Impurity Scattering Rate in Vortex Core of Sign-reversing $s$-wave Superconductors

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We investigate the impurity scattering rates for quasiparticles in vortex cores of sign-reversing $s$-wave superconductors. With use of the Born and Kramer-Pesch approximation for Andreev bound states, we show that the sign-reversed forward scatterings are dominant in vortex cores. Owing to the coherence factor in vortex cores of $\pm s$-wave superconductors, the impurity scattering rate of the Andreev bound states has a characteristic distribution at the Fermi surfaces. For comparison, the impurity scattering rates in vortex cores of $s$-wave and $d$-wave superconductors are also discussed.

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I. INTRODUCTION

The discovery of novel Fe-based superconductors has attracted considerable attention because of high superconducting transition temperature. A $\pm s$-wave pairing symmetry has been theoretically proposed as one of the candidates for the pairing symmetry in Fe-based superconductors.\textsuperscript{2,3,4,5,6,7,8,9,10,11} The $\pm s$ wave symmetry means that the symmetry of pair potentials on each Fermi surface is $s$-wave and the relative phase between them is $\pi$.

It is important for the identification of the $\pm s$-wave symmetry to detect the sign change in the pair potentials between Fermi surfaces. Generally it is difficult to detect the relative phase of the order parameters in spatially uniform systems. As a phenomenon sensitive to the relative phase, the formation of the Andreev bound states at a surface or junction has been discussed by several authors.\textsuperscript{12,13} The low energy excitations localized near vortex cores (Caroli-deGennes-Matricon mode)\textsuperscript{14} can be regarded also as Andreev bound states.\textsuperscript{15,16,17} The impurity scattering effect inside vortex cores is, therefore, expected to provide an efficient phase-sensitive tool.

The effects of the phase-sensitive impurity scattering have been studied experimentally through the quasiparticle interference (QPI) by the scanning tunneling microscopy/spectroscopy (STM/STS) in high-$T_c$ cuprates.\textsuperscript{18,19,20,21,22,23} For example, Hanaguri et al. have detected $d$-wave coherence factors by the magnetic-field dependence of the QPI patterns in Ca$_{2-x}$Na$_x$CuO$_2$Cl$_2$.\textsuperscript{22} With the use of this technique by the STM/STS, one might detect $\pm s$-wave coherence factors in the Fe-based superconductors.\textsuperscript{24}

In QPI experiments, the impurity scattering rates of quasiparticles in the absence and the presence of magnetic field are necessary to identify the pairing symmetry. When the pairing symmetry in the Fe-based superconductors is $\pm s$-wave, the energy spectrum is fully-gapped and hence the low energy excitations are exhausted by the Andreev bound states localized near vortex cores. One should consider the coherence effects of the Andreev bound states in the QPI patterns obtained by the STM/STS experiments. In earlier study,\textsuperscript{25} however, those effects have not been taken into account yet.

The impurity scattering rates of the Andreev bound states in vortex cores have been treated analytically,\textsuperscript{25,26,27,28} within the quasiclassical Eilenberger theory,\textsuperscript{29,30} for $s$-wave,\textsuperscript{25,26} and chiral $p$-wave superconductors.\textsuperscript{27,28} Those analytical results on the impurity scattering rates have been confirmed to be consistent with numerical results of self-consistent Born approximation.\textsuperscript{31,32} The analytical calculation of the Andreev bound states in vortex cores originates from Kramer and Pesch\textsuperscript{15} in pure superconductors and has been generalized to the impure case.\textsuperscript{25,26,27} We thus call the method used in Refs.\textsuperscript{26,27} the Kramer-Pesch approximation in this paper.

The quasiclassical theory is applicable to Fe-based superconductor since the band widths ($\sim$ a few eV) are much larger than the maximum of the superconducting gap ($\sim$ 10meV). The iron-based superconductors are known to be multi-band systems and have multiple Fermi surfaces.\textsuperscript{22} Assuming that the intraband pairings are dominant, one can define the quasiclassical Green functions on each band. One can then solve the equation of motion of the quasiclassical Green function near a vortex core and can obtain the analytical expression of the impurity scattering rate with the Born approximation in multi-band systems by extending the method developed in Refs.\textsuperscript{26,27}.

The aim of this paper is to study impurity effects in vortex cores of two-dimensional multi-band superconductors within the quasiclassical theory, with a particular interest in $\pm s$-wave superconductors. We obtain the impurity scattering rate $\Gamma_{kk'}$ from the initial state $k$ to the final state $k'$ by the Kramer-Pesch approximation,\textsuperscript{15,26,27} in $s$-wave and $d$-wave and $\pm s$-wave superconductors. We discuss the scattering-angle dependence of the sign-conserved and sign-reversed impurity scattering rates.

