \lambda_z (i_y + j_y) - e^{i\pi \lambda_y (i_z + j_z)} \langle a_{i\alpha} a_{j\beta} \rangle (e^{iK(i_x-i_y)}\delta_{i+\hat{z}+\hat{y}, j} - e^{iK(i_x+i_y)}\delta_{i+\hat{z}-\hat{y}, j})$$

(15)

where $j$ is always related to $i$ as N.N.N pairing. Compare this expression with Eq. (7), it is obvious that the GTOPs now form a basis of representation of MTG and the mixing between $s_\pm$ and $d_{x^2-y^2}$ wave pairing states under action of MTG has been eliminated.

The SC ground states, in the absence of magnetic field, can be classified by finding all the invariant subgroups of the symmetry group $G \otimes U(1)$, which have a one-to-one correspondence to IURs of the symmetry group of normal state Hamiltonian. In the case of $D_{4h}$ point group symmetry, such a classification is obtained by the fact that $D_{4h}$ has three invariant subgroups of index 2, and the two dimensional cyclic group, as a subgroup of $U(1)$, compensates the phase change of OPs by $e^{i\pi}$ when the elements of coset representative acts on them. In the same manner, the ground state of a vortex structure can also be classified by finding all the invariant subgroups of symmetry group of the Hamiltonian in a magnetic field, and consequently the winding structure of the vortex core states have symmetry constraints of different classes. The topological characteristics of vortex states are location of pinning center, phase distribution of GTOPs, and winding number. It turns out that the vortex states, as a structural vanishing region with a nontrivial winding feature defined on GTOPs parameter space, always pin at the center of the MUC and the winding number can be calculated from the symmetry properties of GTOPs. In work of M. Ozaki et al. to work of M. Ozaki et al., winding numbers $\mathcal{W}$ of $s^*$ and $d_{x^2-y^2}$ wave pairing GTOPs have been calculated.
The irreducible hopping subsets
Here we calculate the corresponding to on-site atomic energies, hopping along $\hat{x}$ rather than single particle operator space. The derivation differs from transformation.

$\psi_0 = (e + tC_{2\pi})\tilde{C}^d \wedge L^g$

$\tilde{C}^d = \{e^{\pm i k_x}C_{4\pi}, k = 1, 2, 3, 4\}$

Note that $\tilde{C}^d$ always acts on paired field operators space rather than single particle operator space. The derivation is based on the fact that the generator of $\tilde{C}^d$, as a symmetry transformation of GTO's, leaves them invariant.

It has been reported that the electronic structure of iron-based superconductors in the vicinity of the Fermi level is dominated by $d_{xz}$, $d_{yz}$, and $d_{xy}$ orbitals from first-principle calculation, therefore it is feasible to calculate the vortex core states based on an effective three-orbital model.

Taking advantage of the 4-fold rotational symmetry, the Bloch Hamiltonian can be written as following

$$H = \sum_k \psi^d(k)M(k)\psi(k)$$

where $\psi^d(k) = [a^d_x(k), a^d_y(k), a^d_z(k)]$ and the 4-fold rotation is carried out by one of the generators of $D_4h$ group

$$C_{4\pi} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The irreducible hopping subsets (in unit: eV) corresponding to on-site atomic energies, hopping along $\hat{x}$, and $\hat{x} + \hat{y}$ directions are

$$K_0 = \text{diag}[0.00, 0.00, 0.04]$$

$$K_1 = \begin{pmatrix} 0.05 & 0.00 & -0.20 \\ 0.00 & 0.01 & 0.00 \\ 0.20 & 0.00 & 0.20 \end{pmatrix}$$

$$K_2 = \begin{pmatrix} 0.02 & 0.01 & 0.10 \\ 0.01 & 0.02 & 0.10 \\ -0.01 & -0.10 & 0.20 \end{pmatrix}$$

TABLE I: Winding number of GTOPs for different pairing states. $G_{i, j} = 1, 2, 3, 4, 5, 6$ are six maximal little group. $G_{5, 6}$ differs from $G_{5, 6}$ by taking the complex conjugate of gauge transformation.

