s- and $d_{xy}$-wave components induced around a vortex
in $d_{x^2-y^2}$-wave superconductors

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Abstract

Vortex structure of $d_{x^2-y^2}$-wave superconductors is microscopically analyzed in the framework of the quasi-classical Eilenberger equations. If the pairing interaction contains an $s$-wave ($d_{xy}$-wave) component in addition to a $d_{x^2-y^2}$-wave component, the $s$-wave ($d_{xy}$-wave) component of the order parameter is necessarily induced around a vortex in $d_{x^2-y^2}$-wave superconductors. The spatial distribution of the induced $s$-wave and $d_{xy}$-wave components is calculated. The $s$-wave component has opposite winding number around vortex near the $d_{x^2-y^2}$-vortex core and its amplitude has the shape of a four-lobe clover. The amplitude of $d_{xy}$-component has the shape of an octofoil. These are consistent with results based on the GL theory.
In the last years, a number of investigations were carried out theoretically and experimentally to identify the symmetry of pairing state in high-$T_c$ superconductors. Although precise pairing symmetry has not been determined yet, it is recognized that $d_{x^2-y^2}$-wave symmetry is most probable.\(^1\) Recently, the vortex structure of the $d$-wave superconductors attracts much attention because it may have different structure from that of conventional $s$-wave superconductors. One of the related topics is a possibility that other components of the order parameter may be induced around a vortex in $d$-wave superconductors. Based on symmetry considerations, Volovik suggested this possibility.\(^2\) In $d_{x^2-y^2}$-wave superconductors, the amplitude of $s$-wave pairing should be contained at the core region of the vortex, since the $d_{x^2-y^2}$-wave vortex has the same symmetry as that of the opposite winding $s$-wave component. Solving the tight-binding Bogoliubov-de Gennes equation self-consistently, Soininen, Kallin and Berlinsky calculated the vortex structure on a 16×16 lattice and showed that $s$-wave component with an opposite winding number is contained around the vortex core in $d_{x^2-y^2}$-wave superconductors.\(^3\) Ren, Xu and Ting derived the two components Ginzburg Landau (GL) equations for $s$- and $d$-wave superconductivity from the Gor'kov equations, and studied the mixing of the $s$-wave component near a vortex in $d$-wave superconductors.\(^4\) They suggested that the winding number of the induced $s$-wave component around the vortex is 3 far from the vortex core and $-1$ near the center of vortex, and its profile has the shape of a four-lobe clover.

According to the general consideration based on the GL theory, it is possible that the $s$-wave component is coupled with the $d$-wave component through the gradient terms. Therefore, $s$-wave component is induced wherever the $d$-wave order parameter spatially varies, such as near the vortex. The mixing due to the same mechanism also occurs near a surface of $d$-wave superconductors, where $d$-wave component decreases on approaching the surface and $s$-wave component is induced in the surface region. This surface effect was considered by Matsumoto and Shiba using the self-consistent quasi-classical Green function formalism.\(^5\) They also considered the mixing of $d_{xy}$-wave component in addition to the mixing of $s$-wave component.
The purpose of this paper is to analyze $s$- and $d_{xy}$-wave components induced around a vortex in $d_{x^2-y^2}$-wave superconductors using the quasi-classical Eilenberger equations, which can be applied at arbitrary temperatures. The quasi-classical calculations on the vortex structure were carried out for conventional $s$-wave superconductors by Pesch and Kramer, and Klein, and for pure $d_{x^2-y^2}$-wave superconductors by Schopohl and Maki, and the current authors. Here we consider the case of an isolated vortex under a magnetic field applied parallel to the $c$-axis (or $z$-axis) in the clean limit. The Fermi surface is assumed to be two-dimensional, which is appropriate to high-$T_c$ superconductors, and isotropic for simplicity. Throughout the paper, lengths and energies are measured in units of the coherence length $\xi$ and the uniform gap $\Delta_0$ at $T = 0$, respectively.