This paper is organized as follows. The Born approximation and the quasiclassical approximation for multi-band superconductors are presented in Sec. II. The generalization to multi-band superconductors is shown to...
be straightforward when we assume that the intraband pairings are dominant. The impurity self-energy in a single vortex within the Kramer-Pesch approximation is derived in Sec. III. The analytical expression of the impurity scattering rates $\Gamma_{hkk'}$ in vortex cores is derived. The results are shown in Sec. IV. We discuss the coherence effects on the scattering-angle dependence for the cases of the sign-conserved and the sign-reversed scatterings. We also calculate the $q \equiv k' - k$-dependence of the impurity scattering rate for the isotropic $s$-wave, $d$-wave and the isotropic $\pm s$-wave superconductors, respectively. The conclusion is given in Sec. V.

II. BORN APPROXIMATION AND QUASICLASSICAL APPROACH

A. Orbital representation and Band representation

Let us consider two-dimensional superconductors. We consider an $n$-orbital system which is a periodic crystal with $n$ atomic orbitals in unit cell. We introduce the Hamiltonian written as

$$H = \sum_{k,\sigma,\mu,\nu} \epsilon_{k,\mu,\nu}^c c_{k,\mu}^{\dagger} c_{k,\nu}^{\sigma} + \sum_{k,\mu,\nu} \Delta_{k,\mu,\nu} c_{k,\mu}^{\dagger} c_{-k,\nu}^{\sigma} + \text{h.c.},$$  (1)

where the operator $c_{k,\mu}^{\dagger}$ creates an electron with spin $\sigma$ and momentum $k$ on the $\mu$-th orbital. In the matrix form, this Hamiltonian is a $2n \times 2n$ matrix in Nambu and orbital spaces expressed as

$$\hat{H}^N_{\text{orb}}(k_x, k_y) = \begin{pmatrix} \hat{H}^0_{\text{orb}}(k_x, k_y) & \hat{\Delta}^0(\kappa_x, \kappa_y) \\ \hat{\Delta}^0(\kappa_x, \kappa_y) & -\hat{H}^0_{\text{orb}}(k_x, k_y) \end{pmatrix},$$  (2)

in the “orbital representation” where the basis functions are atomic orbitals in crystal unit cell. Here, $\hat{H}^0_{\text{orb}}$ is the Hamiltonian in the normal state represented as an $n \times n$ matrix in the orbital space and $\hat{\Delta}^0$ is the superconducting order parameter. From now on, the subscript “orb” indicates that matrices are represented with the orbital basis, hat $\hat{a}$ denotes an $n \times n$ matrix in the orbital space and check $\check{a}$ denotes a $2n \times 2n$ matrix composed of the $2 \times 2$ Nambu space and the $n \times n$ orbital space. The unperturbed $2n \times 2n$ Green function in the orbital representation is defined as

$$\hat{G}^0_{\text{orb}}(k_x, k_y; \omega_n) = \left[ \omega_n \mathbb{1} - \hat{H}^0_{\text{orb}}(k_x, k_y) \right]^{-1}.$$  (3)

Here, $\omega_n$ is the Fermion Matsubara frequency.

We also introduce an $n \times n$ Hamiltonian in the “band representation” defined by

$$\hat{H}^b_{\text{orb}}(k_x, k_y) \equiv \hat{P}^{-1}(k_x, k_y) \hat{H}^0_{\text{orb}}(k_x, k_y) \hat{P}(k_x, k_y),$$  (4)

$$= \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_n \end{pmatrix}.$$  (5)

Here, $\lambda_i$ $(i = 1, 2, \cdots, n)$ denotes the $i$-th largest eigenvalue. $\hat{P}$ is a unitary matrix consisting of the eigenvectors for the Hamiltonian $\hat{H}^0_{\text{orb}}(k_x, k_y)$. The $2n \times 2n$ Hamiltonian in Nambu and orbital spaces in the “band representation” is also defined by

$$\hat{H}^N_{\text{orb}}(k_x, k_y) \equiv \hat{U}^{-1}(k_x, k_y) \hat{H}^0_{\text{orb}}(k_x, k_y) \hat{U}(k_x, k_y),$$  (6)

$$\hat{U}(k_x, k_y) \equiv \begin{pmatrix} \hat{P}(k_x, k_y) & 0 \\ 0 & \hat{\bar{P}}(k_x, k_y) \end{pmatrix},$$  (7)

where

$$\hat{\bar{P}} \equiv \hat{P}^{-1} \hat{\Delta} \hat{P}. $$  (8)

The unperturbed $2n \times 2n$ Green function in the band representation is written as

$$\hat{G}^0_{\text{orb}}(k_x, k_y; i\omega_n) = \hat{U}(k_x, k_y)^{-1} \hat{G}^0_{\text{orb}}(k_x, k_y; i\omega_n) \hat{U}(k_x, k_y).$$  (9)

In general, $\hat{\Delta}$ contains off-diagonal elements, which correspond to inter-band pairings.