Here we calculate $W$ for $s_\pm$ and $d_{xy}$ wave states and list all the results in Table I, in which

$$\begin{array}{cccc}
G_1 & G_2 & 0 & 0 \\
G_5 & G_6 & -1 & -1 \\
G_3 & G_4 & 2 & 4 \\
\end{array}$$

For simplicity, the spin indices have been dropped. Instead of going along the boundary of the irreducible BZ, an alternative path has been used to show the band structure with dominating orbital weights in Fig. (a). The projected density of states(PDOS) reveal strongly-hybridized bands which are composed of $d_{xz}$ and $d_{yz}$ orbitals along the off-diagonal line of the extend BZ below the Fermi level. The Fermi surface (Fig. (b)), obtained with a chemical potential $\mu = 0.312$ eV corresponding to a filling factor $n = 4.23$, shows four electron pockets which do not have any SC gap node in cases of pairing states belonging to $A_{1g}$ and $B_{1g}$ IURs. The absence of electron hole pockets at Gamma point is consistent with experimental observation.

The Hamiltonian can be diagonalized by conducting the Bogoliubov-Valatin transformation containing $t_{2g}$ orbital degrees of freedom as

$$a_{i\alpha\sigma} = \sum_{\gamma \neq 0} u_{\alpha \alpha}^n \gamma_{\alpha \sigma} + \bar{\sigma} v_{\alpha \alpha}^n \gamma_{\alpha \sigma}^\dagger$$

where the quasiparticle creation operator $\gamma_{\alpha \sigma}^\dagger$ is the lad-
der operator of the eigen-spectrum of the Hamiltonian which satisfies \( [H, \gamma^\dagger_{\sigma \sigma}] = \epsilon_{\sigma \sigma} \gamma^\dagger_{\sigma \sigma} \). The diagonal condition of the Hamiltonian is the BdG equation

\[
\sum_{j, \beta} \begin{pmatrix} \tilde{h}^{\dagger \dagger}_{j \beta}(i \alpha, j \beta) \\ \Delta^{*}_{j \beta}(i \alpha, j \beta) \end{pmatrix} \begin{pmatrix} u_{j \beta}^n \\ v_{j \beta}^n \end{pmatrix} = \epsilon_n \begin{pmatrix} u_{i \alpha}^{n \dagger} \\ v_{i \alpha}^{n \dagger} \end{pmatrix}
\]

(22)

where

\[
\tilde{h}_{\sigma \sigma}(i \alpha, j \beta) = \tilde{t}_{\sigma \sigma}(i \alpha, j \beta) - \mu \delta_{ij} \delta_{\alpha \beta}
\]

and the OPs defined on different orbitals are

\[
\Delta^{*}_{j \beta}(i \alpha, j \beta) = -\frac{V_{ij}(i \alpha, j \beta)}{2} \sum_{\epsilon_{n}>0, <0} u_{i \alpha}^{n \dagger} v_{j \beta}^{n} \tanh(\frac{\epsilon_n}{2k_B T})
\]

(23)

Eq. (20) and (21) give a nontrivial winding boundary condition on quasi-particle amplitudes as

\[
\begin{pmatrix} u_{i \alpha}^{n \dagger} \\ v_{i \alpha}^{n \dagger} \end{pmatrix} = \begin{pmatrix} e^{\frac{i}{2}N_{\nu}[\lambda_{x} \lambda_{y} + \frac{1}{2}(\lambda_{x} i_{y} - \lambda_{y} i_{x})]} u_{i \alpha}^{n \dagger} \\ e^{-\frac{i}{2}N_{\nu}[\lambda_{x} \lambda_{y} + \frac{1}{2}(\lambda_{y} i_{x} - \lambda_{x} i_{y})]} v_{i \alpha}^{n \dagger} \end{pmatrix}
\]

(24)

The GTOPs are calculated by BdG equation self-consistently with the above boundary condition, which is assigned to the matrix element \( \tilde{h}_{\sigma \sigma}(i \alpha, j \beta) \) and \( \Delta^{*}_{j \beta}(i \alpha, j \beta) \) for \( N_{\nu} = 1 \). The self-consistent calculation starts with an arbitrarily distributed GTOPs and the iteration is performed with a convergence criterion that the GTOPs has relative difference less that \( 10^{-3} \) between two consecutive steps. The particle density are calculated via quasi-particle wavefunctions as

\[
\langle n_{i \alpha \tau} \rangle = \frac{1}{2} \sum_{\epsilon_{n}>0, <0} |u_{i \alpha}^{n \dagger}|^2 [1 - \tanh(\frac{\epsilon_n}{2k_B T})]
\]

