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On p-Wave Pairing Superconductivity under Cubic Symmetry

Masa-aki OZAKI, Kazushige MACHIDA and Tetsuo OHMI

Department of Physics, Kyoto University, Kyoto 606

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A group theoretical classification of p-wave pairing superconducting states is made for a system with cubic crystalline symmetry in the absence of the spin-orbit coupling. The 15 inert p-pairing states which make the Ginzburg-Landau free energy stationary are enumerated and characterized, indicating that the energy gap vanishes along lines on the Fermi surface in some of those states. This is contrasted with the strong spin-orbit coupling case by others.

§ 1. Introduction

Recently much attention has been focused on the so-called heavy electron systems with large effective mass experimentally[1)~8)] and theoretically.[9)~22)] In particular, some superconducting properties in these systems exemplified by $CeCu_2Si_2$, UBe_{13} and UPt_3 are unusual and very different from those of the conventional singlet pairing superconductors. Namely the power-law behavior of physical quantities in the low temperature region instead of the exponential one expected for the isotropic pairing state are observed: (1) The specific heat behaves as T^3 in UB_{13}.[2)] (2) The nuclear relaxation rate T_1^{-1} exhibits T^3-dependence for both $CeCu_2Si_2$[3)] and UBe_{13}.[4)] (3) The ultrasonic attenuation coefficient[5)] in UPt_3 is proportional to T^2. All these particular power-law dependences are indicative of an anisotropic superconducting state in which the superconducting energy gap vanishes at points for (1) and along lines for (2) and (3) on the Fermi surface. The observation[6)] of the second superconducting transition in $U_{1-x}Th_xBe_{13}$ ($x \lesssim 0.06$) further leads us to speculate the unconventional pairing states which possess internal degree of freedom.

Corresponding to this experimental situation, several theories both for singlet and triplet pairings have been already proposed. Among others Anderson,[15)] and Ueda and Rice[17)] have given possible pairing states for triplet pairing in cubic crystalline symmetry. Volovik and Gorkov[16)] have discussed quite thoroughly various states for triplet and singlet pairings in cubic, hexagonal and tetragonal symmetries. Taking into account the crystalline field symmetry and spin-orbit coupling simultaneously, they obtain the possible superconducting phases group-theoretically. As for triplet pairing their conclusions agree to yield no phase with lines of the zeros in the energy gap, that is, the gap in the stable phases is nodeless or disappears at isolated points on the Fermi surface.

In this paper we take a view*) that the residual spin-orbit coupling felt by a Cooper pair is relatively weak compared with the pairing energy although the spin-orbit coupling for individual electrons near the Fermi surface is very strong. The spin-orbit coupling, which acts as fixing the relative orientation of the orbital part and spin direction for a pair, are regarded as a perturbation and neglected here.

*) A similar opinion has been expressed by K. Miyake and S. Maekawa.

We shall list up all possible stable triplet pairing states under a certain crystalline symmetry, namely we consider cubic symmetry in this paper. The listed phases are confined to the so-called "inert phases"[23] which make each term of the free energy functional stationary, that is, in an inert phase the order parameter does not vary with the coefficients in the free energy functional. Since the enumeration of the singlet pairing states such as s- and d-wave pairing done by Volovik and Gorkov[16] is valid even for the case in which the spin-orbit coupling is weak, our work together with Volovik and Gorkov's work, exhausts possible inert s-, p- and d-pairing states under cubic crystalline symmetry.

The paper is organized as follows: The Ginzburg-Landau free energy functional for p-wave pairing in cubic symmetry is derived in the next section. Group theoretical classification is made in § 3 by using the Michel theorem[24),25] which is powerful in finding extremum points of an invariant function under compact group action. We characterize the classified phases and examine the relative stability of these phases in § 4. The final section is devoted to discussion and conclusion.

§ 2. Symmetry properties and Ginzburg-Landau functional

In this section we examine the symmetry properties of the order parameter for p-pairing and construct the Ginzburg-Landau (GL) free energy valid up to fourth order in the order parameter.

We first introduce the order parameter $\Delta_{\alpha\beta}(\boldsymbol{k})$ for p-wave pairing which is described by

$$\Delta_{\alpha\beta}(\boldsymbol{k})=\langle a_{\boldsymbol{k}\alpha}a_{-\boldsymbol{k}\beta}\rangle=i(\boldsymbol{\sigma}\cdot\boldsymbol{d}(\boldsymbol{k})\sigma_2)_{\alpha\beta}\,, \tag{2·1}$$

where α and β stand for spin indices. The wave number near the Fermi surface is $\boldsymbol{k}$ and σ_i is the Pauli matrix ($i=x, y$ and z). The vector $\boldsymbol{d}(\boldsymbol{k})$ is expressed by

$$\boldsymbol{d}(\boldsymbol{k})=\boldsymbol{A}\cdot\hat{\boldsymbol{k}}, \tag{2·2}$$

where $\hat{\boldsymbol{k}}$ is a unit vector of $\boldsymbol{k}$. The 3×3 complex matrix $\boldsymbol{A}$ specifies various phases of p-pairing. Denoting $\tau_\lambda=i\sigma_\lambda\sigma_2$ and $\boldsymbol{A}=\boldsymbol{A}^{(1)}+i\boldsymbol{A}^{(2)}$ ($\boldsymbol{A}^{(1)}$ and $\boldsymbol{A}^{(2)}$ are the 3×3 real matrices), we rewrite Eq. (2·1) as

$$\Delta(\boldsymbol{k})=\sum_{\lambda=1}^{3}\sum_{j=1}^{3}\sum_{i=1}^{2}A_{\lambda j}^{(i)}\tau_\lambda\hat{k}_j l_i\,, \tag{2·3}$$

where we have introduced $l_1=1$ and $l_2=i$.

The symmetry properties of the order parameter $\Delta(\boldsymbol{k})$ in Eq. (2·3) determine the functional form of the GL free energy. It is to be noted that the GL functional should be invariant with respect to the combined symmetry group $G_0=\boldsymbol{O}\times S\times M$ in the absence of the spin-orbit coupling where $\boldsymbol{O}$ is the cubic point group, S the spin rotation group and $M=\Phi+t\Phi$, in which Φ and t are the groups of the gauge and time reversal transformations. Therefore, let us examine the transformation properties of $\Delta(\boldsymbol{k})$. We denote an element of $\boldsymbol{O}$ by p, an element of S by $u(\boldsymbol{e}, \theta)$, which corresponds to spin rotation around an axis $\boldsymbol{e}$ by an angle θ and an element of Φ by $\tilde{\varphi}$ which corresponds to a phase change $e^{i\varphi}$. Using this notation we can see that each part $\{\hat{k}_j, \tau_\lambda, l_i\}$ of $\Delta(\boldsymbol{k})$ transforms for a combined group element $g=pu(\boldsymbol{e}, \theta)\tilde{\varphi}$ as

$$p\hat{k}_j=\sum_{j'}D(p)_{j'j}\hat{k}_{j'},$$
$$u(\boldsymbol{e},\theta)\tau_\lambda=\sum_{\lambda'}\check{S}_{\lambda'\lambda}(\boldsymbol{e},\theta)\tau_{\lambda'},$$
$$\tilde{\varphi}l_i=\sum_{i'}\check{M}_{i'i}(\tilde{\varphi})l_{i'},$$
$$t\tilde{\varphi}l_i=\sum_{i'}\check{M}_{i'i}(t\tilde{\varphi})l_{i'}, \tag{2·4}$$

where $D(p)$ is the matrix of the irreducible representation T_1 in $\boldsymbol{O}$, $\check{S}(\boldsymbol{e},\theta)$ is the three dimensional rotation matrix characterized by the angle θ and the axis $\boldsymbol{e}$, and

$$\check{M}(\tilde{\varphi})=\begin{pmatrix}\cos\varphi & -\sin\varphi\\ \sin\varphi & \cos\varphi\end{pmatrix},$$
$$\check{M}(t\tilde{\varphi})=\begin{pmatrix}\cos\varphi & -\sin\varphi\\ -\sin\varphi & -\cos\varphi\end{pmatrix}. \tag{2·5}$$

