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Mixing of the order parameters with \(d_{x^2-y^2}\)- and \(d_{xy}\)-wave symmetry in \(d\)-wave superconductors

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We derive the Ginzburg-Landau equation for two-dimensional \(d\)-wave superconductors with fourfold symmetry. The two \(d\)-wave components of the order parameter with \(d_{x^2-y^2}\) and \(d_{xy}\) symmetry are mixed by the component of a magnetic field perpendicular to the two-dimensional plane. The mixing of the two components causes a significant paramagnetic effect in the strong-field region.

Recently there has been a lot of controversy concerning the symmetry of the order parameter in cuprate superconductors.\(^1\) Some of the recent experiments for the superconducting state in these compounds have been interpreted in terms of \(d\)-wave symmetry.\(^2\)–\(^10\) To investigate the properties of the mixed state in cuprate superconductors phenomenological theories based on the Ginzburg-Landau (GL) approach have been developed for two-dimensional (2D) \(d\)-wave superconductors with four-fold symmetry.\(^11\)–\(^15\) Most of the theories proposed so far assume the order parameter having dominantly \(d_{x^2-y^2}\)-wave symmetry and mixing with the \(s\)-wave component in the mixed state. The possibility that the two \(d\)-wave components \((d_{x^2-y^2} \text{ and } d_{xy})\) are mixed under a magnetic field has not yet been fully considered. In a previous paper\(^16\) we showed that the mixing between the two \(d\)-wave components cause a significant paramagnetic effect in the strong-field region and brings about an anomalous enhancement of the upper critical field. In this paper we examine the derivation of the GL equation in 2D \(d\)-wave superconductors and show that the order parameter with \(d_{x^2-y^2}\)-wave symmetry can mix with the component with \(d_{xy}\)-wave symmetry in the presence of a magnetic field.

In 2D \(d\)-wave superconductors with fourfold symmetry about the \(z\) axis the gap function is expanded in terms of the basis functions having \(d_{x^2-y^2}\) and \(d_{xy}\)-wave symmetry as

\[
\Delta_k = \eta^{(+)\dagger}(\hat{k}^2 - \hat{k}^2_z) + 2i \eta^{(-)} \hat{k}_x \hat{k}_y ,
\]

where \(\hat{k}_x = \cos \theta_k\) and \(\hat{k}_y = \sin \theta_k\), and \(\eta^{(\pm)}\) is the complex amplitude (note \(i^2 = -1\)). The amplitude \(\eta^{(\pm)}\) may be considered as the order parameters of the superconducting state with \(d\)-wave symmetry. Then the order parameter in such a system generally has two components corresponding to \(d_{x^2-y^2}\) and \(d_{xy}\)-wave symmetry parts. Let \(\eta^{(\pm)}(\mathbf{R})\) and \(\eta^{(-)}(\mathbf{R})\) be the GL order parameters with \(d_{x^2-y^2}\) and \(d_{xy}\)-wave symmetry, depending on the spatial variable \(\mathbf{R}\). In the previous paper\(^16\) we pointed out from symmetry considerations that the GL free energy is allowed to include the mixing term

\[
\gamma_p [\eta^{(+)}(\mathbf{R})^\ast \eta^{(-)}(\mathbf{R}) + \eta^{(+)}(\mathbf{R}) \eta^{(-)}(\mathbf{R})^\ast] B_4(\mathbf{R}) , \tag{2}
\]

between the order parameters with \(d_{x^2-y^2}\) and \(d_{xy}\)-wave symmetry in the presence of a magnetic field \(\mathbf{B}\). Here, \(B_4(\mathbf{R})\) is the component of the magnetic field perpendicular to the 2D plane. This term generates a paramagnetic current of the form

\[
\frac{1}{2} \gamma_p \left[ \frac{\partial^2}{\partial y^2} \right] \left[ \eta^{(+)}(\mathbf{R})^\ast \eta^{(-)}(\mathbf{R}) + \eta^{(+)}(\mathbf{R}) \eta^{(-)}(\mathbf{R})^\ast \right] . \tag{3}
\]