(25)

\[
\langle n_{i \alpha k} \rangle = \frac{1}{2} \sum_{\epsilon_{n}>0, <0} |v_{i \alpha}^{n \dagger}|^2 [1 + \tanh(\frac{\epsilon_n}{2k_B T})]
\]

(26)

The energy spectrum of the quasi-particle i.e., the LDOS at site \( i \) for orbital \( \alpha \) is calculated via

\[
\rho_{i \alpha}(\epsilon) = \frac{1}{M_x M_y} \sum_{k \in BZ} \sum_{\epsilon_{n}>0, <0} |u_{i \alpha}^{n \dagger}|^2 \delta(\epsilon - \epsilon_n(\vec{k}))
\]

\[+ |v_{i \alpha}^{n \dagger}|^2 \delta(\epsilon + \epsilon_n(\vec{k}))
\]

(27)

where the supercell method has been used for \( M_x = M_y = 10 \). The Lorentzian smearing method is used to visualize the LDOS with a broadening width \( \sigma = 0.001 \). All the self-consistent calculations are performed on a 28×28 MUCs at temperature \( T = 0.1K \).

Calculation of magnetic exchange couplings shows that the leading pairing instability comes from the intra-orbital pairing contribution, whereas the inter-orbital components are found to be significantly small. Consequently, only intra-orbital pairing potential is considered in our numerical calculation. The pairing symmetry for a multi-orbital superconductor is generally defined in momentum space as

\[
\Delta_{\sigma \beta}^{i}(\vec{k}) = g^{i}(\vec{k}) \Gamma_{\alpha \beta}(i \sigma_2)
\]

where \( g^{i}(\vec{k}) \) is basis of the IURs of \( D_{4h} \) point group, \( i \sigma_2 \) defines a tensor state for singlet pairing, and \( \Gamma_{\alpha \beta} \) is the orbital basis for \( D_{4h} \) transformation. The transformation properties of band structure determine all the symmetry transformation of SC OPs. Another reason that the inter-orbital pairing has been omitted in our calculation is that only if \( \Gamma_{\alpha \beta} \) transform according to \( A_{1g} \) representation, then symmetry of pairing state can be exclusively determined by its spatial component \( g^{i}(\vec{k}) \), such that the calculated vortex states has a classification of Table. I. For isotropic \( s \) wave pairing,

\[
V_{i \downarrow}(i \alpha, j \alpha) = -g_0 \delta_{ij}
\]

(28)

for \( s_{\pm} \) wave pairing,

\[
V_{i \downarrow}(i \alpha, j \alpha) = -\frac{g_1}{4} (\delta_{i+x,j+y} + \delta_{i-x,j-y})
\]

\[+ \delta_{i-x,j+y} + \delta_{i+x,j-y})
\]

(29)

and for \( d_{x^2-y^2} \) wave pairing,

\[
V_{i \downarrow}(i \alpha, j \alpha) = -\frac{g_2}{2} (\delta_{i+x,j+y} + \delta_{i+y,j-x})
\]

\[+ \delta_{i-x,j+y} + \delta_{i+y,j-x})
\]

(30)

where \( g_{0,1,2} \) are pairing amplitudes for each pairing symmetry. Fig. 2 shows the Fermi velocity \( \hbar v_F(\vec{k}) = \nabla_{\vec{k}} \epsilon_n(\vec{k}) \) which is used to determine the pairing potential. In order to mimic the intermediate coupling cases for FeSe and \( A_yFe_{2-x}Se_2 \) (\( A=K \), Rb, or \( Cs \)) superconductors whose coherent length \( \xi = \frac{\hbar v_F}{\pi \Delta(0)} \) ranges from 4a to 12a, the maximum pairing amplitudes are taken to be \( g_0 = 0.62 \), \( g_1 = 2.60 \), and \( g_0 = 1.28 \), respectively, which result in two
gaps SC OPs(eV) in zero-field case for different pairing symmetries with respect to three orbitals as for isotropic $s$ wave

$$|\Delta^s_{xz,yz}(0)| = 0.047; |\Delta^s_{xy}(0)| = 0.026$$

for $s_{\pm}$ wave

$$|\Delta^s_{xz,yz}(0)| = 0.048; |\Delta^s_{xy}(0)| = 0.023$$

and for $d_{x^2-y^2}$ wave

$$|\Delta^{d_{x^2-y^2}}_{xz,yz}(0)| = 0.048; |\Delta^s_{xy}(0)| = 0.025$$

where $a$ is lattice constant.