Putting $e_{\lambda ji}=\tau_\lambda\hat{k}_jl_i$, we have

$$ge_{\lambda ji}=\sum_{\lambda'j'i'}\check{S}_{\lambda'\lambda}(u)D_{j'j}(p)\check{M}_{i'i}(m)e_{\lambda'j'i'} \tag{2·6}$$

for $g=pum$ ($p\in\boldsymbol{O}$, $u\in S$ and $m\in M$). Thus $\{e_{\lambda ji}\}$ is a basis of the irreducible representation over the real number field: $\check{G}_0=T_1\otimes\check{S}\otimes\check{M}$ where $\check{G}$ denotes an irreducible representation over the real number field of G. It is readily shown from Eq. (2·6) that

$$g\cdot A^{(i)}_{\lambda j}=\sum_{\lambda'j'i'}\check{S}_{\lambda\lambda'}(u)D_{jj'}(p)\check{M}_{ii'}(m)A^{(i')}_{\lambda'j'}. \tag{2·7}$$

From the transformation property in Eq. (2·7) for $\boldsymbol{A}$ we can construct the GL free energy $F(\boldsymbol{A})$ which leaves invariant under $\boldsymbol{G}_0$: It is easy to see that the second order term in the order parameter is proportional to $\mathrm{Tr}(\boldsymbol{A}\boldsymbol{A}^+)$. The detailed derivation of the fourth order terms is given in Appendix A. Then we have the free energy valid up to the fourth order:

$$F(\boldsymbol{A})=\alpha\mathrm{Tr}(\boldsymbol{A}\boldsymbol{A}^+)+\sum_{i=1}^{7}\beta_iR_i, \tag{2·8}$$

where α and β_i are the GL coefficients. The five invariants $R_1\sim R_5$ defined in Eqs. (A·18) $\sim$(A·22) have been already discussed by Barton and Moore[23] (B-M) and are invariant also under $SO(3)\times S\times M$ where $SO(3)$ is the spatial rotation group, corresponding to the spherical symmetry of the Fermi surface in He^3. The newly appeared terms R_6 and R_7 in Eqs. (A·23) and (A·24) are attributed to cubic crystal symmetry.

The next task is to find the possible order parameter $\boldsymbol{A}$ which minimizes the GL free energy $F(\boldsymbol{A})$. The minimization problem is difficult to solve completely in general because we must treat 18 dimensional variational problem. Here we look for only the inert phases[23] whose order parameter does not depend on the GL coefficients β_i, that is, we seek a solution which makes each fourth order invariant term stationary. Even if we restrict our solutions to the inert phases, the variation problem is still hard to handle analytically. Instead, we treat it group-theoretically.

We note here that Michel's theorem[24),25] is powerful in finding extrema of a certain function invariant under a group action. Let us introduce Michel's theorem briefly: For a point m in the order parameter space $E_0=\{\boldsymbol{A}\}$ the little group $G(m)$ of m is defined by

$$G(m)=\{g\in G_0|g\cdot m=m\}. \tag{2·9}$$

Then Michel's theorem states that if $G(m)$ is a maximal little group*) and the vector space $V(G(m))=\{\boldsymbol{A}\in E_0|g\boldsymbol{A}=\boldsymbol{A} \text{ for } g\in G(m)\}$ is one-dimensional, the point m is a stationary point of every G_0 invariant function. Therefore we can find the inert phases by looking for the point $\boldsymbol{A}=\boldsymbol{A}^{(1)}+i\boldsymbol{A}^{(2)}$ of E_0 whose little group is maximal. It should be noted that such a point of $\boldsymbol{A}$ is a stationary point even for the general GL function including any higher order terms than fourth order terms. In the next section we derive such points in E_0.

§ 3. Enumeration of the inert states

In order to know possible inert states for p-pairing, we find maximal little groups for the combined group $G_0=\boldsymbol{O}\times S\times M$ by utilizing a similar method developed in the previous papers.[26),27)] We first introduce some notations**) and definitions: $\check{G}$ is an irreducible representation of G over the real number field (we denote it R-rep). An invariance group of $\check{G}$ is defined by a maximal subgroup $G'\subseteq G$ such that

$$g\Lambda=\Lambda \qquad \text{for } g\in G', \tag{3·1}$$

where $\Lambda(\neq 0)$ is some element in the R-rep space of $\check{G}$. We denote such a maximal subgroup G' by $[\check{G}]$ and such an element Λ by $\Lambda[\check{G}]$, which is called the invariance vector of $[\check{G}]$. Similarly we define the anti-invariance extension of $[\check{G}]$ as a subgroup $G''=G'+hG'\subseteq G$ which satisfies the following condition; for $\Lambda=\Lambda[\check{G}]$ and $g\in G'$

$$\begin{aligned} g\Lambda&=\Lambda\,,\\ hg\Lambda&=-\Lambda\,, \end{aligned} \tag{3·2}$$

where h is an element of G. We call such h an anti-invariance extension factor of $[\check{G}]$, denoted by $a[\check{G}]$. In Table I we give $[\check{G}]$, $\Lambda[\check{G}]$ and $a[\check{G}]$ for T_1 of the cubic point group, $\check{S}$ and $\check{M}$, which will be used to deduce maximal little groups later.

Table I. The invariance group, its invariance vector and its anti-invariance extension factor of T_1, $\check{S}$ and $\check{M}$.

G	$\check{G}$	$[\check{G}]$	$\Lambda[\check{G}]$	$a[\check{G}]$
$\boldsymbol{O}$	T_1	$\boldsymbol{C}_4$	$\hat{k}_z$	C_{2x}
		$\boldsymbol{C}_{2a}$	$\hat{k}_x+\hat{k}_y$	C_{2b}
		$\boldsymbol{C}_{31}$	$\hat{k}_x+\hat{k}_y+\hat{k}_z$	C_{2b}
S	$\check{S}$	$A(e_z)$[a)]	τ_z	u_{2x}[b)]
M	$\check{M}$	T[c)]	l_1	$\tilde{\pi}$

a) $A(e_z)=\{u(e_z,\,\theta)|0\leqq\theta\leqq 2\pi\}$.

b) $u_{2i}=u(e_i,\,\pi)$.

c) $T=(1,\,t)$, group of time reversal transformation.