B. Born approximation

We consider the Green function under the influence of a lot of weak impurities. The Green function with the Born approximation in the orbital representation is written as

$$\hat{G}^\alpha_{\text{orb}}(k) = \hat{G}^0_{\text{orb}}(k) + \hat{G}^0_{\text{orb}}(k) \hat{\Sigma}^\alpha_{\text{orb}}(k) \hat{G}^0_{\text{orb}}(k),$$  (11)

where

$$\hat{\Sigma}^\alpha_{\text{orb}}(k) \equiv n_{\text{imp}} \int \frac{dk_1}{(2\pi)^2} \hat{\check{u}}(k - k_1) \hat{G}^0_{\text{orb}}(k_1) \hat{\check{u}}(k_1 - k).$$  (12)

$$\hat{\check{u}}(k) \equiv \begin{pmatrix} \hat{u}(k) & 0 \\ 0 & -\hat{u}(k) \end{pmatrix}. $$  (13)

Here, $n_{\text{imp}}$ is the concentration of impurity atoms, $\hat{u}(k)$ is the impurity potential. By substituting eq. (11) into eq. (11), the Green function in the band representation is written as

$$\hat{G}^b_{\text{orb}}(k) = \hat{G}^b_{\text{orb}}(k) + \hat{G}^b_{\text{orb}}(k) \hat{\Sigma}^b_{\text{orb}}(k) \hat{G}^b_{\text{orb}}(k),$$  (14)

where

$$\hat{\Sigma}^b_{\text{orb}}(k) \equiv n_{\text{imp}} \int \frac{dk_1}{(2\pi)^2} \hat{\check{v}}(k, k_1) \hat{G}^b_{\text{orb}}(k_1) \hat{\check{v}}(k_1, k),$$  (15)

$$\hat{\check{v}}(k, k_1) \equiv \hat{U}(k)^{-1} \hat{\check{u}}(k - k_1) \hat{U}(k_1). $$  (16)

It should be noted that the impurity potential in the band representation $\hat{\check{v}}(k, k_1)$ is a function of $k$ and $k_1$, not a function of $k - k_1$. Assuming that intraband pairings are dominant, we neglect the off-diagonal (interband) elements in $\hat{\Delta}^b$. In this case, the normal and anomalous parts of the self-energy $\hat{\Sigma}^b_{\text{orb}}(k) \Sigma^b_{\text{orb}}(k)$ are expressed as
\[
\Sigma_{ij}(\mathbf{k}) = \eta_{\text{imp}} \int \frac{d\mathbf{k}_1}{(2\pi)^2} \sum_m \hat{v}_{im}(\mathbf{k}_1, \mathbf{k}_1) \hat{G}_{0,mn}(\mathbf{k}_1) \hat{v}_{mj}(\mathbf{k}_1, \mathbf{k}),
\]
\[
\Sigma_{ij}^A(\mathbf{k}) = \eta_{\text{imp}} \int \frac{d\mathbf{k}_1}{(2\pi)^2} \sum_m \hat{v}_{im}(\mathbf{k}_1, \mathbf{k}_1) \hat{F}_{0,mn}(\mathbf{k}_1) \hat{v}_{mj}(\mathbf{k}_1, \mathbf{k}),
\]

where
\[
\hat{v}(\mathbf{k}, \mathbf{k}_1) \equiv \hat{P}(\mathbf{k})^{-1} \hat{u}(\mathbf{k} - \mathbf{k}_1) \hat{P}(\mathbf{k}_1),
\]
\[
\hat{G}_0^b = - \begin{pmatrix} G_0 & F_{\alpha} & 0 \\ 0 & G_\beta & F_{\beta} \\ -F_{\alpha} & 0 & G_\alpha \\ 0 & -F_{\beta} & G_\beta \end{pmatrix}.
\]

Here, the symbols \( i, j, m \) denote the band indices. For simplicity, we assume that the perturbed Green function \( \hat{G}_b \) is diagonal in the band space. For example, the Green function in the two-band system is written as
\[
\hat{G} = \begin{pmatrix} G_\alpha & 0 & F_{\alpha} \\ 0 & G_\beta & F_{\beta} \\ -F_{\alpha} & 0 & G_\alpha \\ 0 & -F_{\beta} & G_\beta \end{pmatrix}.
\]

In this assumption, one can regard the self-energy as diagonal with respect to the band index.

C. Quasiclassical Green functions

We assume \( |\Delta_1| \ll E_F \). This relation is satisfied in most of systems such as conventional superconductors and Fe-based ones since the band width is a few eV and the superconducting order parameter is the order of 10meV in these materials. In this case, one can use a quasiclassical approximation.

