Impurity Effects on the Nodal Structure of Anisotropic Superconductors

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For anisotropic superconductors, the gap function belongs to an irreducible representation of the point group of crystals, which determines the nodal structure of the gap function. Impurity effects on anisotropic superconductors have been treated by the Born or T-matrix approximation by which only a partial sum of the perturbation series is calculated. Instead, we take into account all terms of the perturbation series. As a result, we find that the introduction of nonmagnetic impurities does not change the nodal structure in all cases. We also find how to obtain nodes of the gap function and show the list for $O_h$, $D_{4h}$, and $D_{4h}$.

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I. INTRODUCTION

Measurements of direction dependent specific heat and direction dependent thermal conductivity have enabled us to investigate concrete nodal structures of anisotropic superconductors. For anisotropic superconductors, the gap function is considered to belong to an irreducible representation of the point group of crystals, which determines the nodal structure of the gap function [1-3]. The nodal structure of the gap function has strong influence on low temperature behaviors of physical quantities, for example, specific heat and NMR relaxation rate, which are called the power-laws. Thus, from qualitative point of view, it is more important to investigate nodal structures than to calculate concrete values. Furthermore, since what an irreducible representation the gap function belongs to has close connection with pairing interaction, its identification is crucial for understanding the pairing mechanism.

For conventional s-wave superconductors, low-temperature behaviors are insensitive to small concentrations of nonmagnetic impurities (Anderson’s Theorem) [4]. However, it is not the case with anisotropic superconductors. Particularly, for gaps with line nodes, density of states (DOS) at the Fermi energy is shifted to nonzero value, and therefore low temperature behaviors are modified by arbitrarily small impurity concentrations [5-7]. Thus, impurity effects play an important roll to identify the representation of the gap function.

In this paper, we deal with nonmagnetic impurity effects for anisotropic superconductors. We assume that the gap function as an order parameter is obtained by the generalized Ginzburg-Landau theory (GL). Previously, the correction of self-energy part in the Dyson equation (Gor’kov equation) due to impurities has been treated by the Born or T-matrix approximation. Instead, we take into account all terms of perturbation series of self-energy part, not as an approximation. We prove that the introduction of nonmagnetic impurities does not change the representation of the gap function in section IV. We also show how to obtain nodes of the gap function and show the list for $O_h$, $D_{4h}$, and $D_{4h}$ in appendixes.

II. MODEL

We consider a mean field approximated Hamiltonian which includes nonmagnetic impurity term,

$$H = \sum_{k,s} \epsilon(k) a_{k,s}^\dagger a_{k,s} + \frac{1}{2} \sum_{k,s_1,s_2} (\Delta_{s_1,s_2}(k) a_{k,s_1}^\dagger a_{-k,s_2}^\dagger - \Delta_{s_1,s_2}^*(k) a_{k,s_1} a_{-k,s_2}) + \frac{1}{V} \sum_{k,k',s} V(k - k') \delta \rho(k - k') a_{k,s}^\dagger a_{k',s},$$

(1)

where

$$\Delta_{s,s'}(k) \equiv - \sum_{k_1,k_2} V_{s_1,s_2,s_3}(k,k') (a_{k_1,s_1} a_{-k_2,s_2}).$$

(2)

Here, $k$ is a wave number of electrons, $s$ is pseudospin of electrons, $\epsilon(k)$ is the band energy, $V_{s_1,s_2,s_3}(k,k')$ is an effective electron-electron interaction, $V$ is volume of the system, and $a_{k,s}^\dagger$ ($a_{k,s}$) are annihilation (creation) operators. $\Delta_{s,s'}(k)$ is the gap function. The last term is nonmagnetic impurity term [8]. By $\langle \cdots \rangle$ we mean not only expectation value at temperature $T$, but also disorder-averaging.

Then, equations which temperature Green’s functions satisfy (Gor’kov equation) are

$$\hat{G}(k, i\omega_n) = \hat{G}_0(k, i\omega_n) - \hat{G}_0(k, i\omega_n) \Sigma^{(1)}(k, i\omega_n) \hat{G}(k, i\omega_n)$$

(3)

$$\hat{G}_0(k, i\omega_n) \Sigma^{(2)}(k, i\omega_n) \hat{F}(k, -i\omega_n)^\dagger,$$

$$\hat{F}(k, -i\omega_n)^\dagger = - \hat{G}_0(-k, i\omega_n)^\dagger \Sigma^{(2)}(-k, i\omega_n) \hat{G}(k, i\omega_n)$$

(4)

$$- \hat{G}_0(-k, i\omega_n)^\dagger \Sigma^{(1)}(-k, i\omega_n) \hat{F}(k, -i\omega_n)^\dagger,$$

where $\hat{G}(k, i\omega_n)$ and $\hat{F}(k, i\omega_n)$ are normal and anomalous temperature Green’s functions of matrix form respectively (subscript “0” means that for free fermion system), $\omega_n$ is the Matsubara frequency, and $\Sigma^{(1)}(k, i\omega_n)$ and $\Sigma^{(2)}(k, i\omega_n)$ are the proper self-energy parts.
Note that $\hat{F}(k,-i\omega_n)^\dagger$ is not merely complex conjugate of $\hat{F}(k,-i\omega_n)$, but hermitian conjugate of $\hat{F}(k,-i\omega_n)$ which differs from that in the appendix of ref. 8. Throughout this paper, we take an appropriate regularization if needed.

III. PROPERTIES OF THE GAP FUNCTION OF CLEAN SUPERCONDUCTORS

If temperature $T$ is very close to a transition point $T_c$, the gap equation becomes a linear equation. Therefore while $T$ is close enough to $T_c$, the gap function is a combination of basis functions of an irreducible representation $\Gamma^\alpha$ of the group $G$ (the largest group which does not change lattice), such as

$$\hat{\Delta}(k) = \sum_i c_i \hat{\Delta}_i^\alpha(k).$$  \hfill (5)

$\hat{\Delta}_i^\alpha(k)$ is $i$-th basis of irreducible representation $\Gamma^\alpha$. These coefficients $\{c_i\}$ are determined by GL. Note that basis functions are the ones for following transformation forms faithful representation of $G$:

$$\hat{U}_R \hat{\Delta}_i^\alpha(R^{-1}k) \hat{U}_R^\dagger = \sum_j \hat{\Delta}_j^\alpha(k) D_{ij}^\alpha(R)$$  \hfill (6)

$$\hat{U}_R \equiv \exp(-i\hat{\sigma} \cdot n\theta/2)$$  \hfill (7)

$R$ is a transformation of $G$. $\hat{\sigma}$ is the Pauli’s spin matrix. $\theta$, $n$ are the rotation angle and the unit vector which represent the direction of the rotational part (in the sense of right handed screw) of the transformation $R^{-1}$. $D_{ij}^\alpha(R)$ is an (ij) component of a matrix of irreducible representation $\Gamma^\alpha$ of $G$ for $R$. Transformations for pseudospins are derived from the fact that due to spin-orbit coupling, interaction $V_{s_2s_3s_4}(k,k')$ is not invariant under rotations of wavenumbers unless we rotate pseudospins simultaneously.