*) In the set of all subgroups of G_0 a partial ordering relation "$<$" can be introduced: For two subgroups G_1 and G_2 we shall write $G_1<G_2$ if G_1 is a proper subgroup of gG_2g^{-1} for some element g in G_0. The term "maximal" is defined with respect to this partial ordering "$<$".

**) In the following we use the Schönflies notation[28)] for point groups and their elements.

Table II. The non-product type invariance group of $\check{G}_1\otimes\check{G}_2$.

$G_1\times G_2$	$\check{G}_1\otimes\check{G}_2$	$[\check{G}_1\otimes\check{G}_2]_{\text{non-p}}$	$\Lambda[\check{G}_1\otimes\check{G}_2]_{\text{non-p}}$	$a[\check{G}_1\otimes\check{G}_2]_{\text{non-p}}$
$\boldsymbol{O}\times S$	$T_1\otimes\check{S}$	${}_{II}\boldsymbol{O}$ [a]	$\frac{1}{\sqrt{3}}(\tau_x\hat{k}_x+\tau_y\hat{k}_y+\tau_z\hat{k}_z)$	
		${}_{II}\boldsymbol{D}_4$	$\frac{1}{\sqrt{2}}(\tau_x\hat{k}_x+\tau_y\hat{k}_y)$	$C_{2x}u_{2y}$
		${}_{II}\boldsymbol{C}_{31}$ [b]	$\frac{1}{\sqrt{6}}\{\tau_x(\hat{k}_y-\hat{k}_z)+\tau_y(\hat{k}_z-\hat{k}_x)+\tau_z(\hat{k}_x-\hat{k}_y)\}$	$C_{2b}u_{2b}$
$\boldsymbol{O}\times M$	$T_1\otimes\check{M}$	$(1+tC_{2x})\tilde{\boldsymbol{C}}_4$ [c]	$\frac{1}{\sqrt{2}}(\hat{k}_x+i\hat{k}_y)$	$\tilde{\pi}$
		$(1+tC_{2b})\tilde{\boldsymbol{C}}_{31}$ [d]	$\frac{1}{\sqrt{3}}\{i(\hat{k}_z+\varepsilon\hat{k}_x+\varepsilon^2\hat{k}_y)\}$ [e]	$\tilde{\pi}$
$S\times M$	$\check{S}\otimes\check{M}$	$(1+tu_{2x})\tilde{A}(e_z)$ [f]	$\frac{1}{\sqrt{2}}(\tau_x+i\tau_y)$	u_{2z}

a) ${}_{II}\boldsymbol{P}=\{pu(p)|p\in\boldsymbol{P},\ u(p)$ is the spin rotation about the same rotation axis by rotation angle as $p\}$.
b) $\boldsymbol{C}_{31}=\{E,\ C_{31}^{+},\ C_{31}^{-}\}$.
c) $\tilde{\boldsymbol{C}}_4=\{E,\ C_{4z}^{+}(\widetilde{\pi/2}),\ C_{4z}^{-}(-\widetilde{\pi/2}),\ C_{2z}\tilde{\pi}\}$.
d) $\tilde{\boldsymbol{C}}_{31}=\{E,\ C_{31}^{+}(\widetilde{2\pi/3}),\ C_{31}^{-}(-\widetilde{2\pi/3})\}$.
e) $\varepsilon=e^{(2\pi/3)i}$.
f) $\tilde{A}(e_z)=\{u(e_z,\theta)\tilde{\theta}|0\leqq\theta\leqq2\pi\}$.

As an illustrative purpose of our method to find the maximal little group: $[\check{G}_0]=[T_1\otimes\check{S}\otimes\check{M}]$ we take up a case in which a group is given by a direct product: $G=G_1\times G_2$. Certain types of the maximal little group $[\check{G}]=[\check{G}_1\otimes\check{G}_2]$ are readily constructed from the knowledge of individual $[\check{G}_i]$, $\Lambda[\check{G}_i]$ and $a[\check{G}_i]$ for each group G_i ($i=1$ or 2), namely, the product-type invariance group $[\check{G}]$ and vector $\Lambda[\check{G}]$ given by

$$[\check{G}]=\{1+a[\check{G}_1]a[\check{G}_2]\}([\check{G}_1]\times[\check{G}_2]),$$
$$\Lambda[\check{G}]=\Lambda[\check{G}_1]\Lambda[\check{G}_2] \tag{3·3}$$

are easily seen to be an invariance group of $\check{G}=\check{G}_1\otimes\check{G}_2$ and its invariance vector.

On the other hand, it is rather difficult to obtain the non-product type invariance group in a general form. However, we have constructed the non-product type invariance groups for several particular cases; that is, $T_1\otimes\check{S}$, $T_1\otimes\check{M}$ and $\check{S}\otimes\check{M}$ using the method of the previous paper.[26] The result is summarized in Table II, furnishing enough information from which we can obtain the invariance group of $\check{G}_0=T_1\otimes\check{S}\otimes\check{M}$.

Now let us enumerate the inert states by constructing the maximal little groups according to the method mentioned above. The inert states are classified into two categories, depending on whether the order parameter is real or complex. We consider each state separately.

3.1. *Real states*

The states with a real order parameter are described in general by

$$\Delta(\boldsymbol{k})=(\sum_{\mu j}A_{\mu j}^{(1)}\tau_\mu\hat{k}_j)\,l_1\,. \tag{3·4}$$

Noting that l_1 is the invariance vector of $[\check{M}]=T=(1, t)$ where T is the group of time reversal transformation, we derive the invariance group of the real state from Eq. (3·3) by putting $G_1=\boldsymbol{O}\times S$, $G_2=M$ and $l_1=\Lambda[\check{G}_2]$ as

$$[\check{G}_0]_{\text{real}}=\{1+a[T_1\otimes\check{S}]a[\check{M}]\}([T_1\otimes\check{S}]\times[\check{M}])$$
$$=\{1+a[T_1\otimes\check{S}]\tilde{\pi}\}([T_1\otimes\check{S}]\times T) \tag{3·5}$$

with the basis

$$\Lambda[\check{G}_0]_{\text{real}}=\Lambda[T_1\otimes\check{S}]. \tag{3·6}$$

Let us first consider the product-type invariance group of $[T_1\otimes\check{S}]$ appearing in Eqs. (3·5) and (3·6). This is also obtained by Eq. (3·3) and Table I:

$$[T_1\otimes\check{S}]_{\text{prod}}=\{1+a[T_1]a[\check{S}]\}([T_1]\times[\check{S}])$$
$$=\{1+a[T_1]u_{2x}\}([T_1]\times A(e_z)) \tag{3·7}$$

with the basis

$$\Lambda[T_1\otimes\check{S}]_{\text{prod}}=\Lambda[T_1]\Lambda[\check{S}]$$
$$=\Lambda[T_1]\tau_z \tag{3·8}$$

and

$$a[T_1\otimes\check{S}]_{\text{prod}}=a[T_1] \quad \text{or} \quad a[\check{S}]. \tag{3·9}$$

From Eqs. (3·5)~(3·9) and Table I we have the following spin axial states and the corresponding little groups:

(c_1)

$$\hat{\Delta}(c_1)=\tau_z\hat{k}_z,$$
$$G(c_1)=(1+C_{2x}\tilde{\pi})(1+C_{2x}u_{2x})[\boldsymbol{C}_4\times A(e_z)\times T], \tag{3·10}$$