First, we solve the quasi-classical Eilenberger equations to obtain the Green functions for a given pair potential. For the $d_{x^2-y^2}$ symmetry and not too low temperatures, the pair potential may be assumed by

$$\Delta(\theta, r) = \bar{\Delta}(\theta, r)e^{i\phi},$$
$$\bar{\Delta}(\theta, r) = \Delta(T) \tanh(r) \cos(2\theta),$$

where $r = \sqrt{x^2 + y^2}$ is the distance from the center of vortex line, $\theta$ is the angle of $k$-vector with the $a$-axis (or $x$-axis), and the phase $\phi$ of the pair potential around vortex center is given by $e^{i\phi} = (x + iy)/r$. The quasi-classical Green functions with the Matsubara frequency $\omega_n = (2n+1)\pi T$ are obtained by solving the Eilenberger equations, which are given as follows in the gauge where pair potential is real,

$$\begin{align*}
\{\omega_n + \frac{1}{2}\left(\partial_\parallel + i\partial_\parallel \phi\right)\} \bar{f}(\omega_n, \theta, r) &= \bar{\Delta}(\theta, r) g(\omega_n, \theta, r), \\
\{\omega_n - \frac{1}{2}\left(\partial_\parallel - i\partial_\parallel \phi\right)\} \bar{f}^\dagger(\omega_n, \theta, r) &= \bar{\Delta}(\theta, r) g(\omega_n, \theta, r),
\end{align*}$$

$$g(\omega_n, \theta, r) = \left(1 - \bar{f}(\omega_n, \theta, r) \bar{f}^\dagger(\omega_n, \theta, r)\right)^{1/2},$$

where $\text{Reg}(\omega_n, \theta, r) > 0$ and $\partial_\parallel \phi = -r_\perp/r^2$. Here, we have taken the coordinate system: $\hat{u} = \cos \theta \hat{x} + \sin \theta \hat{y}$, $\hat{v} = -\sin \theta \hat{x} + \cos \theta \hat{y}$, thus a point $r = x\hat{x} + y\hat{y}$ is denoted as $r =$.
The anomalous Green functions $\bar{f}$ and $\bar{f}^\dagger$ in Eqs. (2)-(4) are related to the usual notations $f$ and $f^\dagger$ as $f = \bar{f}e^{i\phi}$ and $f^\dagger = \bar{f}^\dagger e^{-i\phi}$.

Instead of solving Eqs. (2)-(4), it is more convenient to use the following parameterization devised by Schopohl and Maki.

$$\bar{f} = \frac{2a}{1 + \bar{a}b}, \quad \bar{f}^\dagger = \frac{2\bar{b}}{1 + \bar{a}b}. \quad (5)$$

From Eq. (4), $g$ is given by

$$g = \frac{1 - \bar{a}\bar{b}}{1 + \bar{a}b}. \quad (6)$$

Substituting Eqs. (3) and (6) into Eqs. (2) and (3), we obtain the Riccati equation for $\bar{a}$:

$$\partial_{\parallel}\bar{a}(\omega_n, \theta, \mathbf{r}) - \bar{\Delta}(\theta, \mathbf{r}) + \left\{ 2\omega_n + i\partial_{\parallel}\phi + \bar{\Delta}(\theta, \mathbf{r})\bar{a}(\omega_n, \theta, \mathbf{r}) \right\} \bar{a}(\omega_n, \theta, \mathbf{r}) = 0. \quad (7)$$

The other unknown quantity $\bar{b}$ is related to $\bar{a}$ by symmetry: $\bar{b}(r_{\parallel}) = \bar{a}(-r_{\parallel})$. Far from the vortex core, $\bar{a}$ is reduced to the value of a spatially homogeneous situation without magnetic field:

$$\bar{a}_\infty(\theta) = \sqrt{\frac{\omega_n^2 + |\bar{\Delta}|^2}{\bar{\Delta}}} - \omega_n \quad (\omega_n > 0). \quad (8)$$

To obtain the quasi-classical Green functions, we integrate Eq. (7) along the trajectory where $r_{\perp}$ is held constant, using Eq. (8) as the initial value.