Since the Green function \( \hat{G}_{0,mn}(\mathbf{k}_1) \) is localized around Fermi wave-length on the \( m \)-th band \( k_{Fm} \), the self-energy on the \( i \)-th band \( \Sigma_i^b(\mathbf{k}) \) is written as
\[
\Sigma_i^b(\mathbf{k}) \sim \eta_{\text{imp}} \sum_m \int \frac{dS_{F,k,m}}{v_{F,k,m}} \hat{v}_{im}(\mathbf{k}, \mathbf{k}_1) \left( \int d\xi_{k,m} \hat{G}_{0,mn}(\mathbf{k}_1) \right) \hat{v}_{mi}(\mathbf{k}_1, \mathbf{k}).
\]

Here, \( \mathbf{k}_1 \) denotes the unit vector in the direction \( \mathbf{k}_1, v_{F,k,m} \) is the Fermi velocity on the \( m \)-th band and \( dS_{F,k,m} \) is the Fermi-surface area element on the \( m \)-th band. We introduce the functions written as
\[
\Delta(k_F) \equiv \sum_m \delta_{k_F, k_F^m} \Delta_m(k_F^m),
\]
\[
v(k_F, k_F^m) = \sum_m \delta_{k_F, k_F^m} \delta_{k_F^m, k_F^{m'}} \hat{v}_{mm'}(k_F, k_F^m),
\]
\[
g(k_F) = \sum_m \delta_{k_F, k_F^m} \hat{u}(k_F, k_F^m),
\]
\[
f(k_F) = \sum_m \delta_{k_F, k_F^m} \hat{u}_{mm'}(k_F^m),
\]

where \( \int d\xi_{k,m} \) shows that we take the contributions from poles close to the Fermi surface on the \( m \)-th band. With the use of the above functions, the normal and anomalous parts of the self energy are written, respectively, as
\[
\Sigma^N(k_F) = \eta_{\text{imp}} \langle v(k_F, k_{1,F}) g(k_{1,F}) v(k_{1,F}, k_F) \rangle_{FS},
\]
\[
\Sigma^A(k_F) = \eta_{\text{imp}} \langle v(k_F, k_{1,F}) f(k_{1,F}) v(k_{1,F}, k_F) \rangle_{FS},
\]

where
\[
\langle A(k_F') \rangle_{FS} = \int dS_{F,k'} A(k_F').
\]

Here we introduce the effective single-band Fermi surface as shown in Fig. 1 since the relation \( k_F^m \neq k_F^{m'} \) is always satisfied for \( m \neq m' \). Therefore, one can regard the \( n \)-band system as a single-band system omitting the band index \( m \) and be allowed to translate a \( n \times n \) matrix \( \hat{u} \) into a scalar \( u \) from now on.

In the quasiclassical approximation, the self-energy can be determined as a local value \( \Sigma(k_F, r) \). Therefore, one can calculate the self-energy by substituting \( g(\mathbf{k}_1, r) \) into Eq. 27 in inhomogeneous systems.
We introduce the quasiclassical Green function \( \tilde{g} \) defined by

\[
\tilde{g}(z, k_F, r) \equiv \left( \begin{array}{c} g \ \ f \\ -\bar{f} \ -g \end{array} \right),
\]

(30)

which is a \( 2 \times 2 \) matrix in the Nambu space and is a function of complex frequency \( z \), Fermi wave-length \( k_F \), a point \( r = r(\cos \phi, \sin \phi) \) in real space. From now on, check \( \tilde{a} \) denotes a \( 2 \times 2 \) matrix in the Nambu space. The equation of motion for \( \tilde{g} \) written as

\[
-iv_F(k_F) \cdot \nabla \tilde{g} = [\tilde{\tau}_3 - \tilde{\Delta}(r, k_F) - \tilde{\Sigma}, \tilde{g}],
\]

(31)

supplemented by the normalization condition

\[
\tilde{g}^2 = -\pi^2 1.
\]

(32)

Here, \( \tilde{\Delta} \) is given by

\[
\tilde{\Delta}(r, k_F) = \left( \begin{array}{cc} 0 & \Delta(r, k_F) \\ -\Delta^*(r, k_F) & 0 \end{array} \right),
\]

(33)

and \( \tilde{\tau}_3 \) is a Pauli matrix in Nambu space. In this paper, we consider the case where \( \tilde{g} \) is an analytic function of \( z \) in the upper half complex plane. Setting \( z = \epsilon + i\delta \) with real \( \delta \), we obtain the retarded Green function. We use a special parameterization of the quasiclassical Green function to solve the equation (31).\(^{27,36,37,38,39,40}\) The solution \( \tilde{g} \) of eq. (31) can be written as

\[
\tilde{g} = \frac{-i\pi}{1+ab} \left( \begin{array}{cc} 1 - ab & 2ia \\ -2ib & -(1 - ab) \end{array} \right).
\]

(34)

Here, \( a \) and \( b \) are the solutions of the following Riccati differential equations:

\[
v_F(k_F) \cdot \nabla a = -2(-iz + i\Sigma_{11})a -a^2(\Delta^* - \Sigma_{21}) + (\Delta + \Sigma_{12}),
\]

(35)

\[
v_F(k_F) \cdot \nabla b = +2(-iz + i\Sigma_{11})b +b^2(\Delta + \Sigma_{12}) - (\Delta^* - \Sigma_{21}).
\]

(36)

In this parameterization, the normalization condition (32) is automatically satisfied. For simplicity, we solve the Riccati differential equations under a given form of pair function.