(c_2)

$$\hat{\Delta}(c_2)=\frac{1}{\sqrt{2}}\tau_z(\hat{k}_x+\hat{k}_y),$$
$$G(c_2)=(1+C_{2b}\tilde{\pi})(1+C_{2b}u_{2x})[\boldsymbol{C}_{2a}\times A(e_z)\times T], \tag{3·11}$$

(c_3)

$$\hat{\Delta}(c_3)=\frac{1}{\sqrt{3}}\tau_z(\hat{k}_x+\hat{k}_y+\hat{k}_z),$$
$$G(c_3)=(1+C_{2b}\tilde{\pi})(1+C_{2b}u_{2x})[\boldsymbol{C}_{31}\times A(e_z)\times T]. \tag{3·12}$$

We use the same label $a, b, \cdots, h$ for the obtained states as in Barton and Moore[23] (B-M) to emphasize the correspondence between our states and theirs. The three states $c_1\sim c_3$ become equivalent to the c state[23] (or the polar phase) in the absence of the crystal field.

Let us now consider the non-product type invariance group of $[T_1\otimes\check{S}]$ appearing in Eqs. (3·5) and (3·6). The relevant invariance groups are listed in Table II. From the first row of Table II and Eqs. (3·5) and (3·6) we have

(a)

$$\hat{\Delta}(a)=\frac{1}{\sqrt{3}}(\tau_x\hat{k}_x+\tau_y\hat{k}_y+\tau_z\hat{k}_z),$$

$$G(a)={}_{II}\boldsymbol{O}\times T\,. \tag{3·13}$$

This state is identical to the a state in B-M or the so-called B phase in He^3. From the second and third rows in Table II and Eqs. (3·5) and (3·6) we have

(b_1)

$$\hat{\Delta}(b_1)=\frac{1}{\sqrt{2}}(\tau_x\hat{k}_x+\tau_y\hat{k}_y)\,,$$

$$G(b_1)=(1+C_{2x}u_{2y}\tilde{\pi})[{}_{II}\boldsymbol{D}_4\times T]\,, \tag{3·14}$$

(b_2)

$$\hat{\Delta}(b_2)=\frac{1}{\sqrt{6}}\{\tau_x(\hat{k}_y-\hat{k}_z)+\tau_y(\hat{k}_z-\hat{k}_x)+\tau_z(\hat{k}_x-\hat{k}_y)\}\,,$$

$$G(b_2)=(1+C_{2b}u_{2b}\tilde{\pi})[{}_{II}\boldsymbol{C}_{31}\times T]\,. \tag{3·15}$$

We note that in these 6 states obtained so far the order parameters are real and the corresponding invariance groups contain the time reversal group T.

3.2. *Complex states*

The complex states are obtained by non-trivially combining two symmetries of $\boldsymbol{O}\times\check{S}$ and $\check{M}$. Two product-type complex states are derived from Eq. (3·3) by putting $[\check{G}_1]=[T_1\otimes\check{M}]_{non-p}$ and $[\check{G}_2]=[\check{S}]$, or $[\check{G}_1]=[\check{S}\otimes\check{M}]_{non-p}$ and $[\check{G}_2]=[T_1]$.

The f_1 and f_2 states, which are obtained from the second row in Table I, the fourth and fifth rows in Table II and Eq. (3·3), correspond to the f state in B-M or the so-called

Table III. The inert phase and its little group.

state		order parameter	little group $G(\hat{\Delta})$
BW phase	a	$(1/\sqrt{3})(\tau_x\hat{k}_x+\tau_y\hat{k}_y+\tau_z\hat{k}_z)$	${}_{II}\boldsymbol{O}\times T$
planar	b_1	$(1/\sqrt{2})(\tau_x\hat{k}_x+\tau_y\hat{k}_y)$	$(1+C_{2x}u_{2y}\tilde{\pi})\{{}_{II}\boldsymbol{D}_4\times T\}$
phase	b_2	$(1/\sqrt{6}\{\tau_x(\hat{k}_y-\hat{k}_z)+\tau_y(\hat{k}_z-\hat{k}_x)+\tau_z(\hat{k}_x-\hat{k}_y)\}$	$(1+C_{2b}u_{2b}\tilde{\pi})\{{}_{II}\mathrm{C}_{31}\times T\}$
polar	c_1	$\tau_z\hat{k}_z$	$(1+C_{2x}\tilde{\pi})(1+C_{2x}u_{2x})\{\boldsymbol{C}_4\times A(e_z)\times T\}$
phase	c_2	$(1/\sqrt{2})\tau_z(\hat{k}_x+\hat{k}_y)$	$(1+C_{2x}\tilde{\pi})(1+C_{2b}u_{2x})\{\boldsymbol{C}_{2a}\times A(e_z)\times T\}$
	c_3	$(1/\sqrt{3})\tau_z(\hat{k}_x+\hat{k}_y+\hat{k}_z)$	$(1+C_{2b}\tilde{\pi})(1+C_{2b}u_{2x})\{\boldsymbol{C}_{31}\times A(e_z)\times T\}$
α phase	d	$(1/\sqrt{3})(\tau_x\hat{k}_x+\varepsilon\tau_y\hat{k}_y+\varepsilon^2\tau_z\hat{k}_z)$	$(1+tC_{2b})\,{}_{II}\tilde{\boldsymbol{C}}_{31}\,{}_{II}\boldsymbol{D}_2$[a]
bipolar phase	e	$(1/\sqrt{2})(\tau_x\hat{k}_x+i\tau_y\hat{k}_y)$	$(1+tu_{2x})\,{}_{II}\boldsymbol{D}_2\cdot{}_s\tilde{\boldsymbol{C}}_4$[b]
axial	f_1	$(1/\sqrt{2})\tau_z(\hat{k}_x+i\hat{k}_y)$	$(1+u_{2x}\tilde{\pi})(1+tC_{2x})\{\tilde{\boldsymbol{C}}_4\times A(e_z)\}$
phase	f_2	$(1/\sqrt{3})i\tau_z(\hat{k}_z+\varepsilon\hat{k}_x+\varepsilon^2\hat{k}_y)$	$(1+u_{2x}\tilde{\pi})(1+tC_{2x})\{\tilde{\boldsymbol{C}}_{31}\times A(e_z)\}$
β phase	g_1	$(1/\sqrt{2})(\tau_x+i\tau_y)\hat{k}_z$	$(1+C_{2x}u_{2z})(1+tu_{2x})\{\boldsymbol{C}_4\times\tilde{A}(e_z)\}$
	g_2	$(1/2)(\tau_x+i\tau_y)(\hat{k}_x+\hat{k}_y)$	$(1+C_{2b}u_{2z})(1+tu_{2x})\{\boldsymbol{C}_{2a}\times\tilde{A}(e_z)\}$
	g_3	$(1/\sqrt{6})(\tau_x+i\tau_y)(\hat{k}_x+\hat{k}_y+\hat{k}_z)$	$(1+C_{2b}u_{2z})(1+tu_{2x})\{\boldsymbol{C}_{31}\times\tilde{A}(e_z)\}$
γ phase	h_1	$(1/2)(\tau_x+i\tau_y)(\hat{k}_x+i\hat{k}_y)$	$(1+tC_{2x}u_{2x})\{\tilde{\boldsymbol{C}}_4\times\tilde{A}(e_z)\}$
	h_2	$(1/\sqrt{6})i(\tau_x+i\tau_y)(\hat{k}_z+\varepsilon\hat{k}_x+\varepsilon^2\hat{k}_y)$	$(1+tC_{2b}u_{2x})\{\tilde{\boldsymbol{C}}_{31}\times\tilde{A}(e_z)\}$

a) ${}_{II}\tilde{\boldsymbol{C}}_{31}=\{E,\ C_{31}^{+}u(C_{31}^{+})(\widehat{2\pi/3}),\ C_{31}u(C_{31}^{-})(\widehat{-2\pi/3})\}$.