We can write the gap function with $\psi(k)$ or $d(k)$ corresponding to singlet (even parity) or triplet (odd parity), as such $\Delta(k) = i\sigma_y \psi(k)$, $\tilde{\Delta}(k) = i(d(k) \cdot \sigma)\sigma_y$, respectively, where $\sigma$ and $\sigma_y$ are the Pauli’s spin matrices. By comparison with Eq.(6), we find that, instead of $\hat{\Delta}_i(k)$, we can treat $\psi(k)$ or $d(k)$ which satisfy:

singlet:

$$\psi(k) = \sum_i c_i \psi_i^\alpha(k),$$  \hfill (8)

$$\psi_i^\alpha(R^{-1}k) = \sum_j \psi_j^\alpha(k) D_{ji}^\alpha(R),$$  \hfill (9)

triplet:

$$d(k) = \sum_i c_i d_i^\alpha(k),$$  \hfill (10)

$$\tilde{R}^{-1}d_i^\alpha(R^{-1}k) = \sum_j d_j^\alpha(k) D_{ji}^\alpha(R),$$  \hfill (11)

where $\tilde{R}$ is a rotation matrix which does not have the parity transformation part of $R$. Throughout this paper, we take the basis functions $\psi_i^\alpha(k)$ and $d_i^\alpha(k)$ to be real because accidental degeneracy may not occur.

Now, the quasiparticle energy depends on $\Delta(k)$ as

singlet:

$$E_k \equiv \sqrt{\epsilon(k)^2 + \frac{1}{2} \text{tr} \hat{\Delta}(k) \hat{\Delta}(k)^\dagger} = \sqrt{\epsilon(k)^2 + |\psi(k)|^2},$$  \hfill (12)

triplet:

$$E_{k\pm} \equiv \sqrt{\epsilon(k)^2 + |d(k)|^2 \pm |q(k)|},$$  \hfill (13)

where $q(k) = id(k) \times d(k)^\ast$. $\hat{\Delta}(k)$ has zero points derived from its belonging irreducible representation (See Appendix B). The zero points make nodes of the excitation energy on the Fermi surface.

IV. SUPERCONDUCTORS IN THE PRESENCE OF NONMAGNETIC IMPURITIES

Since we can find that the quantity in the presence of nonmagnetic impurities corresponding to the gap function of clean superconductors is the proper self-energy part of anomalous type $\hat{\Sigma}^{(2)}(k, i\omega_n)$, let us consider $\hat{\Sigma}^{(2)}(k, i\omega_n)$. For convenience, we first consider a term $\hat{G}_1 \hat{F}_1 \hat{G}_1^\ast$ of perturbation series of $\hat{\Sigma}^{(2)}(k, i\omega_n)$ (See Fig. B). Note that the subscript “1” means the exact Green’s functions in the absence of impurities.
The transformation of \( \hat{\Sigma}^{(2)}(k, i\omega_n) \) such as
\[
\Sigma^{(2)}(k, \omega) \rightarrow \hat{U}_R \Sigma^{(2)}(R^{-1}k, i\omega_n) \hat{U}_R^* \]
leads to corresponding transformation of \( \hat{G}_i \hat{F}_i \hat{G}_i^* \) term included in \( \hat{\Sigma}^{(2)}(k, i\omega_n) \) as such as
\[
\begin{align*}
&n_i^2 \sum_{k_1, k_2} V(k - k_1)^2 V(k_1 - k_2)^2 \\
&\times \hat{G}_1(k - k_1 + k_2, i\omega_n) \hat{F}_1(k_2, i\omega_n) \hat{G}_1^*(-k_1, i\omega_n) \\
&\rightarrow n_i^2 \sum_{k_1, k_2} V(R^{-1}k - k_1)^2 V(k_1 - k_2)^2 \\
&\times \hat{U}_R \hat{G}_1(R^{-1}k - k_1 + k_2, i\omega_n) \\
&\times \hat{F}_1(k_2, i\omega_n) \hat{G}_1^*(-R^{-1}k_1, i\omega_n) \hat{U}_R^* \\
&= n_i^2 \sum_{k_1, k_2} V(R^{-1}(k - k_1))^2 V(R^{-1}(k_1 - k_2))^2 \\
&\times \hat{U}_R \hat{G}_1(R^{-1}(k - k_1) + k_2, i\omega_n) \hat{U}_R^* \\
&\times \hat{F}_1(R^{-1}k_2, i\omega_n) \hat{G}_1^*(-R^{-1}k_1, i\omega_n) \hat{U}_R^* \\
&\times \hat{G}_1^*(-R^{-1}k_1, i\omega_n) \hat{U}_R^*,
\end{align*}
\]
where \( n_i \) is the impurity concentration. This implies that transformation such as \( \Sigma^{(2)}(k, i\omega_n) \rightarrow \hat{U}_R \Sigma^{(2)}(R^{-1}k, i\omega_n) \hat{U}_R^* \) is equivalent to the transformation of Green’s functions in \( \Sigma^{(2)}(k, i\omega_n) \) such as
\[
\begin{align*}
\hat{G}_1(k, i\omega_n) &\rightarrow \hat{U}_R \hat{G}_1(R^{-1}k, i\omega_n) \hat{U}_R^*, \\
\hat{F}_1(k, i\omega_n) &\rightarrow \hat{U}_R \hat{F}_1(R^{-1}k, i\omega_n) \hat{U}_R^*, \\
\hat{G}_1^*(-k, i\omega_n) &\rightarrow \hat{U}_R \hat{G}_1^*(-R^{-1}k, i\omega_n) \hat{U}_R^*, \\
\hat{F}_1^*(k, -i\omega_n) &\rightarrow \hat{U}_R \hat{F}_1^*(R^{-1}k, -i\omega_n) \hat{U}_R^*.
\end{align*}
\]
Although the current example does not have \( \hat{F}_1^*(k, -i\omega_n) \), we can always treat general terms like this. The reason for this is as follows.