### III. KRAMER-PESCH APPROXIMATION

We calculate the self-energy in a single vortex core with the Kramer-Pesch approximation.\(^{27,42,43}\) Since Eqs. (35) and (36) contain \( \nabla \) only through \( v_F \cdot \nabla \), they reduce to a one-dimensional problem on a straight line, the direction of which is given by that of the Fermi velocity \( v_F(k_F) \). We denote by \( \tilde{a} \) and \( \tilde{b} \) the unit vectors along the crystal axes \( X \) and \( Y \), respectively. We introduce \( s, y, r \) by

\[
r = X\tilde{a} + Y\tilde{b} = s\tilde{v} + y\tilde{u},
\]

(37)

\[
r = \sqrt{X^2 + Y^2} = \sqrt{s^2 + y^2},
\]

(38)

with

\[
\begin{pmatrix} \tilde{v} \\ \tilde{u} \end{pmatrix} \equiv \begin{pmatrix} \cos \theta_v & \sin \theta_v \\ -\sin \theta_v & \cos \theta_v \end{pmatrix} \begin{pmatrix} \tilde{a} \\ \tilde{b} \end{pmatrix}.
\]

(40)

Here, \( \theta_v \) is the angle between \( \tilde{a} \) and the Fermi velocity \( v_F(k_F) \).

In the Kramer-Pesch approximation, we expand the coefficients of Riccati equations \( a \) and \( b \) with respect to the impact parameter \( y \) and the energy \( \epsilon \). Near the vortex, the superconducting pair function in the first order with respect to \( y \) can be written as

\[
\Delta(k_F, r) = f(|s|)\Delta_0 \text{sign}(sd(k_F)) e^{i\theta_v} \left( 1 + \frac{y}{s} \right).
\]

(41)

\[
\equiv \Delta_0 + \Delta_1
\]

(42)

Here, \( f(s) \) describes the spatial variation of the modulus of the pair potential and \( f(0) = 0, \lim_{s \to \infty} f(s) = 1 \) and \( d(k_F) \) describes the variation of the pair potential in momentum space. Following Refs. 27,42, we obtain the coefficients \( a \) and \( b \):

\[
a_0 = -\text{sign}(d(k_F)) e^{i\theta_v},
\]

(43)

\[
b_0 = \text{sign}(d(k_F)) e^{-i\theta_v},
\]

(44)

\[
a_1(s) = \frac{e^{u(s)}}{|v_F(k_F)|} \int_{-\infty}^{s} ds' \left( 2ia_0(\epsilon - \Sigma) + 2iy \frac{\Delta_0}{s} \right) e^{-u(s')},
\]

(45)

\[
b_1(s) = \frac{e^{u(s)}}{|v_F(k_F)|} \int_{s}^{\infty} ds' \left( -2ib_0(\epsilon - \Sigma) + 2iy \frac{\Delta_0}{s'} \right) e^{-u(s')},
\]

(46)

with

\[
\Sigma(s, k_F) = \Sigma_{11} - \frac{i}{2} \text{sign}(d(k_F)) \left( e^{i\theta_v} \Sigma_{21} + e^{-i\theta_v} \Sigma_{12} \right).
\]

(47)

\[
u(s) = \frac{2|d(k_F)|\Delta_0}{|v_F(k_F)|} \int_{0}^{|s|} ds' \tanh(s).
\]

(48)

Here, we set \( f(s) = \tanh(s) \). At a low energy \( \epsilon \) and a small impact parameter \( y \), the Green function is written as\(^{27,42}\)-

\[
\tilde{g} \sim \frac{-2\pi i}{a_1b_0 + a_0b_1} \tilde{M},
\]

(49)

with

\[
\tilde{M} \equiv \begin{pmatrix} 1 & ia_0 \\ -ib_0 & -1 \end{pmatrix}.
\]

(50)
We obtain the impurity self-energy with the quasiparticle momentum $\mathbf{k}$ for the Kramer-Pesch approximation written as:

$$\Sigma_k = \frac{1}{C} \int_{-\infty}^{\infty} ds \tilde{\Sigma}(s) e^{-u(s)}, \quad (51)$$

since the denominator of $\tilde{g}$ can be expressed as

$$a_1 b_0 + a_0 b_1 = \frac{2 C e^{u(s)}}{|v_F(k_F)|} \left( \epsilon - 2y \frac{\xi_0 |d(k_F)|^2 \Delta_s^2}{|v_F(k_F)|} - \Sigma_k \right). \quad (52)$$

Here, $C \equiv |v_F(k_F)|/(2|d(k_F)| \Delta_{\infty})$.