b) ${}_s\tilde{\boldsymbol{C}}_4=\{E,\ C_{4z}^{+}u_{2a}(\widehat{\pi/2}),\ C_{4z}^{-}u_{2a}(\widehat{-\pi/2}),\ C_{2z}\tilde{\pi}\}$.

A phase in He^3.

Similarly from the first row in Table I, the sixth row in Table II and Eq. (3·3) we obtain three states g_1, g_2 and g_3 which are listed in Table III. These correspond to the g state (or the β phase) in B-M. The third type of the complex states h_1 and h_2 is derived from the product: $\Lambda[T_1\otimes\check{M}]_{\text{non-p}}\Lambda[\check{S}\otimes\check{M}]_{\text{non-p}}$ correnponding to the h state (or the γ phase) in B-M.

Finally the fourth type of the complex state are obtained by a nontrivial combination of all the three groups: $\boldsymbol{O}$, S and M. By rather cumbersome application of the method in the previous paper[26] we obtain two states d and e, which coincide with the d state (or a phase) and the e state (or bipolar phase) in B-M.

All these results are summarized in Table III. As is seen in the next section each state enumerated here indeed makes all $R_i(i=1\sim7)$ in the GL free energy functional extremum.

§ 4. Characterization of the states and relative stability

In this section we give some characterization of the p-pairing states listed in the previous section. The temparature dependence of physical quantities at low temperatures such as the specific heat, the ultrasonic attenuation or the nuclear relaxation rate is mainly determined by the topology of zeros in the energy gap. The zeros in the energy gap are given by $\boldsymbol{d}^2(\boldsymbol{k})=0$ on the Fermi surface. In Table IV we show the topology of zeros in the energy gap (lines or points) for each state. It is to be noted that lines of zeros exist for several states. This is contrasted with the strong spin-orbit coupling case treated by others[16),17] where the states with only nodeless or points of zeros in the energy gap are realized for p-pairing.

The unitarity of a state is defined by the condition: $\Delta\Delta^+\propto\sigma_0$ where σ_0 is the 2×2 unit matrix. This can be rewritten[29] as $\boldsymbol{d}(\boldsymbol{k})\times\boldsymbol{d}^*(\boldsymbol{k})=0$. The unitarity property is shown in Table IV. For the non-unitary states a Cooper pair at a point k on the Fermi surface has a net average spin:

$$\boldsymbol{S}(\boldsymbol{k})\propto i\boldsymbol{d}(\boldsymbol{k})\times\boldsymbol{d}^*(\boldsymbol{k})\,. \tag{4·1}$$

Integrating $\boldsymbol{S}(\boldsymbol{k})$ over the Fermi surface we have

$$\langle S_\mu\rangle\propto i\sum_{\nu\lambda l}\varepsilon_{\mu\nu\lambda}A_{\nu l}A^*_{\lambda l}=i\sum_{\nu\lambda}\varepsilon_{\mu\nu\lambda}(AA^+)_{\nu\lambda}\,, \tag{4·2}$$

where μ is the component of the spin direction. This is the coefficient of the linear term of the external field $H=(H_x, H_y, H_z)$ in the GL free energy. The third column in Table IV shows the presence or absence of $\langle S_\mu\rangle$.

The deviation of the zero-field susceptibility χ_{ij} from the normal state value is proportional to $(\boldsymbol{AA}^+)_{ij}$. Therefore the eigenvalues of $\boldsymbol{AA}^+$ determine the magnetic susceptibility in the superconducting state. If none of three eigenvalues vanishes, the susceptibility differs from the normal state value. The three eigenvalues are listed in the fourth column of Table IV.

The fifth column in Table IV shows the symmetry property under the time reversal transformation. Since in the states $d\sim h_2$ the order parameters are complex, the time reversal symmetry is broken in these states.

Table IV.

state	topology of zero gap	unitarity and $\langle \boldsymbol{S} \rangle$	eigenvalues of $\boldsymbol{A}\boldsymbol{A}^+$	time reversal	R_1	R_3[a]	R_4	R_5	R_6	R_7
a	no node	u[b]	$\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$	+[e]	1	1/3	1/3	1/3	1/3	1/3
b_1	points	u	$0, 1, 1$	+	1	1/2	1/2	1/2	1/2	1/2
b_2	points	u	$0, \frac{1}{2}, \frac{5}{6}$	+	1	1/2	1/2	1/2	1/3	1/3
c_1	lines	u	$0, 0, 1$	+	1	1	1	1	1	1
c_2	lines	u	$0, 0, 1$	+	1	1	1	1	1/2	1/2
c_3	lines	u	$0, 0, 1$	+	1	1	1	1	1/3	1/3
d	points	$n, \langle \boldsymbol{S} \rangle = 0$[c]	$\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$	−[f]	0	1/3	1/3	1/3	1/3	1/3
e	points	$n, \langle \boldsymbol{S} \rangle = 0$	$0, \frac{1}{2}, \frac{1}{2}$	−	0	1/2	1/2	1/2	1/2	1/2
f_1	points	u	$0, 0, 1$	−	0	0	1	1	1/2	1/2
f_2	points	u	$0, 0, 1$	−	0	0	1	1	1/3	1/3
g_1	lines	$n, \langle S_z \rangle \neq 0$[d]	$0, 0, 1$	−	0	1	1	0	0	1
g_2	lines	$n, \langle S_z \rangle \neq 0$	$0, 0, 1$	−	0	1	1	0	0	1/2
g_3	lines	$n, \langle S_z \rangle \neq 0$	$0, 0, 1$	−	0	1	1	0	0	1/3
h_1	points	$n, \langle S_z \rangle \neq 0$	$0, 0, \frac{1}{2}$	−	0	0	1	0	0	1/2
h_2	points	$n, \langle S_z \rangle \neq 0$	$0, 0, 1$	−	0	0	1	0	0	1/3

a) Note that $R_2 = [\mathrm{Tr}\boldsymbol{A}\boldsymbol{A}^+]^2 = 1$.
b) u denotes a unitary state.
c) n denotes a non-unitary state. $\langle \boldsymbol{S} \rangle$ is the value defined by Eq. (4·2).
d) $\langle S_z \rangle \neq 0$ means that $\langle S_z \rangle \neq 0$ and $\langle S_x \rangle = \langle S_y \rangle = 0$.
e) + denotes the state which has time reversal symmetry.
f) − denotes the state in which the time reversal symmetry is broken.