FIG. 3: (color online) Amplitudes(color mapping) and phase distribution of GTOPs for isotropic $s$ wave pairing state for $d_{xz}$ orbital (a) and (b), $d_{yz}$ orbital (c) and (d), and $d_{xy}$ orbital (e) and (f), respectively. The phase distribution of GTOPs have been mapped to a complex vector field on 2-d lattice and the length of arrows, which represent the amplitude of GTOPs, have been amplified in order to obtain enough resolution.

FIG. 4: (color online) Eigenvalues as function of indices of BdG equation at around Fermi level in the cases of isotropic $s$ wave pairing state for zero-field states, shown in green circles, and vortex states, shown in red square, respectively.

III. RESULTS AND DISCUSSION

The vortex structures for isotropic $s$ wave pairing state are shown in Fig. 3 for different orbitals, respectively. The vortex states exhibit orbital anisotropy in that for $d_{xz}$ and $d_{yz}$ orbitals the amplitudes show two plateaus with a difference about 0.005eV along $\hat{y}$ and $\hat{x}$ direction on both sides of the core region and the pinning center of these two orbitals deviates slightly from the center of MUC, while $d_{xy}$ vortex pins exactly at (14,14) site. The phase distribution show a winding number $W = 1$, such that the symmetry subgroup of such a vortex structure is $G_{\mathcal{B}2d}$. The winding structure of the $s$ wave vortex, as mapped to a complex vector field, has a sink-type core center. Fig. 4 shows the eigenvalues obtained from vortex and zero-field states, where it has been found there are 16 in-gap eigenstates for both positive and negative eigenvalues due to $SU(2)$ symmetry. We examine the behavior of the quasi-particle wavefunction $u^{\alpha\uparrow\uparrow}_{\alpha\alpha'}$ and $v^{\alpha\downarrow\uparrow}_{\alpha\alpha'}$ and it turns out that all the 32 in-gap states are extended to the entire MUC(Fig. 4, eigenstate $|e_{2353}\rangle$). The orbital anisotropy again appears as for $d_{xz}$ and $d_{yz}$ orbitals, the wavefunction extends to $\hat{x}$ and $\hat{y}$ direction because the spatial orientation of d-orbital harmonics, whereas for $d_{xy}$ orbital, the spreading of wavefunction is symmetric in $\hat{x}$ and $\hat{y}$ directions. These extended wavefunctions amount to a relatively large vortex core region and consequently large scale variation of GTOPs within the entire MUC.

The structures of $s_{\pm}$ wave vortices are shown in Fig. 5. The core regions of $d_{xz}$ and $d_{yz}$ orbital vortices are not a geometric point any more. Instead, they have been stretched along $\hat{x}$ and $\hat{y}$ directions due to the fact that although the pairing bonds are defined on adjacent N.N.N sites, the electrons forming cooper pair come from distinguishable-oriented orbitals. The symmetry sub-
group of $s_{\pm}$ wave vortices is still $G_5$, but orbital asymmetry results in a line-type topological defect for $d_{xz}$ and $d_{yz}$ orbital vortices, whereas $d_{xy}$ orbital vortex is still of sink-type. One special fact worth noting is that there is a suppression of GTOPs at corners of MUC, which also exits for pairing bond along $-\hat{x} \pm \hat{y}$ and $\hat{x} - \hat{y}$ directions. In order to understand the physical origin of this phenomena, we examine the phase variation along two loops around the vortex core at the center and corner of MUC, respectively. The loop around the corner of MUC is well-defined in order parameter space since the nontrivial winding periodic boundary condition Eq. [21] has been applied. Since the homotopy group of order parameter space of a vortex state is $\pi_1(R) = \mathbb{Z}$ and that the winding number $N_v = 1$ has been fixed when the self-consistent calculation is carried out, we expect that the variation along the loop around the corner is definitely not homotopic equivalent to that around vortex at center. Fig. 7(a) shows the phase variation around the vortex core, where the phases change slowly on a number of lattice sites at the very beginning of the loop as shown in Fig. 6(a) in the vicinity of site (25,3). We have deliberately chosen a loop far away from the core region, since a stable topological defect always leaves its signature arbitrarily away from it. However, the phase variation of GTOPs around the corner of MUC exhibits some turning-back points, from which the clockwise increments contribute negative phase winding. Therefore the total winding around the corner is zero, which proves that the suppression of GTOPs on corners of MUC is not a vortex. Detailed analysis about the phase difference on each lattice sites shows that such singularities at corners is actually caused by the discontinuity feature of boundary condition of wavefunction of each orbitals when the calculation is carried out on $N_x \times N_y$ lattice. From Eq. [21], we know that the variation of boundary condition along $\hat{y}$ direction for adjacent ($\lambda_x = 1, \lambda_y = 0$) MUC is