Combinations of adjoining two Green’s functions appearing in \( \Sigma^{(2)}(k, i\omega_n) \) are restricted as left raw below because of particle number conservation at each point.

And we can insert spin rotation matrices into two Green’s functions as right raw below. Moreover, it is always possible to transform internal wave numbers as well as \( G_1 \hat{F}_1 \hat{G}_1^* \) because internal wave numbers are merely integral variables.

\[
\begin{align*}
G_1 \hat{G}_1 &\rightarrow \hat{G}_1 \hat{U}_R^* \hat{U}_R \hat{G}_1^*, \\
G_1 \hat{F}_1 &\rightarrow \hat{G}_1 \hat{U}_R^* \hat{U}_R \hat{F}_1 \hat{G}_1^*, \\
\hat{F}_1 \hat{G}_1 &\rightarrow \hat{F}_1 \hat{U}_R^* \hat{U}_R \hat{G}_1 \hat{F}_1, \\
\hat{F}_1 \hat{F}_1 &\rightarrow \hat{F}_1 \hat{U}_R^* \hat{U}_R \hat{F}_1 \hat{F}_1.
\end{align*}
\]

Therefore examination on what irreducible representations these Green’s functions have for above transformations \( \Gamma_\beta \) will make it clear that what irreducible representations \( \Sigma^{(2)}(k, i\omega_n) \) has for above transformations for \( \Sigma^{(2)}(k, i\omega_n) \).

Here, we define \( G', \Gamma'_\beta, \) and \( D'_\beta \). By \( G' \) we mean the maximal subgroup of \( G \) where the quasiparticle energy of clean superconductor is invariant. We can find that \( G' \) is not only maximal but also the largest. Because if \( G'' \) where the excitation energy is invariant is not contained by \( G' \), the quasiparticle energy is also invariant under the subgroup which is generated from \( G' \cup G'' \), this contradicts the fact that \( G' \) is maximal. \( \Gamma'_\beta \) is an irreducible representation subspace of \( G' \).

\( D'_\beta \) is a subspace of \( \Gamma'_\beta \) generated from elements which have a form of \( \sum_i c_i \psi_i^{(\beta)} = \sum_i c_i \psi_i^{(\alpha)} \). The coefficients \( \{ c_i \} \) are determined by GL. \( \{ c_i \} \) are determined uniquely from \( \{ e_i \} \).

Let us examine what irreducible representations Green’s functions have under above assumption. In what follows, \( \Delta(k) \) is called unitary if the product \( \Delta(k) \Delta(k)^\dagger \) is proportional to the unit matrix, otherwise it is called nonunitary. Note that only triplet case can be nonunitary.

It can be proved that regardless of the absence or the presence of impurities, \( \Delta(k) \in D'_\beta \subset \Gamma'_\beta \) until level crossing (including by another bifurcation from the solution) occurs for any GL solution. In what follows, we shall consider two cases (i) and (ii) separately.

(i) In case order parameter coefficients \( \{ c_i \} \) obtained as a solution of GL are all real (complex number multiplied overall is neglected), only unitary case applies to this case.

Exact Green’s functions of clean superconductors are
\[
\begin{align*}
\hat{G}_1(k, i\omega_n) &= -\frac{i\omega_n + \epsilon(k)}{\omega_n^2 + E_k^2} \sigma_0, \\
\hat{F}_1(k, i\omega_n) &= -\frac{i\Delta(k)}{\omega_n^2 + E_k^2}.
\end{align*}
\]

Because the excitation energy of clean superconductors and the band energy satisfies \( E_k = \epsilon(k') = \epsilon(k) \).
under transformations of \( G' \) respectively, Green’s functions are transformed by \( G' \) as

\[
\hat{U}_R \hat{G}_1(R^{-1}k, i\omega_n) \hat{U}_R^\dagger = -\frac{i\omega_n + \epsilon(R^{-1}k)}{\omega_n^2 + E_k^2} \hat{U}_R \hat{\sigma}_0 \hat{U}_R^\dagger = \hat{G}_1(k, i\omega_n),
\]

\[
\hat{U}_R \hat{F}_1(R^{-1}k, i\omega_n) \hat{U}_R^T = \frac{\hat{U}_R \Delta(R^{-1}k) \hat{U}_R^T}{\omega_n^2 + E_k^2},
\]

(26)

Hence,

\[
\hat{G}_1(k, i\omega_n) \in \Gamma_1^{++},
\]

(28)

\[
\hat{F}_1(k, i\omega_n) \in D_{\beta}',
\]

(29)

Because \( \{c_i\} \) are all real,

\[
[D_{\beta}' \otimes D_{\beta}']_{AS} = 0,
\]

(30)

where \([\cdots]_{AS}\) means antisymmetric tensor product. Furthermore, since we can find that the condition which the excitation energy for unitary case is invariant under \( G' \) is equivalent to

\[
[D_{\beta}' \otimes D_{\beta}']_S \subset \Gamma_1^{++}.
\]

(31)

Therefore,

\[
D_{\beta}' \otimes D_{\beta}' = [D_{\beta}' \otimes D_{\beta}']_S + [D_{\beta}' \otimes D_{\beta}']_{AS}
\]

\[
\subset \Gamma_1^{++} + 0 = \Gamma_1^{++}.
\]

(32)

Now, the representation of each term of \( \hat{\Sigma}^{(2)}(k, i\omega_n) \) is

\[
D_{\beta}' \otimes D_{\beta}' \otimes D_{\beta}' \otimes \cdots \otimes D_{\beta}' \otimes D_{\beta}' \otimes D_{\beta}' \subset D_{\beta}'.
\]

(33)

Here, we neglect \( \hat{G}_1(k, i\omega_n) \) and \( \hat{G}_1^*(k, i\omega_n) \) since they belong to \( \Gamma_1^{++} \).

And the facts that \( \hat{F}(k, i\omega_n) \) and \( \hat{F}^\dagger(k, -i\omega_n) \) appear in turn, and the number of \( \hat{F}(k, i\omega_n) \) is always greater than \( \hat{F}^\dagger(k, -i\omega_n) \) by one are used.