In order to know the relative stability of the state in Table IV, it is convenient to rewrite the free energy: Eq. (2·8) in the form

$$F(\Delta, \boldsymbol{A}) = \alpha\Delta^2 + K\Delta^4, \tag{4·3}$$

so that the matrix $\boldsymbol{A}$ can have a standard normalization

$$\mathrm{Tr}\ \boldsymbol{A}\boldsymbol{A}^+ = 1, \tag{4·4}$$

$$K = \sum_{i=1}^{7} \beta_i R_i \tag{4·5}$$

with $R_2 = [\mathrm{Tr}\boldsymbol{A}\boldsymbol{A}^+]^2 = 1$. The parameter Δ is determined by minimizing Eq. (4·3) with respect to Δ at fixed K and α and is given by

$$\Delta^2 = \frac{\alpha'}{2K}\left(1 - \frac{T}{T_c}\right). \tag{4·6}$$

We have taken α in its customary form $-\alpha'(1 - T/T_c)$ where T_c is the transition temperature. The free energy is completely minimized by finding the matrix $\boldsymbol{A}$ for given β_i's, subject to the normalization constraint Eq. (4·4). Such a matrix yields the smallest value of K.

In Table IV we give the values of $R_i(i=1\sim7)$ for each state. Barton and Moore[23] have shown that at the inert stationary point R_1 has the values 0 or 1, R_3 and R_5 have the values 0, 1/3, 1/2 and 1, R_4 has the values 1/3, 1/2 and 1. The new terms R_6 and R_7 are investigated in Appendix B, showing that R_6 has the stationary values 0, 1/3, 1/2 and 1 and that R_7 has the values 1/3, 1/2 and 1. We can see from Table IV that the listed inert states indeed take the stationary values for each $R_i(i=1\sim7)$.

We can also see that the b_1, b_2 and c_2 states cannot give the absolute minimum of the free energy F because $F(b_1)$ lies between $F(a)$ and $F(c_1)$, $F(b_2)$ lies between $F(a)$ and $F(c_3)$ and $F(c_2)$ lies between $F(c_1)$ and $F(c_3)$ irrespective of the values of $\beta_i(i=1\sim7)$. The relative stability of the states is determined once a set of the values of β_i is given which should be calculated by a microscopic model Hamiltonian.

It should be noted that in the listed states the spin direction is arbitrary, therefore each state has continuous degeneracy with respect to the spin rotation. This is contrasted with the case by others[15)~17] in which their states have discrete degeneracy with respect to the spin rotation because the orbital and spin parts in the order parameters are not independent and are coupled due to the spin-orbit coupling.

§ 5. Discussion and conclusion

We compare the p-pairing states which are derived by Volovik and Gorkov,[16] and Ueda and Rice[17] when the spin-orbit coupling is strong. In the strong spin-orbit coupling the 18 dimensional irreducible representation space: $E_0=\{\boldsymbol{A}=\boldsymbol{A}^{(1)}+i\boldsymbol{A}^{(2)}\}$ of the order parameter is decomposed into the irreducible components of ${}_{II}\boldsymbol{O}\times M$, that is, $A_1\otimes\check{M}+E\otimes\check{M}+T_1\otimes\check{M}+T_2\otimes\check{M}$ which have dimensions 2, 4, 6 and 6 respectively. They have solved the variational problem in each irreducible space to find stable states.[17] Here according to the notation by Ueda and Rice[17] (U-R), let us compare their states with ours: The A_1 states in U-R is equivalent to the a state in our theory. One of the states among the three E states in U-R (the first one in Table II in U-R,[17] we denote it $E^{(1)}$ and so on hereafter) is equivalent to the b_1 states because the equivalence can easily be seen from the following transformation:

$$u_{2x}\hat{\Delta}(E^{(1)})=u_{2x}\frac{1}{\sqrt{2}}(\tau_x\hat{k}_x-\tau_y\hat{k}_y)$$

$$=\frac{1}{\sqrt{2}}(\tau_x\hat{k}_x+\tau_y\hat{k}_y)=\hat{\Delta}(b_1)\ .$$

In the same way we can see that $T_1^{(1)}$ and $T_2^{(1)}$ are equivalent to b_1, and that $E^{(3)}$ and $T_1^{(2)}$ are equivalent to d and b_2 respectively. The other states in U-R are not stationary point in our larger variational space E_0 anymore. The obtained p-pairing states have continuous degeneracy with respect to the spin rotation while in the strong spin-orbit case U-R degeneracy is discrete as is mentioned before. In some of our states the energy gap vanishes on lines of the Fermi surface in contrast with the strong spin-orbit case[17] where the zeros of the energy gap are isolated points or none.

In summary, we have enumerated all the possible inert p-wave pairing states under cubic symmetry. Volovik and Gorkov[16] enumerate both singlet and triplet pairing states in the strong spin-orbit coupling case. Their classification of the singlet pairing states is

valid also for the case in the absence of the spin-orbit coupling. Therefore our work, together with Volovik and Gorkov exhausts all possible non-trivial s-, p- and d-pairing states under cubic crystalline symmetry.

The present work might help to examine the nature of exotic superconductivity observed in heavy Fermion materials.

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Appendix A

——Derivation of the Fourth Order Terms——

We derive the fourth order terms in the GL free energy. We first note that in order that the fourth order term is invariant under gauge transformation, it must be written by a sum of the form $A_{\mu i}A_{\nu j}A^*_{\rho k}A^*_{\lambda l}$. Since $A_{\mu i}$ transforms by the T_1 representation of $\boldsymbol{O}$ with respect to the suffix i, the space $\{A_{\mu i}A_{\nu j}\}^{(\mu,\nu)}$, spanned by $A_{\mu i}A_{\nu j}$ $(i,j=x,y\,z)$ for fixed μ and ν over the complex number field, is decomposed into the irreducible components of $\boldsymbol{O}$ according to $T_1\times T_1=A_1+E+T_1+T_2$. The basis φ of each component is explicitly written with the aid of the Clebsch-Gordan coefficient as

A_1:

$$\varphi(A_1,\mu,\nu)=\frac{1}{\sqrt{3}}(A_{\mu 1}A_{\nu 1}+A_{\mu 2}A_{\nu 2}+A_{\mu 3}A_{\nu 3})\,, \tag{A·1}$$

E:

$$\varphi_1(E,\mu,\nu)=\frac{1}{\sqrt{6}}(A_{\mu 1}A_{\nu 1}+A_{\mu 2}A_{\nu 2}-2A_{\mu 3}A_{\nu 3})\,,$$

$$\varphi_2(E,\mu,\nu)=\frac{1}{\sqrt{2}}(-A_{\mu 1}A_{\nu 1}+A_{\mu 2}A_{\nu 2})\,, \tag{A·2}$$

T_1:

$$\varphi_1(T_1,\mu,\nu)=\frac{1}{\sqrt{2}}(A_{\mu 2}A_{\nu 3}-A_{\mu 3}A_{\nu 2})\,,$$

$$\varphi_2(T_1,\mu,\nu)=\frac{1}{\sqrt{2}}(A_{\mu 3}A_{\nu 1}-A_{\mu 1}A_{\nu 3})\,,$$

$$\varphi_3(T_1,\mu,\nu)=\frac{1}{\sqrt{2}}(A_{\mu 1}A_{\nu 2}-A_{\mu 2}A_{\nu 1})\,, \tag{A·3}$$