FIG. 5: (color online) Amplitudes and phases(color mapping) of quasi-particle wavefunctions $u_{i\alpha}^n$ and $u_{i\alpha}^n$ for isotropic $s$ wave pairing symmetry of index $n=2353$ for $d_{xz}$ orbital (a) and (b), $d_{yz}$ orbital (c) and (d), and $d_{xy}$ orbital (e) and (f), respectively.
FIG. 7: (color online) Phase mapping onto complex plane of $s_\pm$ pairing bond along $\hat{x} + \hat{y}$ direction. Loop around center of MUC is $(25,3) \rightarrow (25,25) \rightarrow (3,25) \rightarrow (3,3) \rightarrow (25,3)$ (a) and around corner of MUC is $(3,1) \rightarrow (3,3) \rightarrow (1,3) \rightarrow (28,3) \rightarrow (25,3) \rightarrow (25,1) \rightarrow (25,28) \rightarrow (25,25) \rightarrow (28,25) \rightarrow (1,25) \rightarrow (3,25) \rightarrow (3,28) \rightarrow (3,1)$. The loop direction has been shown in color mapping of each steps.

FIG. 8: (color online) Eigenvalues as function of indices of BdG equation at around Fermi level in the cases of $s_\pm$ wave pairing state for zero-field states, shown in green circles, and vortex states, shown in red square, respectively.

FIG. 9: (color online) Amplitudes and phases(color mapping) of quasi-particle wavefunctions $\psi_{n\alpha}^s$ and $\psi_{n\alpha}^d$ for $s_\pm$ wave pairing state of index $n=2353$ for $d_{xz}$ orbital (a) and (b), $d_{yz}$ orbital (c) and (d), and $d_{xy}$ orbital (e) and (f), respectively.
the wavefunction of these two orbitals transform under

$$C_{4z}|d_{xz}\rangle = |d_{yz}\rangle$$

$$C_{4z}|d_{yz}\rangle = -|d_{xz}\rangle$$

while $d_{xy}$ orbital does not mix with them under transformation. Here we give an example of numerical results of GTOPs for each orbitals on site (3,3), as shown in Table II. In zero-field case, phase difference of $e^{i\pi}$ is observed between $\pi_x$ and $\pi_y$, $\sigma_x$ and $\sigma_y$ bonds, which are defined on different orbitals, whereas in vortex state, such a phase exits along with the gauge modification induced by magnetic field. Moreover, the winding structures shown in Fig. 10 and 11 for different orbitals share this common feature for all GTOPs defined on entire MUC. For $d_{xy}$ orbitals, $G_5^{-}$ vortices which are defined on pairing bonds $\Delta_{xy}(\hat{x})$ and $\Delta_{xy}(\hat{y})$ are of sink- and source-type because of the phase difference $e^{i\pi}$ as GTOPs transform according to $B_{1g}$ IUR. In the presence of magnetic field, the sign change of $d_{x^2-y^2}$ wave pairing symmetry, along with the orbital-hybridized GTOPs together give rise to a $G_6^*$ winding structure for $d_{xz}$ and $d_{yz}$ orbitals, which seems like a solenoidal complex vector field. The phase difference of $e^{i\pi}$ in terms of GTOPs has been observed between $\Delta_{xz}(\sigma_x)$ as shown in Fig. 10 (b) and $\Delta_{yz}(\pi_y)$ as shown in Fig. 10 (h), and also between $\Delta_{xz}(\sigma_y)$ as shown in Fig. 10 (d) and $\Delta_{yz}(\pi_z)$ as shown in Fig. 10 (f). Among

FIG. 10: (color online) Amplitudes(color mapping) and phase distribution of $d_{x^2-y^2}$ wave pairing bonds for $d_{xz}$ orbital along $\hat{x}$ direction (a) and (b), $\hat{y}$ direction (c) and (d), and for $d_{yz}$ orbital along $\hat{x}$ direction (e) and (f), $\hat{y}$ direction (g) and (h), respectively. Results of pairing bonds along the other two directions of N.N. pairing are same with these results.