Because all terms appearing in \( \hat{\Sigma}^{(2)}(k, i\omega_n) \) belong to the same \( D_{\beta}' \) as the original \( \hat{\Delta}(k) \), if equation (32) holds, \( \hat{\Sigma}^{(2)}(k, i\omega_n) \) belongs to the same \( D_{\beta}' \) as the original \( \hat{\Delta}(k) \) under \( G' \). It should be noted that in the present case, in the table in Sigrist-Ueda, \( \Gamma_{\beta}' \) are all 1D irreducible representation, hence \( D_{\beta}' = \Gamma_{\beta}' \).

(ii) Whereas, in the case of complex coefficients \( \{c_i\} \), equation (32) does not hold. Because there is no such 1D representation of \( G \), it is enough for us to prove the case of 2D and 3D.

For \( G' \), any gap function which has complex coefficients is 2D irreducible representation. Now, \([D_{\beta}' \otimes D_{\beta}']_{AS}\) is a certain 1D representation other than \( \Gamma_{\beta}' \) because of its dimension and it can be proved that it is not \( \Gamma_1^{++} \). Hence, we find

\[
[D_{\beta}' \otimes D_{\beta}']_{AS} \subset \Gamma_{1D}',
\]

(34)

where \( \Gamma_{1D}' \) is defined as a certain 1D representation other than \( \Gamma_1^{++} \) which has \([D_{\beta}' \otimes D_{\beta}']_{AS}\) as a subset. It is worth mentioning that in this case, nonunitary cases arise, and it is easy to verify that

\[
\hat{G}_1(k, i\omega_n) \in \Gamma_1^{++} + [D_{\beta}' \otimes D_{\beta}']_{AS},
\]

(35)

\[
\hat{F}_1(k, i\omega_n) \in D_{\beta}',
\]

(36)

in nonunitary cases.

In any case of (ii), i.e., unitary or nonunitary, general term of \( \hat{\Sigma}^{(2)}(k, i\omega_n) \) has the following representation:

\[
D_{\beta}' + \Gamma_{1D}' \otimes D_{\beta}'.
\]

(37)

We can find that in all cases, this is \( D_{\beta}' \), and the solution of the gap equation is not affected by the introduction of nonmagnetic impurities.

After all, in any case, we can find that \( \hat{\Sigma}^{(2)}(k, i\omega_n) \in D_{\beta}' \).

V. SUMMARY AND DISCUSSION

We proved that the introduction of nonmagnetic impurities does not change the nodal structure of anisotropic superconductors. We also show why zeros of \( \hat{\Sigma}^{(2)}(k, 0) \) are related to the nodal structure in Appendix A, how to obtain nodal structures in Appendix B and show them in the case of \( O_h \), \( D_{oh} \), and \( D_{th} \) in the table II, III, and IV of Appendix C respectively. Calculations in Appendix C and D were done by using MATHEMATICA.

Although theoretical calculations for anisotropic s-wave gaps show that the gap anisotropy is smeared out by introducing nonmagnetic impurities, and anisotropic s-wave superconductivity is therefore anticipated to exhibit experimental evidences of \( YNi_2B_2C \), it is no wonder that the nodes disappear because the nodes are not the ones as an irreducible representation.

We should pay attention to that even if nodes of gaps disappear due to impurities, we do not say anything about the amplitudes of gaps. Hence, the fact obtained in this paper does not contradict the fact that the axial-like gap (gap with point node(s)) and the polar-like gap (gap with line node(s)) are suppressed partially by introducing nonmagnetic impurities in the case of the Born approximation, and in the case of the T-matrix approximation. Especially, a theoretical calculation by Haas et al. and an experiment by Hashimoto et al. agrees with our theory, although these are too simple to be evidences.
This work is based on the prior research by Takahiro Aoyama, Masatoshi Sato, and Mahito Kohmoto. The author acknowledges them for helpful discussions.

Appendix A: The Existence of the nodes

From Gor’kov equation, we can derive that

\[
((i\omega_n - \epsilon(k))\tilde{\sigma}_0 - \tilde{\Sigma}^{(1)}(k, i\omega_n) + \tilde{\Sigma}^{(2)}(k, i\omega_n))
\times ((-i\omega_n - \epsilon(k))\tilde{\sigma}_0 + \tilde{\Sigma}^{(1)}(-k, i\omega_n)^*)^{-1}
\times \tilde{\Sigma}^{(2)}(-k, i\omega_n)^*\tilde{G}(k, i\omega_n)
= \tilde{\sigma}_0
\]  

(A1)

Putting \(\omega\) to 0, we can obtain zero energy excitation. Consider a point where \(\Sigma^{(2)}(k, 0) = 0\). At that point, if \((-\epsilon(k))\tilde{\sigma}_0 + \tilde{\Sigma}^{(1)}(-k, 0)^*)^{-1}\) is divergent more strongly than two \(\Sigma^{(2)}(k, 0)\)s on both side, the Green’s function has no pole there. In this case, there is no node.

If it is divergent less strongly than or equal to two \(\Sigma^{(2)}(k, 0)\)s on both side, or not at all divergent, the equation becomes

\[
((\epsilon(k)\tilde{\sigma}_0 + \tilde{\Sigma}^{(1)}(k, 0))\tilde{G}(k, 0)
= -\tilde{\sigma}_0,
\]  

(A2)

where we renormalize the residue into \(\Sigma^{(1)}(k, 0)\) if it exists.