It was shown that this paramagnetic current largely cancels the diamagnetic current originating from the motion of the center of mass of the Cooper pairs in the strong-field region and causes an anomalous enhancement of the upper critical field \(H_c2\) at low temperatures.\(^16\) It was demonstrated\(^16\) that the calculated results for \(H_c2\) well explain the anomalous enhancement observed both in overdoped Tl-2201 (Ref. 17) and Bi-2201 compounds.\(^18\)

In this paper we present a derivation of the mixing term given in Eq. (2) from Gorkov’s equation for a two-dimensional \(d\)-wave superconductor with fourfold symmetry. To our knowledge no one has yet derived such a term in the GL equation from Gorkov’s equation for unconventional superconductors. This term originates from the internal orbital motion of the pairing electrons under a magnetic field as shown in the following.

We start with the following Gorkov’s equation:

\[
\left[ i \omega_n - \frac{\hbar^2}{2m} \left(-i \nabla + \frac{e}{\hbar c} \mathbf{A}(\mathbf{r}) \right)^2 \right] G(\mathbf{r}, \mathbf{r}'; i \omega_n) \\
+ \int d\mathbf{x} \Delta(\mathbf{r}, \mathbf{x}) F^\dagger(\mathbf{x}, \mathbf{r}'; i \omega_n) = \delta(\mathbf{r} - \mathbf{r}') , \tag{4}
\]

\[
- i \omega_n - \frac{\hbar^2}{2m} \left(-i \nabla + \frac{e}{\hbar c} \mathbf{A}(\mathbf{r}) \right)^2 \right] F(\mathbf{r}, \mathbf{r}'; i \omega_n) \\
- \int d\mathbf{x} \Delta(\mathbf{r}, \mathbf{x}) G(\mathbf{x}, \mathbf{r}'; i \omega_n) = 0. \tag{5}
\]

Here, the bilocal gap function \(\Delta(\mathbf{r}, \mathbf{r}')\) is defined by

\[
\Delta^\ast(\mathbf{r}, \mathbf{r}') = V(\mathbf{r} - \mathbf{r}') T \sum_{\omega_n} F(\mathbf{r}, \mathbf{r}'; i \omega_n) , \tag{6}
\]

where \(V(\mathbf{r} - \mathbf{r}')\) is the interaction between electrons causing the \(d\)-wave superconductivity. In the following we investigate the linearized GL equation because the mixing term (2) leads to a linear term in the GL equation. The linearized equation for \(\Delta^\ast(\mathbf{r}, \mathbf{r}')\) is obtained from Eqs. (4)–(6) as follows:
\[ \Delta^*(r, r') = V(r - r') T \sum_{\omega_n} \int dx \int dx' \times G^N(x, r - i \omega_n) G^N(x', r'; i \omega_n) \Delta^*(x, x'). \]

where \( G^N(x, r; i \omega_n) \) is the temperature Green function in the normal state. As usual we utilize the quasiclassical approximation for \( G^N(x, r; i \omega_n) \) in the presence of a magnetic field

\[
\Delta^*(r, r') = V(r - r') T \sum_{\omega_n} \int dx \int dx' \times G^N(x, r - i \omega_n) G^N(x', r'; i \omega_n) G^N_0(x - r; i \omega_n) G^N_0(x' - r'; i \omega_n) \exp[ -i (x - r) \cdot \Pi^1(\nabla_r) - i (x' - r') \cdot \Pi^1(\nabla_{r'})] \Delta^*(r, r'),
\]

with

\[
\Pi^1(\nabla_r) = i \frac{\partial}{\partial r} - \frac{e}{\hbar c} A(r). \]

Let us now introduce the center-of-mass coordinates, \( \mathbf{R} \) and \( \mathbf{X} \), and the relative coordinates, \( \mathbf{u} \) and \( \mathbf{s} \), as

\[
\mathbf{R} = (\mathbf{r} + \mathbf{r}')/2, \quad \mathbf{X} = (\mathbf{x} + \mathbf{x}')/2
\]

\[
\mathbf{u} = \mathbf{r} - \mathbf{r}', \quad \mathbf{s} = \mathbf{x} - \mathbf{x}'.
\]