Second, we calculate the pair potential from the resulting quasi-classical Green functions by the self-consistent condition

$$\bar{\Delta}(\theta, \mathbf{r}) = N_0 2\pi T \sum_{\omega_n > 0} 2\pi \int_0^{2\pi} \frac{d\theta'}{2\pi} V(\theta, \theta') \bar{f}(\omega_n, \theta', \mathbf{r}), \quad (9)$$

where $N_0$ is the density of states at the Fermi surface. The pair potential and the pairing interaction are decomposed into $s$-, $d_{x^2-y^2}$- and $d_{xy}$-wave components,

$$V(\theta, \theta') = V_s + V_{x^2-y^2} \cos(2\theta) \cos(2\theta') + V_{xy} \sin(2\theta) \sin(2\theta'), \quad (10)$$

$$\bar{\Delta}(\theta, \mathbf{r}) = \bar{\Delta}_s(\mathbf{r}) + \bar{\Delta}_{x^2-y^2}(\mathbf{r}) \cos(2\theta) + \bar{\Delta}_{xy}(\mathbf{r}) \sin(2\theta). \quad (11)$$
Substituting Eqs. (10) and (11) into Eq. (9), we obtain

$$\bar{\Delta}_s(r) = V_s N_0 2\pi T \sum_{\omega_n > 0} \int_0^{2\pi} \frac{d\theta}{2\pi} \tilde{f}(\omega_n, \theta, r),$$  \hspace{1cm} (12)$$

$$\bar{\Delta}_{x^2-y^2}(r) = V_{x^2-y^2} N_0 2\pi T \sum_{\omega_n > 0} \int_0^{2\pi} \frac{d\theta}{2\pi} \tilde{f}(\omega_n, \theta, r) \cos(2\theta),$$  \hspace{1cm} (13)$$

$$\bar{\Delta}_{xy}(r) = V_{xy} N_0 2\pi T \sum_{\omega_n > 0} \int_0^{2\pi} \frac{d\theta}{2\pi} \tilde{f}(\omega_n, \theta, r) \sin(2\theta).$$  \hspace{1cm} (14)$$

As already mentioned, at not too low temperatures, $T/T_c \geq 0.5$, the resulting profile of $\bar{\Delta}_{x^2-y^2}(r)$ calculated from Eq. (13) after solving the Eilenberger equations is almost the same as that of Eq. (1), ensuring the self-consistency in that temperature region.

As seen from Eqs. (12) and (14), the Green function $\tilde{f}$ solved under the given pair potential immediately yields the induced $s$-wave (or $d_{xy}$-wave) component. Figures 1 and 2 show the $s$-wave component $\bar{\Delta}_s(r)$ induced around a vortex in $d_{x^2-y^2}$-wave superconductors. As seen from Fig. 1, the amplitude has the shape of a four-lobe clover. Near the vortex center $|\bar{\Delta}_s| \propto r$ and far from the vortex core $|\bar{\Delta}_s| \propto r^{-2}$. As shown in Fig. 2, the term with $e^{-2i\phi}$ is dominant near the vortex center and the term with $e^{2i\phi}$ is dominant far from the vertex core. The induced $s$-wave component, therefore, can be written as

$$\Delta_s(r) = \bar{\Delta}_s(r) e^{i\phi} = \left( c_1(r) e^{-2i\phi} + c_2(r) e^{2i\phi} \right) e^{i\phi},$$  \hspace{1cm} (15)$$

where $c_1(r)$ and $c_2(r)$ are factors depending on $r$. Near the center of vortex $|c_1| > |c_2|$, and far from the vortex core $|c_1| < |c_2|$. These are consistent with the results given by Ren, Xu and Ting based on the GL theory.\textsuperscript{13} On lowering temperature, the amplitude $|\bar{\Delta}_s(r)|$ increases and the inner area where $e^{-2i\phi}$ is dominant spreads out.