Moreover, \(\Sigma^{(1)}(k, 0)^* = \Sigma^{(1)}(k, 0)\) because the transformation \(\Sigma^{(1)}(k, 0) \rightarrow \Sigma^{(1)}(k, 0)^*\) causes transformations on internal Green’s functions such as,

\[
(-\tilde{G}_1(k_1, 0))(-\tilde{G}_1(k_2, 0))\rightarrow
(-\tilde{G}_1(k_2, 0))^*(-\tilde{G}_1(k_1, 0))^*
= (-\tilde{G}_1(k_2, 0))(-\tilde{G}_1(k_1, 0)),
\]

\[
(-\tilde{G}_1(k_1, 0))\tilde{F}_1(k_2, 0)\rightarrow
\tilde{F}_1(k_2, 0)^*(-\tilde{G}_1(k_1, 0))^*
= \tilde{F}_1(k_2, 0)(-\tilde{G}_1(k_1, 0)),
\]

\[
\tilde{F}_1(k_1, 0)\tilde{G}_1(-k_2, 0)^*\rightarrow
\tilde{G}_1(-k_2, 0)^*\tilde{F}_1(k_1, 0)^*
= \tilde{G}_1(-k_2, 0)^*\tilde{F}_1(k_1, 0)^*,
\]

\[
\tilde{F}_1(k_1, 0)\tilde{F}_1(k_2, 0)\rightarrow
\tilde{F}_1(k_2, 0)^*\tilde{F}_1(k_1, 0)^*,
\]

\[
\tilde{G}_1(-k_1, 0)^*\tilde{G}_1(-k_2, 0)^*\rightarrow
\tilde{G}_1(-k_2, 0)^T\tilde{G}_1(-k_1, 0)^T
= \tilde{G}_1(-k_2, 0)^*\tilde{G}_1(k_2, 0)^*,
\]

\[
\tilde{G}_1(-k_1, 0)^*\tilde{F}_1(k_2, 0)^*\tilde{G}_1(-k_2, 0)^*
\]

Note that in \(\Sigma^{(1)}(k, 0)\), the number of \(F_1\) and \(F_1^\dagger\) is equal. Similar to the argument of \(\Sigma^{(2)}(k, 0)\), the transformation causes a change with dually corresponding term with no sign change.

Thus, \(\Sigma^{(1)}(k, 0)^\dagger = \Sigma^{(1)}(k, 0)\), and \((\epsilon(k)\tilde{\sigma}_0 + \tilde{\Sigma}^{(1)}(k, 0))\) can be diagonalized by a unitaty matrix.

Let us write the eigenvalues as \(\epsilon(k) + \Sigma^{(1)}(k, 0), (i = 1, 2)\).

\(\epsilon(k)\) changes its sign on the Fermi surface, while \(\Sigma^{(1)}(k, 0)\) should be slowly varying in the vicinity of the Fermi surface if impurity concentration is sufficiently small although this needs to be proved. Therefore, there should be a point near the Fermi surface where \(\epsilon(k) + \Sigma^{(1)}(k, 0) = 0\). At that point, zero energy excitation exists.

Appendix B: How to obtain nodes of the gap functions

The fact that \(\Sigma^{(2)}(k, 0)\) has the same parity as the gap function is almost trivial. This condition and the condition \(\Sigma^{(2)}(-k, 0)^T = -\Sigma^{(2)}(k, 0)\) leads to the fact that \(\Sigma^{(2)}(k, 0)\) can be written in the same form as the gap function, i.e., \(\Sigma^{(2)}(k, 0) = i\sigma_y \psi(k)\) or \(\Sigma^{(2)}(k, 0) = i(d(k) \cdot \sigma_0)\sigma_y\) with certain functions \(\psi(k)\) or \(d(k)\), corresponding to the parity, respectively.

Searching for zeros of \(\Sigma^{(2)}(k, 0)\) is reduced to searching for those of \(\psi(k)\) or \(d(k)\). The fact \(\Sigma^{(2)}(-k, 0)^T = -\Sigma^{(2)}(k, 0)\) is proved in the latter half of this appendix.

Although there are many sets of basis functions of irreducible representations, it may occur that any basis functions become zero at certain points. Here, we consider such zero points.

singlet case:

We write basis functions \(\{\psi^{(a)}\}_{i=1,2,\cdots,d_\alpha}\) of the irreducible representation \(\Gamma^\alpha\) \((d_\alpha\) dimension) of the point group \(G\) in the form:

\[
\psi(k) = \begin{pmatrix}
\psi^{(a)}_1 \\
\psi^{(a)}_2 \\
\vdots \\
\psi^{(a)}_{d_\alpha}
\end{pmatrix}.
\]  

(B1)
And \( \psi(k) \) satisfies
\[
\psi(R^{-1}k) = \hat{D}(R)^T \psi(k),
\]
where \((\hat{D}(R))_{ij} = D_{ij}^{(\alpha)}(R)\) is a representation matrix of the group element \( R \) of the irreducible representation \( \Gamma^\alpha \).

The equation \((B2)\) gives relationships between values of \( \psi(k) \) at points which is moved by elements of \( G \).

Now, let us consider a point \( k \) which is not invariant under any element \( R \) of \( G \). Then, \( \{R^{-1}k\}_{R \in G} \) consists of points of the same number \( g \) as the order of \( G \), and values of \( \psi(k) \) at \( \{R^{-1}k\}_{R \in G} \) have relationships. Since there are at most \( d_\alpha(g - 1) \) independent linear equations for \( d_\alpha g \) variables \( \{\psi(R^{-1}k)\}_{R \in G} \)

\[
\begin{pmatrix}
\hat{1} & -\hat{D}(R_2)^T & \cdots & -\hat{D}(R_d)^T \\
\hat{1} & -\hat{D}(R_3)^T & \cdots & -\hat{D}(R_d)^T \\
\vdots & \vdots & \ddots & \vdots \\
\hat{1} & -\hat{D}(R_d)^T & \cdots & -\hat{D}(R_d)^T
\end{pmatrix}
\begin{pmatrix}
\psi(R_1^{-1}k) \\
\psi(R_2^{-1}k) \\
\vdots \\
\psi(R_d^{-1}k) \\
\psi(k)
\end{pmatrix}
= 0,
\]

the solutions are
\[
\begin{pmatrix}
\psi(R_1^{-1}k) \\
\psi(R_2^{-1}k) \\
\vdots \\
\psi(R_d^{-1}k) \\
\psi(k)
\end{pmatrix}
= \left(\begin{pmatrix}
\hat{D}(R_2)^T \\
\hat{D}(R_3)^T \\
\vdots \\
\hat{D}(R_d)^T
\end{pmatrix} \right) a
\]

where \( a \) is an arbitrary \( d_\alpha \) dimensional vector, and \( \hat{D}(R_d) = \hat{1} \) (\( d_\alpha \) dimensional unit matrix). Therefore no restriction that forces \( \{\psi(R^{-1}k)\}_{R \in G} \) to be zeros appears.

Next we consider a point \( k \) which is invariant under some elements of \( G \). These points can exist only when they are on rotational axes or mirror reflection planes. In contrast to previous case, since \( \psi(k) \) with the condition \( R^{-1}k = k \) satisfies
\[
\psi(k) = \hat{D}(R)^T \psi(k),
\]
the value of \( \psi(k) \) is restricted.