Assuming that the magnetic field is almost constant in the scale less than the size of the Cooper pairs, we approximate \( A(r) \) as

\[
A(r) = A(|\mathbf{R}|) - \frac{i}{2} (\mathbf{u} \cdot \nabla_{\mathbf{R}}) A(|\mathbf{R}|).
\]

In this approximation the differential operator in Eq. (10) is reduced to

\[
- i (x - r) \cdot \Pi^1(\nabla_r) - i (x' - r') \cdot \Pi^1(\nabla_{r'})
\]

\[
= - i (\mathbf{X} - \mathbf{R}) \cdot \hat{\Pi}^1(\nabla_{\mathbf{R}}) + (\mathbf{s} - \mathbf{u}) \cdot \nabla_{\mathbf{u}} + \frac{i e}{2 \hbar c} (\mathbf{s} - \mathbf{u})
\]

\[
\cdot [\mathbf{u} \cdot \nabla_{\mathbf{R}}] A(|\mathbf{R}|),
\]

where

\[
\hat{\Pi}^1(\nabla_{\mathbf{R}}) = i \frac{\partial}{\partial \mathbf{R}} - \frac{2 e}{\hbar c} A(\mathbf{R}).
\]

Then we have

\[
\Delta^*(\mathbf{R}, \mathbf{u}) = V(\mathbf{u}) T \sum_{\omega_n} \int d\mathbf{X} \int d\mathbf{s} \sum_p \sum_q \exp[ i (q + p) \cdot \mathbf{X} + i (q - p) \cdot \mathbf{s}/2] \frac{\exp[ -i (q + p) \cdot \mathbf{X} + i (q - p) \cdot \mathbf{s}/2]}{(\epsilon_q + i \omega_n)(\epsilon_p - i \omega_n)}
\]

\[
\times \exp \left[ - i \mathbf{X} \cdot \hat{\Pi}^1(\nabla_{\mathbf{R}}) + \mathbf{s} \cdot \nabla_{\mathbf{u}} + \frac{i e}{2 \hbar c} \mathbf{s} \cdot [\mathbf{u} \cdot \nabla_{\mathbf{R}}] A(|\mathbf{R}|) \right] \Delta^*(\mathbf{R}, \mathbf{u})
\]

\[
= V(\mathbf{u}) T \sum_{\omega_n} \int d\mathbf{X} \int d\mathbf{s} \sum_p \sum_q \exp[ i (q + p) \cdot \mathbf{X} + i (q - p) \cdot \mathbf{s}/2] \frac{\exp[ -i (q + p) \cdot \mathbf{X} + i (q - p) \cdot \mathbf{s}/2]}{(\epsilon_q + i \omega_n)(\epsilon_p - i \omega_n)}
\]

\[
\times \exp \left[ - i \mathbf{X} \cdot \hat{\Pi}^1(\nabla_{\mathbf{R}}) + \frac{i e}{2 \hbar c} \mathbf{s} \cdot [\mathbf{u} \cdot \nabla_{\mathbf{R}}] A(|\mathbf{R}|) \right] \exp \left[ - \frac{i e}{4 \hbar c} \mathbf{s} \cdot [\mathbf{s} \cdot \nabla_{\mathbf{R}}] A(|\mathbf{R}|) \right] \Delta^*(\mathbf{R}, \mathbf{u} + \mathbf{s}).
\]

In deriving the last expression in Eq. (17) we used the formula

\[
\exp(\hat{A} + \hat{B}) = \exp \hat{A} \exp \hat{B} \exp(-[\hat{A}, \hat{B}]/2)
\]

and the relation

\[
\exp([\mathbf{s} \cdot \nabla_{\mathbf{u}}] \Delta^*(\mathbf{R}, \mathbf{u}) = \Delta^*(\mathbf{R}, \mathbf{u} + \mathbf{s}).
\]
Assuming the slow spatial variation, we expand the exponential operator to the second order in \( \hat{\nabla}_R \) and to the first order in \( \nabla \mathbf{A}(\mathbf{R}) \),