Figures 3 and 4 show the $d_{xy}$-wave component $\bar{\Delta}_{xy}(r)$ induced around a vortex in $d_{x^2-y^2}$-wave superconductors. As shown in Fig. 3, the amplitude has the shape of an octofoil. Near the vortex center $|\bar{\Delta}_s| \propto r^3$ and far from the vortex core $|\bar{\Delta}_s| \propto r^{-4}$. As seen from Fig. 4, the term with $e^{-4i\phi}$ is dominant near the vortex center and the term with $e^{4i\phi}$ is dominant far from the vortex core. The induced $d_{xy}$-wave component, therefore, can be written as
\[ \Delta_{xy}(r) = \bar{\Delta}_{xy}(r)e^{i\phi} = \left( d_1(r)e^{-4i\phi} + d_2(r)e^{4i\phi}\right)e^{i\phi}, \] (16)

where \(d_1(r)\) and \(d_2(r)\) are factors depending on \(r\). Near the center of vortex \(|d_1| > |d_2|\), and far from the vortex core \(|d_1| < |d_2|\). Our results of the induced \(d_{xy}\)-component are also explained by the GL theory, if the non-local correction terms are included. As far as the gradient terms are concerned, the mixing of \(d_{x^2-y^2}\) and \(d_{xy}\)-components is absent in the usual second derivative terms and first appears in the fourth-order derivative terms.

Let us now interpret our microscopic calculations so far in terms of the GL framework for ease of the understanding. The GL equations are derived from the Gor’kov equations by the same calculation as in the case of \(s\)- and \(d_{x^2-y^2}\)-components. For \(d_{x^2-y^2}\) and \(d_{xy}\)-components which are simultaneously non-vanishing, we obtain

\[ \alpha_{xy}\Delta_{xy} - (\partial_x^2 + \partial_y^2)\Delta_{xy} - \gamma \left\{ \left( \frac{5}{8}(\partial_x^2 + \partial_y^2) + \partial_x^2\partial_y^2 \right)\Delta_{xy} + \frac{1}{2}\partial_x\partial_y(\partial_x^2 - \partial_y^2)\Delta_{x^2-y^2} \right\} + |\Delta_{xy}|^2\Delta_{xy} + \frac{2}{3}|\Delta_{x^2-y^2}|^2\Delta_{xy} + \frac{1}{3}\Delta_{x^2-y^2}\Delta_{xy}^* = 0, \] (17)

\[ - \ln\left( \frac{T_c}{T} \right) \Delta_{x^2-y^2} - (\partial_x^2 + \partial_y^2)\Delta_{x^2-y^2} - \gamma \left\{ \left( \frac{7}{8}(\partial_x^2 + \partial_y^2) - \partial_x^2\partial_y^2 \right)\Delta_{x^2-y^2} + \frac{1}{2}\partial_x\partial_y(\partial_x^2 - \partial_y^2)\Delta_{xy} \right\} + |\Delta_{x^2-y^2}|^2\Delta_{x^2-y^2} + \frac{2}{3}|\Delta_{xy}|^2\Delta_{x^2-y^2} + \frac{1}{3}\Delta_{xy}\Delta_{x^2-y^2}^* = 0 \] (18)

in the dimensionless form, where \(\gamma = 62\zeta(5)/49\zeta(3)^2\), \(\alpha_{xy} = 2\{(V_{xy}N_0)^{-1} - (V_{x^2-y^2}N_0)^{-1}\}\).

Far from the vortex core, we can assume \(\Delta_{x^2-y^2} = \Delta_{\infty}e^{i\phi}\), and the leading order terms of the GL equations (17) and (18) are written as

\[ (\alpha_{xy} + \frac{1}{3}\Delta_{\infty}^2)\Delta_{xy} + \frac{\Delta_{\infty}^2}{3}e^{2i\phi}\Delta_{xy}^* - \frac{\gamma\Delta_{\infty}}{2}\partial_x\partial_y(\partial_x^2 - \partial_y^2)e^{i\phi} = 0, \] (19)

\[ - \ln(T_c/T)\Delta_{\infty} + \Delta_{\infty}^3 = 0. \] (20)