(i) In the case that there exist \( R \) such that the rank of the matrix \( (\hat{D}(R)^T - \hat{1}) \) equals \( d_\alpha \), that is, determinant of the matrix is not equal to zero, then \( \psi(k) = 0 \). In this case, for any set of coefficients \( \{c^\alpha_i\} \), \( \sum_i c^\alpha_i \psi_i(k) = c \cdot \psi(k) = 0 \). For example, \((0, 0, 1)\) (line) and \((0, 0, 1)\) (point) of \( \Gamma^{5+} \) of \( D_{0h} \) applies to this case.

(ii) In the case that there is no \( R \) such that the rank of the matrix \( (\hat{D}(R)^T - \hat{1}) \) equals \( d_\alpha \). In this case, if the rank of the matrix for an \( R \) equals \( n < d_\alpha \), the solutions of the equation \((B2)\) must lie in \( d_\alpha - n \) dimensional subspace. If \( k \) has several \( R \) which satisfies \( R^{-1}k = k \), the subspace of solutions of the equation is the common subspace of subspaces for each \( R \). \( \psi(k) \) is not always \( 0 \) in this case. However, if coefficients \( c \equiv (c_1^\alpha c_2^\alpha \cdots c_d^\alpha)^T \) belongs to the orthocomplement of the common subspace, then \( c \cdot \psi(k) = \sum_i c^\alpha_i \psi_i(k) = 0 \). This means that the gap function is zero at the point \( k \).

The proof for \( \Sigma^{(2)}(-k, 0)^T = -\Sigma^{(2)}(k, 0) \):

A transformation \( \Sigma^{(2)}(k, 0) \to \Sigma^{(2)}(-k, 0)^T \) induces transformations on internal Green’s functions such as:
\((\hat{G}_1(k_1,0))(-\hat{G}_1(k_2,0))\) \(\xrightarrow{\text{transformation}}\) \((-\hat{G}_1(-k_2,0))^T(\hat{G}_1(-k_1,0))^T\) 
\(= \hat{G}_1(-k_2,0)^* \hat{G}_1(-k_1,0)^*\),

\((-\hat{G}_1(k_1,0))\hat{F}_1(k_2,0) \xrightarrow{\text{transformation}} \hat{F}_1(-k_2,0)^T(\hat{G}_1(-k_1,0))^T\) 
\(= -\hat{F}_1(-k_2,0)^* \hat{G}_1(-k_1,0)^*\),

\(\hat{F}_1(k_1,0)\hat{G}_1(-k_2,0)^* \xrightarrow{\text{transformation}} \hat{G}_1(k_2,0)^\dagger \hat{F}_1(-k_1,0)^T\) 
\(= \hat{G}_1(-k_2,0)^*(-1)\hat{F}_1(k_1,0),\)

\(\hat{G}_1(-k_1,0)^* \hat{F}_1(k_2,0)^\dagger \xrightarrow{\text{transformation}} \hat{F}_1(-k_2,0)^* \hat{F}_1(-k_1,0)^T\) 
\(= \hat{F}_1(k_2,0)^\dagger \hat{F}_1(k_1,0),\)

\(\hat{G}_1(-k_1,0)^* \hat{G}_1(-k_2,0)^* \xrightarrow{\text{transformation}} \hat{G}_1(k_2,0)^\dagger \hat{G}_1(k_1,0)^\dagger\) 
\(= (-\hat{G}_1(k_2,0))(-\hat{G}_1(k_2,0)),\)

\(\hat{G}_1(-k_1,0)^* \hat{F}_1(k_2,0)^\dagger \xrightarrow{\text{transformation}} \hat{F}_1(-k_2,0)^* \hat{G}_1(k_1,0)^\dagger\) 
\(= (-1)\hat{F}_1(-k_2,0)^\dagger \hat{G}_1(k_1,0),\)

\(\hat{F}_1(k_1,0)^\dagger (-\hat{G}_1(k_2,0)) \xrightarrow{\text{transformation}} (-\hat{G}_1(-k_2,0)^* \hat{F}_1(-k_1,0)^* = \(-\hat{G}_1(k_2,0)(-1)\hat{F}_1(k_1,0)^\dagger\),

\(\hat{F}_1(k_1,0)^\dagger \hat{F}_1(k_2,0) \xrightarrow{\text{transformation}} \hat{F}_1(-k_2,0)^T \hat{F}_1(-k_1,0)^* = \hat{F}_1(k_2,0)^\dagger \hat{F}_1(k_1,0)^\dagger\).

Here, the transformation of external wave number \(k \rightarrow -k\) is equivalent to the transformation of internal wave number \(k_i \rightarrow -k_i\).

Thus, by the transformation \(\Sigma^{(2)}(k,0) \xrightarrow{\text{transformation}} \Sigma^{(2)}(-k,0)^T\), each term in \(\Sigma^{(2)}(k,0)\) is multiplied by a factor \(-1\), because \(-1\) is multiplied “the summation of the number of \(\hat{F}_1\) and \(\hat{F}_1^\dagger\) n times, and they are always odd.

In the case of a diagrammatically symmetric term, the transformation causes only the change of internal wave number indices, and thus \(-1\) is multiplied.

In the case of a diagrammatically asymmetric term, the transformation causes a change with dually corresponding term, and thus \(-1\) is multiplied.

Thus, \(\Sigma^{(2)}(-k,0)^T = -\Sigma^{(2)}(k,0)\).