\[
\Delta^\ast(\mathbf{R}, \mathbf{u}) = V(\mathbf{u}) T \sum_{\alpha_n} \int d\mathbf{X} \int ds \sum_{\mathbf{p}} \sum_q \frac{\exp[i(\mathbf{q} + \mathbf{p}) \cdot \mathbf{X} + i(\mathbf{q} - \mathbf{p}) \cdot \mathbf{s}/2]}{\left( \epsilon_\mathbf{q} + i \omega_n \right) \left( \epsilon_\mathbf{p} - i \omega_n \right)} \times \left[ 1 - [\mathbf{X} \cdot \hat{\nabla}_R(\mathbf{V}_R)]^2 + \frac{ie}{2hc} \mathbf{s} \cdot [\mathbf{u} \cdot \hat{\nabla}_R] \mathbf{A}(\mathbf{R}) - \frac{ie}{4hc} \mathbf{s} \cdot [\mathbf{s} \cdot \hat{\nabla}_R] \mathbf{A}(\mathbf{R}) \right] \Delta^\ast(\mathbf{R}, \mathbf{u} + \mathbf{s}). \tag{20}
\]

Let us now introduce the Fourier transformations for the relative coordinates,

\[
\Delta(\mathbf{R}, \mathbf{u}) = \sum_k \Delta(\mathbf{R}, \mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{u}), \tag{21}
\]

\[
V(\mathbf{u}) = \sum_k V(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{u}). \tag{22}
\]

Substituting Eqs. (21) and (22) into Eq. (20), we obtain

\[
\Delta^\ast(\mathbf{R}, \mathbf{k}) = \sum_k V(\mathbf{k} - \mathbf{k}') T \sum_{\alpha_n} \left( \frac{1}{\epsilon_{\mathbf{k}'}^n + \omega_n^2} \Delta^\ast(\mathbf{R}, \mathbf{k}') + \sum_k V(\mathbf{k} - \mathbf{k}') T \sum_{\alpha_n} \left( \frac{1}{2m} \frac{\epsilon_{\mathbf{k}'}^n}{(\epsilon_{\mathbf{k}'}^n + \omega_n^2)^2} \hat{\nabla}_R^2(\mathbf{V}_R)^2 \right) \right) \Delta^\ast(\mathbf{R}, \mathbf{k}) \right.
\]

\[
- \sum_k T \sum_{\alpha_n} \frac{\epsilon_{\mathbf{k}'}^n}{(\epsilon_{\mathbf{k}'}^n + \omega_n^2)^2} \left[ \frac{i}{2m} \sum_{\mathbf{k}''} V(\mathbf{k} - \mathbf{k}'') T \sum_{\alpha_n} \left( \frac{1}{\epsilon_{\mathbf{k}''}^n + \omega_n^2} \Delta^\ast(\mathbf{R}, \mathbf{k}'') \right) \right] \Delta^\ast(\mathbf{R}, \mathbf{k}'). \tag{23}
\]

Since the system is assumed to have fourfold symmetry about the \( z \) axis, the terms proportional to \( k_x'k_y' \) in the integrand vanish after the integration by \( \mathbf{k}' \). Then Eq. (23) is simplified in the Coulomb gauge, \( \nabla \mathbf{A}(\mathbf{R}) = 0 \), as

\[
\sum_k \left[ \epsilon_{\mathbf{k}'}^n \Delta^\ast(\mathbf{R}, \mathbf{k}') \right] T \sum_{\alpha_n} \left( \frac{1}{\epsilon_{\mathbf{k}'}^n + \omega_n^2} \Delta^\ast(\mathbf{R}, \mathbf{k}') \right) = \sum_k V(\mathbf{k} - \mathbf{k}') T \sum_{\alpha_n} \left( \frac{1}{2m} \frac{\epsilon_{\mathbf{k}'}^n}{(\epsilon_{\mathbf{k}'}^n + \omega_n^2)^2} \hat{\nabla}_R^2(\mathbf{V}_R)^2 \right) \Delta^\ast(\mathbf{R}, \mathbf{k}') \right.
\]

\[
- \sum_k T \sum_{\alpha_n} \frac{\epsilon_{\mathbf{k}'}^n}{(\epsilon_{\mathbf{k}'}^n + \omega_n^2)^2} \left[ \frac{k_y'}{m} \left( \frac{\partial A_y(\mathbf{R})}{\partial R_y} \right) \right] \Delta^\ast(\mathbf{R}, \mathbf{k}'). \tag{24}
\]