T_2:

$$\varphi_1(T_2,\mu,\nu)=\frac{1}{\sqrt{2}}(A_{\mu 2}A_{\nu 3}+A_{\mu 3}A_{\nu 2})\,,$$

$$\varphi_2(T_2,\mu,\nu)=\frac{1}{\sqrt{2}}(A_{\mu 3}A_{\nu 1}+A_{\mu 1}A_{\nu 3}),$$

$$\varphi_3(T_2,\mu,\nu)=\frac{1}{\sqrt{2}}(A_{\mu 1}A_{\nu 2}+A_{\mu 2}A_{\nu 1}). \qquad (A\cdot 4)$$

Similarly $\{A^*_{\rho k}A^*_{\lambda l}\}^{(\rho,\lambda)}$ for fixed ρ and λ is decomposed into the irreducible components: $A_1+E+T_1+T_2$ with the basis $\varphi^*(A_1,\rho,\lambda)$, $\varphi_1{}^*(E,\rho,\lambda)$ etc. Since the invariant of the product representation comes only from the product of the same representation, we obtain the following four types of the fourth order invariants under $\boldsymbol{O}$ for fixed μ, ν, ρ and λ:

$$I(A_1)=\varphi(A_1,\mu,\nu)\varphi^*(A_1,\rho,\lambda), \qquad (A\cdot 5)$$

$$I(E)=\sum_{s=1}^{2}\varphi_s(E,\mu,\nu)\varphi_s{}^*(E,\rho,\lambda), \qquad (A\cdot 6)$$

$$I(T_1)=\sum_{s=1}^{3}\varphi_s(T_1,\mu,\nu)\varphi_s{}^*(T_1,\rho,\lambda), \qquad (A\cdot 7)$$

$$I(T_2)=\sum_{s=1}^{3}\varphi_s(T_2,\mu,\nu)\varphi_s{}^*(T_2,\rho,\lambda). \qquad (A\cdot 8)$$

Rearranging the combination of the four invariants in Eqs. (A·5)~(A·8) as $I_1=3I(A_1)$, $I_2=I(A_1)+I(E)$, $I_3=I(A_1)+I(E)+I(T_1)+I(T_2)$ and $I_4=I(A_1)+I(E)-I(T_1)+I(T_2)$, we have

$$I_1=\sum_{i,j}(A_{\mu i}A_{\nu i})(A^*_{\rho j}A^*_{\lambda j}), \qquad (A\cdot 9)$$

$$I_2=\sum_{i}A_{\mu i}A_{\nu i}A^*_{\rho i}A^*_{\lambda i}, \qquad (A\cdot 10)$$

$$I_3=\sum_{i,j}(A_{\mu i}A^*_{\rho i})(A_{\nu j}A^*_{\lambda j}), \qquad (A\cdot 11)$$

$$I_4=\sum_{i,j}(A_{\mu i}A^*_{\lambda i})(A_{\nu j}A^*_{\rho j}). \qquad (A\cdot 12)$$

On the other hand, $A_{\mu i}$ transforms by the representation ($L=1$) of $SO(3)$ with respect to the suffix μ. Therefore the space $\{A_{\mu i}A_{\nu i}\}^{(i,j)}$ for fixed i and j is decomposed as

$$\{A_{\mu i}A_{\nu j}\}^{(i,j)}=\{A_{\mu i}A_{\nu j}\}^{(i,j)}_{L=2}+\{A_{\mu i}A_{\nu j}\}^{(i,j)}_{L=1}+\{A_{\mu i}A_{\nu j}\}^{(i,j)}_{L=0}, \qquad (A\cdot 13)$$

where $\{A_{\mu i}A_{\nu j}\}^{(i,j)}_{L=n}$ denotes the $L=n$ irreducible representation space of $SO(3)$ spanned by $A_{\mu i}A_{\nu j}$ ($\mu,\nu=x,y,z$) for fixed i and j. In the same way we have

$$\{A^*_{\rho k}A^*_{\lambda l}\}^{(k,l)}=\{A^*_{\rho k}A^*_{\lambda l}\}^{(k,l)}_{L=2}+\{A^*_{\rho k}A^*_{\lambda l}\}^{(k,l)}_{L=1}+\{A^*_{\rho k}A^*_{\lambda l}\}^{(k,l)}_{L=0}. \qquad (A\cdot 14)$$

Using a similar discussion in the case $\boldsymbol{O}$, we obtain three $SO(3)$ invariants: K_1, K_2 and K_3 of the product representation as

$$K_1=\sum_{\mu,\nu}(A_{\mu i}A_{\mu j})(A^*_{\nu k}A^*_{\nu l}), \qquad (A\cdot 15)$$

$$K_2=\sum_{\mu,\nu}(A_{\mu i}A^*_{\mu k})(A_{\nu j}A^*_{\nu l}), \qquad (A\cdot 16)$$

$$K_3=\sum_{\mu,\nu}(A_{\mu i}A^*_{\mu l})(A_{\nu j}A^*_{\nu k}) \qquad (A\cdot 17)$$

for fixed i, j, k and l.

From the compatibility condition of both sets of the invariants: $\{I_1, I_2, I_3, I_4\}$ and $\{K_1, K_2, K_3\}$ we finally obtain the following seven kinds of the fourth order invariants under $G_0 = \boldsymbol{O} \times S \times M$:

$$R_1 = \sum_{\mu\nu}\sum_{ij} A_{\mu i} A_{\mu i} A^*_{\nu j} A^*_{\nu j} = (\mathrm{Tr}\boldsymbol{A}\tilde{\boldsymbol{A}})(\mathrm{Tr}\boldsymbol{A}\tilde{\boldsymbol{A}})^*, \tag{A·18}$$

$$R_2 = \sum_{\mu\nu}\sum_{ij} A_{\mu i} A_{\nu j} A^*_{\mu i} A^*_{\nu j} = [\mathrm{Tr}\boldsymbol{A}\boldsymbol{A}^+]^2, \tag{A·19}$$

$$R_3 = \sum_{\mu\nu}\sum_{ij} A_{\mu i} A_{\nu i} A^*_{\mu j} A^*_{\nu j} = \mathrm{Tr}[\boldsymbol{A}^+\boldsymbol{A}(\boldsymbol{A}^+\boldsymbol{A})^*], \tag{A·20}$$

$$R_4 = \sum_{\mu\nu}\sum_{ij} A_{\mu i} A_{\nu j} A^*_{\nu i} A^*_{\mu j} = \mathrm{Tr}[\boldsymbol{A}\boldsymbol{A}^+\boldsymbol{A}\boldsymbol{A}^+], \tag{A·21}$$

$$R_5 = \sum_{\mu\nu}\sum_{ij} A_{\mu i} A_{\mu j} A^*_{\nu j} A^*_{\nu i} = \mathrm{Tr}[\boldsymbol{A}\boldsymbol{A}^+(\boldsymbol{A}\boldsymbol{A}^+)^*], \tag{A·22}$$

$$R_6 = \sum_{\mu\nu}\sum_{i} A_{\mu i} A_{\mu i} A^*_{\nu i} A^*_{\nu i} = \sum_i (\tilde{\boldsymbol{A}}\boldsymbol{A})_{ii} (\tilde{\boldsymbol{A}}\boldsymbol{A})^*_{ii}, \tag{A·23}$$

$$R_7 = \sum_{\mu\nu}\sum_{i} A_{\mu i} A_{\nu i} A^*_{\mu i} A^*_{\nu i} = \sum_i (\boldsymbol{A}^+\boldsymbol{A})^2_{ii}, \tag{A·24}$$

where $\tilde{\boldsymbol{A}}$ is the transposed, $\boldsymbol{A}^+$ hermitian conjugate and $\boldsymbol{A}^*$ complex conjugate matrices of $\boldsymbol{A}$.