### Appendix C: Table of Nodal Structures of \(O_h\), \(D_{6h}\), and \(D_{4h}\) Anisotropic Superconductors

We choose basis functions of irreducible representations for \(O_h\), \(D_{6h}\), and \(D_{4h}\) as follows.

| \(\Gamma\) | \(\psi(k)/d(k)\) |
|---|---|
| \(\Gamma^0\) | \(\psi^{(1+)}(k) = 1\) |
| \(\Gamma^1\) | \(\psi^{(2+)}(k) = (k_x^2 - k_y^2)(k_z^2 - k_y^2)\) |
| \(\Gamma^2\) | \(\psi^{(3+)}(k) = 2k_x^2 - k_y^2\) |
| \(\Gamma^3\) | \(\psi^{(4+)}(k) = k_x k_y (k_z^2 - k_y^2)\) |
| \(\Gamma^4\) | \(\psi^{(5+)}(k) = k_x k_y (k_x^2 - k_y^2)\) |
| \(\Gamma^5\) | \(\psi^{(6+)}(k) = k_x k_y\) |

### Table 1: basis functions of irreducible representations for \(O_h\), \(D_{6h}\), and \(D_{4h}\)

| \(\Gamma\) | \(\psi(k)/d(k)\) |
|---|---|
| \(\Gamma^0\) | \(\psi^{(1+)}(k) = 1\) |
| \(\Gamma^1\) | \(\psi^{(2+)}(k) = (k_x^2 - k_y^2)(k_z^2 - k_y^2)\) |
| \(\Gamma^2\) | \(\psi^{(3+)}(k) = 2k_x^2 - k_y^2\) |
| \(\Gamma^3\) | \(\psi^{(4+)}(k) = k_x k_y (k_z^2 - k_y^2)\) |
| \(\Gamma^4\) | \(\psi^{(5+)}(k) = k_x k_y (k_x^2 - k_y^2)\) |
| \(\Gamma^5\) | \(\psi^{(6+)}(k) = k_x k_y\) |

Order parameters for \(O_h\), \(D_{6h}\), and \(D_{4h}\) obtained from GL and the change of their nodal structure following the introduction of nonmagnetic impurities are given in the following tables. For example, \((1, \omega, \omega^2)\) is a combination of expansion coefficients for basis functions defined here, where \(\omega = e^{i\pi/3}\). (a) means numbers of order parameters being solutions of GL simultaneously.

(b) means the largest subgroup \(G'\) where the excitation energy is invariant (\(\Gamma^1\)). (c) means zeros in \(k\)-space.
immediately under the transition point $T_c$ in the absence of impurities. \([k_x, k_y, k_z]\) in the table means a straight line generated by a vector \((k_x, k_y, k_z)\). \((k_x, k_y, k_z)\) in the table means a plane which is perpendicular to a vector \((k_x, k_y, k_z)\) and goes through the origin of \(k\)-space. (d) means zeros below $T_c$ in the absence and the presence of impurities. Nodes are generated where zeros and Fermi surface intersect. “none” means nonexistence of node, and left arrow means that the nodes on the left-hand side does not disappear. In the right edge, which representation appears is written in the case of complex coefficients.

\[
\text{TABLE III: } D_{sh}
\]

| \(\Gamma^+\) | \(\psi(k)/d(k)\) | (a) | (b) | (c) | (d) |
|------------|-----------------|-----|-----|-----|-----|
| \(\Gamma^+_1\) | 1 | 1 | \(D_{sh}(\Gamma^+_1)\) | none | none |
| \(\Gamma^+_2\) | 1 | 1 | \(O_3(\Gamma^+_2)\) | (1, \(\pm 1, 0\)), (0, 1, \(\pm 1\)), (\(\pm 1, 0, 1\)) | \(\leftarrow\) |
| \(\Gamma^+_3\) | (0, 1) | 3 | \(D_{sh}^{(0,0,1)}(\Gamma^+_3)\) | (1, \(\pm 1, 0\)) | \(\leftarrow\) |
| \(\Gamma^+_4\) | (1, 0) | 3 | \(D_{sh}^{(0,0,1)}(\Gamma^+_4)\) | \([1,1,1],[1,1,1],[1,1,1],[1,1,1],[1,1,1]\) | none |
| \(\Gamma^+_5\) | (1, \(\epsilon\)) | 2 | \(O_3(\Gamma^+_5)\) | \([1,1,1],[1,1,1],[1,1,1],[1,1,1],[1,1,1]\) | \(\leftarrow\) |
| \(\Gamma^+_6\) | (1, \(\omega^2\)) | 8 | \(D_{sh}^{(1,1,1)}(\Gamma^+_6)\) | \([1,1,1],[1,1,1],[1,1,1],[1,1,1],[1,1,1]\) | \(\leftarrow\) |
| \(\Gamma^+_7\) | (1, \(\omega^2\)) | 8 | \(D_{sh}^{(1,1,1)}(\Gamma^+_7)\) | \([1,1,1],[1,1,1],[1,1,1],[1,1,1],[1,1,1]\) | \(\leftarrow\) |
| \(\Gamma^+_8\) | (1, \(\omega^2\)) | 8 | \(D_{sh}^{(0,0,1)}(\Gamma^+_8)\) | \([0,1,0],[0,1,0],[0,1,0],[0,1,0],[0,1,0]\) | \(\leftarrow\) |
| \(\Gamma^+_9\) | (0, 1, 0) | 6 | \(D_{sh}^{(0,0,1)}(\Gamma^+_9)\) | \([0,1,0],[0,1,0],[0,1,0],[0,1,0],[0,1,0]\) | none |
| \(\Gamma^+_10\) | (1, \(\omega^2\)) | 8 | \(D_{sh}^{(1,1,1)}(\Gamma^+_10)\) | none | none |
| \(\Gamma^+_11\) | \(\pm \omega\) | 2 | \(O_3(\Gamma^+_11)\) | none | none |
| \(\Gamma^+_12\) | \(\pm \omega\) | 2 | \(O_3(\Gamma^+_12)\) | none | none |
| \(\Gamma^+_13\) | \(\omega^2\) | 8 | \(D_{sh}^{(1,1,1)}(\Gamma^+_13)\) | none | none |
| \(\Gamma^+_14\) | \(\omega^2\) | 8 | \(D_{sh}^{(1,1,1)}(\Gamma^+_14)\) | none | none |
| \(\Gamma^+_15\) | \(\omega^2\) | 8 | \(D_{sh}^{(1,1,1)}(\Gamma^+_15)\) | none | none |
D has three kinds of subgroup times rotation axis each other, for example, D parameter, we write only subgroups for representative order parameters.

Although such subgroups are different for every order parameter, we write only subgroups for representative order parameters.

The largest subgroup where the quasiparticle energy of a given order parameter is invariant can be obtained as follows. First, examine all maximal subgroups whether the excitation energy is invariant or not under the subgroups. If there exits, that is the largest subgroup.
If not, examine all second maximal subgroups, and so on. The maximal subgroup obtained like this is also the largest subgroup as mentioned in section IV.

Appendix D: Expansion of Order Parameters of Complex Coefficients with respect to $G'$ where the Quasiparticle Energy of Clean Superconductor is Invariant

We examined $\{c'_i\}$ of $\sum_i c'_i \psi_i^{(\beta)} = \sum_i c_i \psi_i^{(\alpha)}$. $\psi_i^{(\beta)}$ means that it belongs to $i$th basis of $\beta$th irreducible representation of $G'$ where the quasiparticle energy of clean superconductor is invariant. These results can be understood from the GL theory.