Note that the last term on the right-hand side of the above equation is a term that has not yet been considered in previous works.\(^{11,12,14}\)

To proceed with the calculation, we expand the interaction, \( V(\mathbf{k} - \mathbf{k}') \), in terms of the powers of \( \hat{k}_x \) and \( \hat{k}_y \) in the following form with fourfold symmetry:

\[
V(\mathbf{k} - \mathbf{k}') = V_0 + V_1(\hat{k}_x\hat{k}_y' + \hat{k}_y\hat{k}_x') + V_2^+((\hat{k}_x^2 - \hat{k}_y^2)(\hat{k}_y^2 - \hat{k}_x^2))
\]

\[
+ 4 V_2^-\hat{k}_x\hat{k}_y\hat{k}_x'\hat{k}_y'. \tag{25}
\]

In the case where a pure \( d \)-wave symmetry state, \( \eta^+(\mathbf{R}) \) or \( \eta^-\mathbf{(R)} \), is realized, the term with the coefficient \( V_2^+ \) or \( V_2^- \) is the dominant interaction causing the superconductivity. However, we include the bilinear term \( V^{(1)}(\mathbf{k} - \mathbf{k}') \)

\[
= V_1(\hat{k}_x\hat{k}_y' + \hat{k}_y\hat{k}_x') \] in Eq. (25). As seen later, this term causes the mixing between the two \( d \)-wave symmetry states in the presence of the magnetic field through the last term on the right-hand side of Eq. (24). Noting that

\[
\nabla \mathbf{k} V^{(1)}(\mathbf{k} - \mathbf{k}') = \frac{V_1}{k_0} \left( \frac{\hat{k}_x\hat{k}_y' - \hat{k}_y\hat{k}_x'}{\hat{k}_x^2 - \hat{k}_y^2} \right), \tag{26}
\]

we can rewrite the last term on the right-hand side of Eq. (24) as follows:
where \( N(e) \) is the density of states. Performing the summation by \( k' \) in Eq. (24) and projecting it on the basis functions, \((k_x' - k_x)\) and \(k_y'\), we find the following coupled equations for the order parameters, \( \eta^+(R) \) and \( \eta^-(R) \):

\[
\begin{align*}
\frac{1}{2} V_2 N(0) \ln \frac{2 \gamma h \omega_D}{\pi T} & \eta^+(R) \\
& - \frac{21 \zeta(3)}{128 \pi^2 T^2} V_2 N(0) \hat{I} \hat{I} (\nabla_R)^2 \eta^+(R) \\
& + \frac{V_1}{8 mk_F} \int_{-\omega_D}^{\omega_D} d\epsilon \frac{dN(e)}{de} \frac{1}{2\epsilon} \tan\left(\frac{\epsilon}{2T}\right) \eta^-(R) \\
& \times (R) \ast B_z(R),
\end{align*}
\]

\[ (28) \]

\[
\begin{align*}
\frac{1}{2} V_2 N(0) \ln \frac{2 \gamma h \omega_D}{\pi T} & \eta^-(R) \\
& - \frac{21 \zeta(3)}{128 \pi^2 T^2} V_2 N(0) \hat{I} \hat{I} (\nabla_R)^2 \eta^-(R) \\
& + \frac{V_1}{8 mk_F} \int_{-\omega_D}^{\omega_D} d\epsilon \frac{dN(e)}{de} \frac{1}{2\epsilon} \tan\left(\frac{\epsilon}{2T}\right) \eta^+(R) \\
& \times (R) \ast B_z(R),
\end{align*}
\]

\[ (29) \]