Now we calculate the imaginary part of the impurity induced self-energy with the Born approximation. In pure superconductors ($\Sigma_k = 0$), the Green function near a vortex core can be written as

$$\tilde{g}_0(s, k_F, \epsilon) = \frac{\pi |v_F(k_F)| e^{-u(s')}}{C(k_F)} \left( \epsilon - E(y', k_F) - i\delta \right) \frac{1}{(\epsilon - E(y, k_F))^2 + \delta^2 M}, \quad \text{where}$$

$$E(y, k_F) = \frac{2 \xi_0 \Delta_{\infty}^2 |d(k_F)|^2}{|v_F(k_F)|}. \quad (54)$$

By substituting Eq. (53) into Eq. (27), the self-energy expressed in Eqs. (45) and (40) becomes

$$\Sigma_{ij}(s, y, k_F) = n_{\text{imp}} \left\langle v_{k_F, k_{1, F}}^* v_{k_{1, F}, k_F} \frac{\pi |v_F(k_{1, F})| e^{-u(s')}}{C(k_{1, F})} \left( \epsilon - E(y', k_{1, F}) - i\delta \right) \frac{1}{(\epsilon - E(y, k_{1, F}))^2 + \delta^2 M} \right\rangle_{\text{FS}}. \quad (55)$$

Here, we introduce the coordinates $(s'', y')$ in the direction to the momentum $k_{1, F}$:

$$y' = s \sin(\theta_v - \theta_{v'}), \quad s'' = s \cos(\theta_v - \theta_{v'}), \quad (56)$$

where $\theta_{v'}$ is the angle between $\hat{a}$ and the Fermi velocity $v_F(k_{1, F})$. With the use of the above equation and $\delta \to 0$, $\text{Im}\tilde{\Sigma}(s, k_F)$ is written as

$$\text{Im} \tilde{\Sigma}(s, y, k_F) = n_{\text{imp}} \left\langle v_{k_F, k_{1, F}}^* v_{k_{1, F}, k_F} \frac{\pi^2 |v_F(k_{1, F})| e^{-u(s'')}}{C(k_{1, F})} \delta(\epsilon - E(y', k_{1, F})) (1 - \text{sign}[d(k_F) d(k_{1, F})]) \cos(\theta_v - \theta_{v'}) \right\rangle_{\text{FS}}. \quad (58)$$

Therefore, by performing the $s'$-integration in Eq. (51), we finally obtain the imaginary part of the impurity induced self-energy:

$$\text{Im} \Sigma_k = n_{\text{imp}} \left\langle v_{k, k'} v_{k', k} (1 - \text{sign}[d(k) d(k')]) \cos(\theta_v - \theta_{v'}) \right\rangle \left( \frac{2\pi^2}{\xi_0} \frac{|d(k)|}{\sin(\theta_v - \theta_{v'})} \frac{|v_F(k')|}{|d(k')|} \frac{|v_F(k)|}{|F_{\text{FS}}(k)|} e^{-u(s_0)} e^{-u(s'_0)} \right), \quad (59)$$

with

$$s_0(k, k') = \frac{\epsilon}{\sin(\theta_v - \theta_{v'})} \left( \frac{|v_F(k')|}{2 \Delta_{\infty}^2 |d(k')|^2 \xi_0} - \frac{|v_F(k)|}{2 \Delta_{\infty}^2 |d(k)|^2 \xi_0} \cos(\theta_v - \theta_{v'}) \right), \quad (60)$$

$$s'_0(k, k') = s_0(k, k') \cos(\theta_v - \theta_{v'}) - \epsilon \frac{|v_F(k)|}{2 \Delta_{\infty}^2 |d(k)|^2 \xi_0} \sin(\theta_v - \theta_{v'}). \quad (61)$$

The impurity scattering rate for the quasiparticles from the initial state $k$ to the final state $k'$ in a vortex core $\Gamma_{k, k'}$ is given by

$$\Gamma_{k, k'}(\epsilon) = n_{\text{imp}} v_{k, k'} v_{k', k} (1 - \text{sign}[d(k) d(k')]) \cos(\theta_v - \theta_{v'}) \left( \frac{2\pi^2}{\xi_0} \frac{|d(k)|}{\sin(\theta_v - \theta_{v'})} \frac{|v_F(k')|}{|d(k')|} \frac{|v_F(k)|}{|F_{\text{FS}}(k)|} e^{-u(s_0)} e^{-u(s'_0)} \right). \quad (62)$$

Then, the coherence factor for the impurity scattering in a vortex core is described by

$$1 - \text{sign}[d(k) d(k')] \cos(\theta_v - \theta_{v'}). \quad (63)$$

The impurity scattering rate \[(62)\] mainly depends on the impurity scattering matrix $v_{k, k'} v_{k', k}$, the scattering angle $(\theta_v - \theta_{v'})$ and the sign-change of the scattering $\text{sign}[d(k) d(k')]$.