$O_h$

(2D) even

$\Gamma^0_4 (3)$ (subgroup $G' = O_h$)

\[
k^2_x + \omega k^2_y + \omega^2 k^2_z = \frac{1}{2}(2k^2_x - k^2_y) + \frac{i}{2}(\sqrt{3}(k^2_x - k^2_y))
\]

= $\psi_1^{(3+)} + i\psi_2^{(3+)}$  \hspace{1cm} (D1)

(2D) odd

$\Gamma^0_5 (3)$ (subgroup $G' = O_h$)

\[
x\omega y k_y + \omega^2 z k_z = \psi_1^{(3-)} + i\psi_2^{(3-)}  \hspace{1cm} (D2)
\]

(3D) even

$\Gamma^0_4 (1)$ (subgroup $G' = D_{3d}$ which has (1,1,1) of $O_h$ as a three times rotation axis)

\[
k_y k_z(k_y^2 - k_z^2) + \omega k_z k_x(k_x^2 - k_y^2) + \omega^2 k_x k_y(k_x^2 - k_y^2)
\]

= $3 - \frac{i\sqrt{3}}{4}(k_x + k_y)k_z(k_x^2 - k_y^2) + k_y(k_y^2 - k_z^2) - k_z(k_x^2 + k_y^2)
\]

\[
= \psi_1^{(3+)} + i\psi_2^{(3+)}  \hspace{1cm} (D3)
\]

$\Gamma^0_4 (4)$ (subgroup $G' = D_{4h}$ which has (0,0,1) of $O_h$ as a four times rotation axis)

\[
k_y k_z(k_y^2 - k_z^2) + i k_z k_x(k_x^2 - k_y^2)
\]

= $\psi_1^{(5+)} + i\psi_2^{(5+)}$  \hspace{1cm} (D4)

$\Gamma^0_5 (1)$ (subgroup $G' = D_{3d}$ which has (1,1,1) of $O_h$ as a three times rotation axis)

\[
k_y k_z + \omega k_z k_x + \omega^2 k_x k_y
\]

= $-\frac{1 + i\sqrt{3}}{4}(2k_x k_y - k_x k_y - k_y k_y)
\]

\[
- \frac{1 - i\sqrt{3}}{4}(\sqrt{3}(k_x - k_y)k_z)
\]

= $\psi_1^{(3+)} + i\psi_2^{(3+)}$  \hspace{1cm} (D5)

$\Gamma^0_4 (4)$ (subgroup $G' = D_{4h}$ which has (0,0,1) of $O_h$ as a four times rotation axis)

\[
k_y k_z + i k_z k_x
\]

= $\psi_1^{(5+)} + i\psi_2^{(5+)}$  \hspace{1cm} (D6)

(3D) odd

$\Gamma^0_4 (1)$ (subgroup $G' = D_{3d}$ which has (1,1,1) of $O_h$ as a three times rotation axis)

\[
\hat{x}(\omega k_y - \omega^2 k_z) + \hat{y}(k_z - \omega k_x) + \hat{z}((\omega^2 k_x - k_y)
\]

= $3 + \frac{i\sqrt{3}}{4}(\hat{x}(-k_y) + \hat{y}(-k_z) + \hat{z}(k_x + k_y)) + \frac{-1 - i\sqrt{3}}{4}(\hat{x}(-2k_y - k_z) + \hat{y}(2k_z + k_z) + \hat{z}(k_z - k_y))
\]

= $\psi_1^{(3-)} + i\psi_2^{(3-)}$  \hspace{1cm} (D7)

$\Gamma^0_4 (4)$ (subgroup $G' = D_{4h}$ which has (1,0,0) of $O_h$ as a four times rotation axis)

\[
\hat{x}(k_y + i k_z) + \hat{y}(-k_z) + \hat{z}(-i k_z)
\]

= $\psi_1^{(5-)} + i\psi_2^{(5-)}$  \hspace{1cm} (D8)

$\Gamma^0_5 (1)$ (subgroup $G' = D_{3d}$ which has (1,1,1) of $O_h$ as a three times rotation axis)

\[
\hat{x}(\omega k_y + \omega^2 k_z) + \hat{y}(k_z + \omega k_x) + \hat{z}((\omega^2 k_x + k_y)
\]

= $-\frac{1 - i\sqrt{3}}{4}(\hat{x}(k_x - 2k_y) + \hat{y}(k_z - 2k_x) + \hat{z}(k_x + k_y)) + \frac{\sqrt{3} + i}{4}(\sqrt{3} \hat{x}k_z + \hat{y}(-k_z) + \hat{z}(k_x - k_y))
\]

= $\psi_1^{(3-)} - i\psi_2^{(3-)}$  \hspace{1cm} (D9)
\[ \Gamma_5^-(4) \text{(subgroup } G' = D_{4h} \text{ which has } (0,0,1) \text{ of } O_{h} \text{ as a four times rotation axis)} \]
\[ \hat{x}(k_y + ik_z) + \hat{y}k_x + \hat{z}(ik_x) = \psi_1^{(5-)} + i\psi_2^{(5-)} \]  
(D10)

\[ \Gamma_6^-(3) \text{(subgroup } G' = D_{6h} \text{)} \]
\[ (\hat{x} + i\hat{y})(k_x + ik_y) = \psi_1^{(6-)} + i\psi_2^{(6-)} \]  
(D14)

\[ D_{6h} \]
(2D)even
\[ \Gamma_5^+(3) \text{(subgroup } G' = D_{6h} \text{)} \]
\[ k_z(k_x + ik_y) = \psi_1^{(5+)} + i\psi_2^{(5+)} \]  
(D11)

\[ \Gamma_6^+(3) \text{(subgroup } G' = D_{6h} \text{)} \]
\[ (k_x + ik_y)^2 = \psi_1^{(6+)} + i\psi_2^{(6+)} \]  
(D12)

\[ \text{(2D)odd} \]
\[ \Gamma_5^- (3) \text{(subgroup } G' = D_{6h} \text{)} \]
\[ \hat{x}k_z + i\hat{y}k_z = \psi_1^{(5-)} + i\psi_2^{(5-)} \]  
(D13)