Solving Eqs. (19) and (20), we obtain

\[ \Delta_{xy}(r) = -\frac{16i}{15\pi^4}\left( d'_1e^{-4i\phi} + d'_2e^{4i\phi}\right)e^{i\phi}, \] (21)

where \(d'_1 = d'(\alpha_{xy} + 3\Delta_{\infty}^2), d'_2 = d'(7\alpha_{xy} + 5\Delta_{\infty}^2), d' = \{(\alpha_{xy} + 2\Delta_{\infty}^2)^2 - (\frac{1}{3}\Delta_{\infty}^2)^2\}^{-1}\gamma\Delta_{\infty}\) and \(\Delta_{\infty} = \{(\ln(T_c/T))\}^{1/2}\). Since \(|d'_2| > |d'_1|\), the term with \(e^{4i\phi}\) is dominant. Near the center
of vortex, the leading order of Eqs. (17) and (18) are second and fourth order derivative terms, and the general solution of the GL equations is given as follows. For a $d_{x^2-y^2}$-wave component, $\Delta_{x^2-y^2} = (a_0 r + b_0 r^3 + O(r^5)) e^{i\phi}$, where $a_0$ and $b_0$ are constants. For a $d_{xy}$-wave component, assuming the form of Eq. (16) for $\Delta_{xy}$, we obtain $d_1 = d_0 r^3 + O(r^5)$ and $d_2 = O(r^5)$, where $d_0$ is a constant. Therefore, the term with $e^{-4i\phi}$ is dominant and $|\Delta_{xy}| \propto r^3$. These results are consistent with our quasi-classical calculations.

Our numerical results are quantitatively valid for small $|V_s/V_{x^2-y^2}|$ and $|V_{xy}/V_{x^2-y^2}|$, and for not too low temperatures. From Eqs. (12) and (14), $\bar{\Delta}_s(r)$ and $\bar{\Delta}_{xy}(r)$ are proportional to $V_s$ and $V_{xy}$, respectively. If $|V_s/V_{x^2-y^2}|, |V_{xy}/V_{x^2-y^2}| \ll 1$, $\bar{\Delta}_s(r)$ and $\bar{\Delta}_{xy}(r)$ are negligibly small. The s- and $d_{xy}$-wave components, then, do not affect $d_{x^2-y^2}$-wave superconductivity. In the case that $V_s$ or $V_{xy}$ is comparable to $V_{x^2-y^2}$, self-consistent calculations including s- and $d_{xy}$-wave components are needed. It should be noticed that at low temperatures, a self-consistent calculation for $\bar{\Delta}_{x^2-y^2}(r)$ is needed since the pair potential may deviate from Eq. (4).

A vortex in $d_{x^2-y^2}$-wave superconductors has a four-folded symmetric structure by the mixing of the s- or $d_{xy}$-wave component. However, this anisotropy clearly appears only when $V_s$ or $V_{xy}$ is comparable to $V_{x^2-y^2}$. It may not be probable that this condition is satisfied in high-$T_c$ superconductors. Lastly, we note that the cylindrical symmetry around a vortex line is spontaneously broken in $d_{x^2-y^2}$-wave superconductors even when $V_s$ and $V_{xy}$ are absent. The four-folded symmetric structure of $d_{x^2-y^2}$-wave vortex becomes clear on lowering temperature, which is confirmed by our quasi-classical calculations.

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FIGURES

FIG. 1. (a) Amplitude of the s-wave component, $|\tilde{\Delta}_s(r)|/(V_s/V_{x^2-y^2})$, induced around a vortex in $d_{x^2-y^2}$-wave superconductors at $T/T_c = 0.5$. It has the shape of a four-lobe clover. (b) The core region of (a) is focused. Near the center of vortex, $|\Delta_s| \propto r$.

FIG. 2. Phase of the induced s-wave component, $\arg \tilde{\Delta}_s(r)$. Far from the vortex core, the term with $e^{2i\phi}$ is dominant. Near the center of vortex, the term with $e^{-2i\phi}$ is dominant.

FIG. 3. (a) Amplitude of the $d_{xy}$-wave component, $|\tilde{\Delta}_{xy}(r)|/(V_{xy}/V_{x^2-y^2})$, induced around a vortex in $d_{x^2-y^2}$-wave superconductors at $T/T_c = 0.5$. It has the shape of an octofoil. (b) The core region of (a) is focused. Near the center of vortex, $|\Delta_{xy}| \propto r^3$.

FIG. 4. Phase of the induced $d_{xy}$-wave component, $\arg \tilde{\Delta}_{xy}(r)$. Far from the vortex core, the term with $e^{4i\phi}$ is dominant. Near the center of vortex, the term with $e^{-4i\phi}$ is dominant.