The impurity scattering rate $\Gamma_{k, k'}$ also depends on the product of the local density of states for the quasiparticle with momentum $\mathbf{k}$ and that with $\mathbf{k}'$. The local density of states can be characterized by the impact parameters for
the quasiparticles. The quasiparticles with momentum $k$ form a bound state around a vortex core. The impact parameter $y$ for these quasiparticles is defined from Eq. (54) and depends on the energy $\epsilon$ and the magnitude of the Fermi velocity $|\mathbf{v}_F(k)|$. In the isotropic $s$-wave single-band superconductors, the pattern of the local density of states around a vortex core becomes circuler since the impact parameters for various quasiparticles are same. In the fully-gapped superconductors with multiple Fermi surfaces, there are several circuler patterns of the local density of states around a vortex core. At any case, one can clearly define the trajectory for the quasiparticles forming the Andreev bound states as shown in Fig. 2. Therefore, we can discuss the impurity scattering in vortex cores, in detail.

IV. RESULTS

A. Sign-conserved scattering

We consider the case of $d(k)d(k') > 0$. In this case, the sign of the pair function does not change after the scattering. When the momentum dependence of the impurity scattering matrix $v_{k,k'}v_{k',k}$ is not so large, the scattering angle $(\theta_v - \theta_{v'})$ is important for the impurity scattering rate. The dependence of the scattering angle $(\theta_v - \theta_{v'})$ in Eq. (62) can be written as

$$\Gamma_{k,k'} \propto \frac{1 - \cos(\theta_v - \theta_{v'})}{|\sin(\theta_v - \theta_{v'})|}. \quad (64)$$

One can find that the forward scattering $(\theta_v - \theta_{v'} = 0)$ is completely suppressed since the coherence factor becomes zero:

$$\frac{1 - \cos(\theta_v - \theta_{v'})}{|\sin(\theta_v - \theta_{v'})|} \sim |\theta_v - \theta_{v'}|. \quad (65)$$

In the case of the backward scattering $(\theta_v - \theta_{v'} = \pi)$, in spite of the large coherence factor, the scattering rate is small since the point of the scattering is far from the vortex core so that the amplitude of the bound-state DOS becomes small as shown in Fig. 2(b).

B. Sign-reversed scattering

In the case of $d(k)d(k') < 0$, the dependence of the scattering angle $(\theta_v - \theta_{v'})$ in Eq. (62) can be written as

$$\Gamma_{k,k'} \propto \frac{1 + \cos(\theta_v - \theta_{v'})}{|\sin(\theta_v - \theta_{v'})|}. \quad (66)$$

In contrast with the sign-conserved scattering, the backward scattering $(\theta_v - \theta_{v'} = \pi)$ is important for the impurity scattering matrix $v_{k,k'}v_{k',k}$ since the intensity of the sign-reversed forward scatterings hardly occur in single-band superconductors because quasiparticles close to each other in momentum space feel the same sign of the pair function. In multiband superconductors with electron and hole circular-like Fermi surfaces such as Fe-based materials, the interband scatterings can become the sign-reversed forward scatterings. The $q$-dependence of the impurity scattering rate is anomalous in sign-reversing $s$-wave superconductors since the intensity of the sign-reversed forward scatterings is much larger than that of all other scatterings. Here, $q$ denotes the difference of the quasiparticle’s momentum $q \equiv k' - k$.

C. Numerical result

We show the $q$-dependence of the impurity scattering rate $\Gamma_{k,k+q}$ in the two-band superconductors as a simplified model for Fe-based superconductors. We consider the system with two hole Fermi surfaces and two electron Fermi surfaces as shown in Fig. 3 since Fe-based superconductors have the multiple Fermi surfaces. We rotate crystal axes by $45^\circ$. The hole Fermi surface $\alpha_1$ ($\alpha_2$) is located around $(k_x, k_y) = (0, 0)$ with the diameter $1.2/\sqrt{2}$, $0.6/\sqrt{2}$ and the electron Fermi surface $\beta_1$ ($\beta_2$) is located around $(k_x, k_y) = (\pi/\sqrt{2}, \pi/\sqrt{2})$, $(k_x, k_y) = (-\pi/\sqrt{2}, \pi/\sqrt{2})$ with the diameter $0.8/\sqrt{2}$. For simplicity, the amplitude of the Fermi velocity is isotropic in momentum space $|\mathbf{v}_F(k)| = 1$ and we set the impurity scattering matrix $v_{k,k'}v_{k',k}$ by its average ($v_{k,k'}v_{k',k} = 1$). We consider various superconducting
FIG. 3: (Color online) Two hole Fermi surfaces $\alpha_1, \alpha_2$ and
two electron Fermi surfaces $\beta_1, \beta_2$. The dashed (blue) square
denotes the first Brillouin zone.