where \( B_z = (\partial A_x/\partial R_x - \partial A_y/\partial R_y), \) \( \omega_D \) is the cutoff energy, \( \gamma \) and \( \zeta(n) \) are, respectively, the Euler number and the \( \zeta \) function. The last terms on the right-hand sides of Eqs. (28) and (29) indicate that the GL free energy should contain a term of the form

\[
\gamma_p (\eta^+(R) \ast \eta^-(R) + \eta^+(R) \eta^-(R) \ast B_z(R),
\]

\[ (30) \]

where

\[
\gamma_p = \frac{V_1}{8 mk_F} \int_{-\omega_D}^{\omega_D} d\epsilon \frac{dN(e)}{de} \frac{1}{2\epsilon} \tan\left(\frac{\epsilon}{2T}\right). \]

\[ (31) \]

It is thus concluded that the order parameters with \( d_{x^2-y^2} \) and \( d_{xy} \)-wave symmetry are mixed under a magnetic field perpendicular to the 2D plane. As seen from the above derivation, the mixing term has its origin in the freedom of the relative motion of the pairing electrons. To understand the origin we introduce the transformation, \( \eta^{\pm}(R) \rightarrow \eta_{\mp}(R) \), defined by

\[
\begin{align*}
\eta^+(R) &= \eta_2(R) + \eta_{-2}(R) \\
\eta^-(R) &= \eta_2(R) - \eta_{-2}(R),
\end{align*}
\]

\[ (32) \]

Note that the gap function defined in Eq. (1) is rewritten in terms of these new parameters as

\[
\Delta(R, k) = \eta_2(R) \exp(2i \theta_k) + \eta_{-2}(R) \exp(-2i \theta_k),
\]

\[ (33) \]

Thus the parameters, \( \eta_{\pm}(R) \), are understood to be the order parameters corresponding to the states with orbital angular momentum \( L_z = \pm 2 \). The mixing term in Eq. (30) is then expressed as

\[
\gamma_p (|\eta_2(R)|^2 - |\eta_{-2}(R)|^2) B_z(R),
\]

\[ (34) \]

indicating that the magnetic field stabilizes the state with orbital angular momentum \( L_z = 2 \) \( (\gamma_p < 0) \). From these observations one may conclude that the mixing term arises from the “orbital Zeeman effect” for the pairing electrons with finite orbital angular momentum.

Since the coefficient \( \gamma_p \) contains a factor \( dN(e)/de \), the mixing term is expected to play an important role in a \( d \)-wave superconductor with a narrow band. The upper critical field \( H_c2 \) is calculated in the presence of the mixing term as

\[
H_{c2} = \frac{\phi_0}{2 \pi \xi^{+1}(T)^2} \frac{1}{2(1 - \nu_p)} \left[ 1 - \left( \frac{\xi^{+1}(T)}{\xi^{-1}(T)} \right)^2 \right] \pm \sqrt{\left[ 1 + \left( \frac{\xi^{+1}(T)}{\xi^{-1}(T)} \right)^2 \right] - 4 \nu_p \left( \frac{\xi^{+1}(T)}{\xi^{-1}(T)} \right)^2}
\]

\[ (35) \]

for \( \nu_p \neq 1 \) and

\[
H_{c2} = \frac{\phi_0}{2 \pi \xi^{+12}(T)[1 - (\xi^{+1}(T)/(\xi^{-1}(T))]}
\]

\[ (36) \]

for \( \nu_p = 1 \), where \( \xi^{+1}(T) [\xi^{-1}(T)] \) is the coherence length of the state with \( d_{x^2-y^2} (d_{xy}) \)-wave symmetry, \( \nu_p \) is a constant proportional to \( \gamma_p^2 \) and \( \phi_0 \) is the unit flux \( (hc/2e) \). As seen in
the above equations an anomalous enhancement appears in the temperature dependence of $H_{c2}$ when $\xi^{d+1}(T) \sim \xi^{d+1}(T)$ in the case of $\nu_p \sim 1$. As discussed in the previous paper the enhancement arises from the cancellation of the increase in the kinetic energy under a magnetic field by the paramagnetic energy originating from the internal orbital motion of the pairing electrons.

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