FIG. 11: (color online) Amplitudes(color mapping) and phase distribution of $d_{x^2-y^2}$ wave pairing bond for $d_{xy}$ orbital along $\hat{x}$ direction (a) and (b), and $\hat{y}$ direction (c) and (d), respectively. Results of paring bonds along the other two directions of N.N. pairing are same with these results.
The hole asymmetry is evidently for approaching vortex core and then away from it for each particle states between different pairing symmetries, we compare the orbital-resolved LDOS along off-diagonal line orbital for particle part. The most localized vortex bound state has three peaks for particle part and two peaks for hole part. The most localized vortex bound state has been observed for $d_{xy}$ orbital for particle part.

In order to have a understanding of distinction of vortex states between different pairing symmetries, we compare the orbital-resolved LDOS along off-diagonal line approaching vortex core and then away from it for each pairing states. Fig. 13 (a) shows results for isotropic $s$ wave, where vortices of $d_{xz}$ and $d_{yz}$ orbitals pinning at site (15,15) are characterized by symmetrically located two peaks while $d_{xy}$ orbital single peak. The two peaks start to shrink towards Fermi level from site (7,7) and then transit back to SC coherence peak at site (19,19), therefore the isotropic $s$ wave vortices have a relative large core region as compared with $s_{\pm}$ and $d_{x^2-y^2}$ vortices as shown in Fig. 13 (a), (c), and (d). Another characteristics of $s$ wave vortices is that the LDOS shows no Landau oscillation due to on-site pairing. However, since

| Zero-field SC state | Vortex state |
|--------------------|-------------|
| $\Delta_{xz}(\sigma_z)$ | (0.43, 0.43) (-0.12, 0.58) |
| $\Delta_{xz}(\pi_y)$ | (0.032, 0.032) (-0.14, 0.11) |
| $\Delta_{yz}(\pi_z)$ | (-0.032, -0.032) (-0.12, 0.34) |
| $\Delta_{yz}(\sigma_y)$ | (-0.43, -0.43) (-0.58, 0.11) |
| $\Delta_{xy}(\tilde{x})$ | (0.17, 0.17) (0.091, 0.24) |
| $\Delta_{xy}(\tilde{y})$ | (-0.17, -0.17) (-0.24, 0.096) |
FIG. 15: (color online) Orbital-resolved LDOS along off-diagonal line from site (3,3) \(\rightarrow\) (26,26). Each subfigure from left to right are LDOS for \(d_{xz}\), \(d_{yz}\), and \(d_{xy}\) orbitals in the cases of isotropic \(s\) wave (a), \(s_{\pm}\) wave (b) and (d), and \(d_{x^2-y^2}\) wave (c) pairing states, respectively. The Fermi level has been set to zero and sites in vortex region have been highlighted in red.

FIG. 16: (color online) Orbital-resolved electron density for \(d_{xz}\) and \(d_{xy}\) orbitals for \(s\) wave (a) and (b) , \(s_{\pm}\) wave (c) and (d), and \(d_{x^2-y^2}\) wave (e) and (f) vortices, respectively. Electron density for \(d_{yz}\) orbital is same as \(d_{xz}\) orbital.

The wavefunction of all the in-gap states for both positive and negative eigenstates are not localized, such vortex states may not be favored in iron-based SCs. Additionally, the particle-hole symmetry protects electron density from accumulating or losing in the vortex core region as shown in Fig. 16 (a) and (b) and consequently although the region is large than the coherent length, the chemical potential within and outside the core region are same. For \(s_{\pm}\) vortices, an oscillation phenomena of LDOS for \(d_{xy}\) orbital has been observed. As approaching the core center, the density of states exactly at the Fermi level vary alternately from zero to a finite value, and then oscillates until being stabilized at the core center. At site (13,13) and (14,14) the core states always manifest itself as double peaks, which is different from result of isotropic \(s\) and \(d_{x^2-y^2}\) wave pairing states. Such an alternating appearance of bound state at Fermi level, as a signature of charge density oscillation in the local area around vortex core, may comes from the fact that for orbital \(d_{xz}\)
and $d_{yz}$, as shown in Fig. 16 (c) there is a charge density accumulation, while for $d_{xy}$ orbitals electron density is suppressed inside the core region, as shown in Fig. 16 (d). Finally, Fig. 16 (c) shows LDOS of $d_{xz} - d_{yz}$ wave vortices. It has been found that for $d_{xz}$ and $d_{yz}$ orbitals, the vortex bound states is exactly localized at site (14,14), with stable SC coherence locates at $\pm 0.05$ eV, and for $d_{xy}$ orbital the core region includes site (13,13). Similarly to the cases of $s_{\pm}$ vortices, charge accumulation on orbitals $d_{xz}$ and $d_{yz}$ and loss on orbital $d_{xy}$ have been observed as shown in Fig. 16 (e) and (f), which indicate the signature of charged core states. However, no particle density oscillation appears in LDOS spectrum. The overlap of in-gap bound states at site (14,14) will reproduce a peak on the center of vortex if the broadening width $\sigma$ is enlarged. The LDOS of $d_{xz} - d_{yz}$ wave vortices, especially for $d_{xy}$ orbital, have a same pattern with STM observation done by C. L. Song et al. (Fig. 2 C and D).