Appendix B

—— *Extrema of* R_6 *and* R_7 ——

We write the complex element $A_{\mu i}$ of the 3×3 matrix $\boldsymbol{A}$ in terms of the amplitude and its phase; $A_{\mu i} \equiv C_{\mu i} \exp i\varphi_{\mu i}$. The normalization condition $\mathrm{Tr}\boldsymbol{A}\boldsymbol{A}^+ = 1$ is written as

$$\sum_i (C^2_{xi} + C^2_{yi} + C^2_{zi}) = 1. \tag{B·1}$$

Let us first consider extrema of R_7 which is expressed as

$$\begin{aligned} R_7 &= \textstyle\sum_i (\boldsymbol{A}^+\boldsymbol{A})_{ii} (\boldsymbol{A}^+\boldsymbol{A})_{ii} \\ &= \textstyle\sum_i \sum_{\mu\nu} A^*_{\mu i} A_{\mu i} A^*_{\nu i} A_{\nu i} \\ &= \textstyle\sum_i (C^2_{xi} + C^2_{yi} + C^2_{zi})^2 . \end{aligned} \tag{B·2}$$

Introducting the Lagrange multiplier λ, we examine the extremum of the function Ψ:

$$\Psi = R_7 - \lambda\{\textstyle\sum_i (C^2_{xi} + C^2_{yi} + C^2_{zi}) - 1\}. \tag{B·3}$$

The extremum conditions with respect to $C_{\mu i}$ and $\varphi_{\mu i}$ $(\mu = x, y, z)$ yield

$$\begin{aligned} C_{xi}(C^2_{xi} + C^2_{yi} + C^2_{zi}) &= \lambda C_{xi}, \\ C_{yi}(C^2_{xi} + C^2_{yi} + C^2_{zi}) &= \lambda C_{yi}, \\ C_{zi}(C^2_{xi} + C^2_{yi} + C^2_{zi}) &= \lambda C_{zi}. \qquad (i = x, y, z) \end{aligned} \tag{B·4}$$

When all the $C_{\mu i}$'s are non-vanishing, then we obtain

$$C^2_{xi} + C^2_{yi} + C^2_{zi} = \lambda. \quad (i = x, y, z) \tag{B·5}$$

Therefore the extrema of R_7 are $R_7^{ex}=1/3$ when Eq. (B·5) is satisfied for all $i(i=x, y, z)$, $R_7^{ex}=1/2$ and 1 when two of i and one of i among $i=x, y$ and z satisfy Eq. (B·5).

Let us consider R_6 which is rewritten as

$$\begin{aligned}R_6&=\sum_i(\tilde{A}A)_{ii}(\tilde{A}A)^*_{ii}\\&=\sum_i\sum_{\mu\nu}A^*_{\mu i}A^*_{\mu i}A_{\nu i}A_{\nu i}\\&=\sum_i[C^4_{xi}+C^4_{yi}+C^4_{zi}+2C^2_{xi}C^2_{yi}\cos2(\varphi_{xi}-\varphi_{yi})\\&\quad+2C^2_{yi}C^2_{zi}\cos2(\varphi_{yi}-\varphi_{zi})+2C^2_{zi}C^2_{xi}\cos2(\varphi_{zi}-\varphi_{xi})]\,.\end{aligned}\tag{B·6}$$

The extremum conditions for $C_{\mu i}$ and $\varphi_{\mu i}$ $(\mu=x, y, z)$ yield

$$\begin{aligned}&C_{xi}[C^2_{xi}+C^2_{yi}\cos2(\varphi_{xi}-\varphi_{yi})+C^2_{zi}\cos2(\varphi_{xi}-\varphi_{zi})]=\lambda C_{xi}\,,\\&C_{yi}[C^2_{xi}\cos2(\varphi_{yi}-\varphi_{xi})+C^2_{yi}+C^2_{zi}\cos2(\varphi_{yi}-\varphi_{zi})]=\lambda C_{yi}\,,\\&C_{zi}[C^2_{xi}\cos2(\varphi_{zi}-\varphi_{xi})+C^2_{yi}\cos2(\varphi_{zi}-\varphi_{yi})+C^2_{zi}]=\lambda C_{zi}\,;\end{aligned}\tag{B·7}$$

$$\begin{aligned}&C^2_{xi}[C^2_{yi}\sin2(\varphi_{xi}-\varphi_{yi})+C^2_{zi}\sin2(\varphi_{xi}-\varphi_{zi})]=0\,,\\&C^2_{yi}[C^2_{zi}\sin2(\varphi_{yi}-\varphi_{zi})+C^2_{xi}\sin2(\varphi_{yi}-\varphi_{xi})]=0\,,\\&C^2_{zi}[C^2_{xi}\sin2(\varphi_{zi}-\varphi_{xi})+C^2_{yi}\sin2(\varphi_{zi}-\varphi_{yi})]=0\,,\end{aligned}\tag{B·8}$$

where λ is a Lagrange multiplier.

(i) $\varphi_{xi}=\varphi_{yi}=\varphi_{zi}$

In this case Eqs. (B·7) and (B·8) are reduced to Eq. (B·4), thus giving rise to $R_6^{ex}=\frac{1}{3}$, $\frac{1}{2}$ and 1.

(ii) $\varphi_{xi}=\varphi_{yi}\neq\varphi_{zi}$

From Eq. (B·8) we obtain $C_{xi}=C_{yi}=0$ or $C_{zi}=0$, then Eq. (B·7) becomes independent of φ_{xi} and φ_{yi}. The problem is reduced to that of R_7, giving rise to $R_6^{ex}=1/3$, $1/2$ and 1.

(iii) $\varphi_{xi}\neq\varphi_{yi}\neq\varphi_{zi}$

When $C_{zi}=0$, then $C_{yi}=0$ or $C_{xi}=0$. Therefore the problem is reduced again to that of R_7. When $C_{xi}\neq0$, $C_{yi}\neq0$ and $C_{zi}\neq0$, Eq. (B·8) becomes

$$\begin{aligned}C^2_{yi}&=-C^2_{xi}\frac{\sin2(\varphi_{zi}-\varphi_{yi})}{\sin2(\varphi_{zi}-\varphi_{xi})}\,,\\C^2_{zi}&=-C^2_{xi}\frac{\sin2(\varphi_{yi}-\varphi_{zi})}{\sin2(\varphi_{yi}-\varphi_{xi})}\,.\end{aligned}\tag{B·9}$$

This readily yields $R_6^{ex}=\lambda=0$ by using Eq. (B·7).

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