FIG. 4: (Color online) Schematic figures of the sign of the
pair functions for (a):d-wave and (b):$\pm s$-wave symmetries.

pairing symmetries; the isotropic s-wave $d(k) = 1$, the
d-wave $d(k) = 2k_xk_y/(k_x^2 + k_y^2)$ and the isotropic $\pm s$ wave
$d(k) = -1$ for $\alpha$ bands and $d(k) = 1$ for $\beta$ bands.

First, we consider the isotropic $s$-wave superconductivity.
In this case, all scatterings are sign-conserved scatterings.
As shown in Fig. 5, the impurity scattering rate is finite everywhere in $q$-space. This result is consistent with the result in Sec. IV. (A).

Next, we consider the $d$-wave superconductivity as shown in Fig. 4(a). In this case, the scatterings between $\beta_1$ and $\beta_2$ Fermi surfaces are dominant since some of these scatterings are the sign-reversed forward scatterings. More specifically, the scattering from $(k_x, k_y) = (-\pi + 0.8, \pi)/\sqrt{2}$ ($\theta_v = 0$) on the $\beta_2$ Fermi surface to $(k_x, k_y) = (-\pi + 0.8, -\pi)/\sqrt{2}$ ($\theta_v = 0$) on the $\beta_1$ Fermi surface is the sign-reversed forward scattering as shown in Fig. 4(a). Here, we define the scatterings satisfying the relation $v \sim v'$ as the forward scatterings. From Eq. (66), one see that the impurity scattering rate diverges for this scattering. It should be noted that the condition for these sign-reversed forward scatterings to exist is sensitive to the shape of the Fermi surface and/or the direction of the Fermi velocity in the $d$-wave superconductors.

Finally, we consider the isotropic $\pm s$-wave supercon-
ductivity as shown in Fig. 4(b). In this case, the interband scatterings are dominant. As shown in Fig. 4 there are the arc-like strong intensity distributions in $q$-space. These intensity distributions are caused by the sign-reversed forward scatterings from the arc-like regions on the $\alpha_1$ or $\alpha_2$ Fermi surfaces to those on the $\beta_1$ or $\beta_2$ Fermi surfaces. The regions where the sign-reversed...
forward scatterings occur for the ±s-wave superconductors are broader than those for the d-wave superconductors. These properties are robust since the ±s-wave superconductors always have two or more Fermi surfaces. As shown in Eq. (60), one of the most important factors for the sign-reversed scatterings is the relation of the directions of the Fermi velocity of the quasiparticles before and after scatterings. In the systems with electron and hole Fermi surfaces such as Fe-based superconductors, the more the shapes of Fermi surfaces become similar to each other, the regions of the strong intensity become broader in q-space.

One can easily extend our formulation into three-dimensional systems with use of the Fermi velocities projected on the plane perpendicular to a vortex. The Riccati equations (65)(66) for three-dimensional system turn into the same form as that for two-dimensional system because of a translational symmetry along the direction of the vortex.

Our numerical results do not change qualitatively even when the gap-amplitudes on each Fermi surface are different or anisotropic. The impurity scattering rate depends on the anisotropy of gap-amplitudes only through the ratio of the gap-amplitudes between the initial states and final states |d(k)/d(k′)| expressed in Eq. (62).

We discuss the possibility to observe the effects of the characteristic impurity scattering rate in vortex cores in ±s-wave superconductors. The impurity scattering is one of the origins of the actual measurements by the STM/STS known as the QPI effects. It should be noted that the impurity scattering rate without vortex cores has not been understood clearly since the impurity scatterings depend on not only the properties of superconductivity but also the normal-states properties (i.e., the band-structure) and the type of the impurities. The STM/STS measurements can observe these effects as the QPI effects by applying magnetic fields. The results with vortex cores are more easily to understand. If the very strong arc-like peaks are observed and the intensity near q = 0 is relatively small in the q-map of the dI/dV, this is one of the direct evidences of the ±s-wave superconductivity. These peaks become large decreasing the energy. One should find the samples where the Andreev bound states can be observed more clearly so that the intensity of the sign-reversed forward scatterings becomes much stronger.

V. CONCLUSION

We studied the impurity effects in vortex cores of various kinds of superconducting pairing symmetries. We found that the sign-reversed forward scatterings are dominant for these impurity scatterings by the Andreev bound states in the low energy. The ±s-wave superconductivity yields strong arc-like peaks and weak intensity near q = 0 in the q-map of the dI/dV by the STM/STS measurements. We showed that it is important for the detection of the phase sensitive effects to investigate the system with magnetic fields.

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