We have noted that the self-consistent calculation gives different winding structures of vortex states with respect to different pairing symmetries. However, isotropic $s$ and $s_{\pm}$ wave vortices, share a common winding structure, which is characterized by a sink-type core state as shown in Fig. 3 and 4. But in the case of $d_{xz} - d_{yz}$ wave pairing, vortices contributed from $d_{xz}$ and $d_{yz}$ orbitals show a solenoidal complex vector field distribution, and $d_{xy}$ orbital also gives a sink- and source-type winding structure along $\hat{x}$ and $\hat{y}$ directions. Topologically, all these vortices correspond homotopy group $\pi_1(R) = \mathbb{Z}(W = 1)$ as shown in Table I, and vortices of $s$ and $s_{\pm}$ pairing symmetry belong to symmetry group $G_5^{s\pm}$, and $d_{xz} - d_{yz}$ wave pairing symmetry has $d_{xz}$ and $d_{yz}$ orbital vortices belonging to $G_6^s$ group and $d_{xy}$ orbital vortices $G_5^x$. Such results reveal that the local surgery, i.e. the continuous transformation between element within same homotopic class, is actually carried out by a gauge transformation, or equivalently the co-representation transformation between $G_5^s(G_6^s)$ and $G_6^s(G_6^s)^{\pm\pm}$. Therefore, the relative phase difference between $d_{xz}$, $d_{yz}$ orbitals and $d_{xy}$ vortex in the case of $d_{xz} - d_{yz}$ wave pairing may be observed experimentally. We have assured that such a relative phase difference is an invariant by artificially changing the relative phase of $d_{xz}$, $d_{yz}$ orbitals and $d_{xy}$ orbital hoppings in band structure as

$$ t_{\alpha\beta}(i\alpha, j\beta) \rightarrow t_{\alpha\beta}(i\alpha, j\beta)e^{i\theta_{\alpha\beta}} $$

where $\theta_{\alpha\beta}$ is set as $\frac{\pi}{4}$ or $\frac{\pi}{2}$, the winding pattern of $d_{xz}$, $d_{yz}$ orbital vortices remain almost unchanged, while $d_{xy}$ orbital vortex changes obviously.

IV. SUMMARY

In summary, using a three-orbital model, we present a comprehensive investigation of single vortex core states in FeSe superconductors by means of BdG theory. The numerical results have been classified by invariant subgroups of MTG. It turns out that isotropic $s$ and $s_{\pm}$ wave pairing symmetry give rise to $G_5^s$ vortex states. $G_6^s$ vortex states are obtained for $d_{xz}$ and $d_{yz}$ orbitals due to orbital hybridization, and $G_5^x$ vortex states for $d_{xy}$ orbital in the cases of $d_{xz} - d_{yz}$ pairing. By analyzing behavior of orbital-resolved quasi-particle wavefunctions and LDOS and comparing the results with STM observation, we propose that $d_{xz} - d_{yz}$ wave vortices are most likely candidate. Further experimental verification can be made to examine the difference of charging feature between $d_{xz} - d_{yz}$ and $s_{\pm}$ wave vortices and the electron density oscillation induced by the latter. The phase difference of winding structures between hybridized $d_{xz}$, $d_{yz}$ orbitals and $d_{xy}$ orbital can also be testified as a signature of $d_{xz} - d_{yz}$ wave pairing symmetry in iron selenide superconductors.

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