Group Theoretical Analysis of the Lattice Distorsion in Anisotropic Superconductivity

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ABSTRACT

This report describes the group theoretical determination of the possible type of the uniform lattice distortion associated with the superconducting transition when the order parameter belongs to a degenerate representation of the symmetry group of the system. The method uses the symmetrical property of the Ginzburg-Landau functional with the lattice distortion. Systems with hexagonal (D_6) and tetragonal (D_4) symmetry are studied in the presence of the spin-orbit coupling. It is shown that all states (except 3 states) with the order parameter of the degenerate representation in regard to D_6 or D_4 are unstable to the lattice distortion which breaks the symmetrical configuration.

§1 Introduction

Recently much attention has been focused on heavy electron system such as UBe_{13}, UPt_3 and Ce Cu_2 Si_2. One of the most controversial points is the nature of the superconductivity : Whether it is a conventional singlet or triplet pairing. Volovik and Gor'kov[1)], Ueda and Rice[2)], Blount[3)], Ozaki et al[4)] have investigated the possible anisotropic pairing states using a Ginzburg-Landau theory. A clear identification of the phase has not until now been achieved. Recently Joynt and Rice[5)] have pointed out that a uniform lattice strain is associated with the superconducting transition when the order parameter is anisotropic. In my previous paper[6)] I have described the group theoretical method for determining of the spontaneous crystal symmetry lowering at the phase transition to the anisotropic superconductivity. In the paper the cubic system was studied in detail in the presence and the absence of the spin-orbit coupling. In this report I examine both of hexagonal (D_6) and tetragonal (D_4) systems in the presence of the spin-orbit coupling by this group theoretical method.

§2 The Ginzburg-Landau (GL) functional with the lattice distortion.

At the original lattice configuration $R=R_0$, the system has the symmetry group $G_0={}_{II}P\times M$ due to the spin-obit coupling, where ${}_{II}P=\{pu(p)|p\varepsilon P\}$, $u(p)$ is the spin rotation about the same rotation axis by the same rotation angle as $p\varepsilon P$, P is D_6 or D_4, $M=\Phi+t\Phi$, $\Phi=\{\gamma\}$ and t are the group of the gauge and the time reversal transformation. For either case of singlet (s=0) or triplet (s=1) the superconductivity transition is classified by the single valued irreducible representation Γ of ${}_{II}P$ such as A_1, A_2, B_1, B_2, E_1 and E_2 for ${}_{II}D_6$, A_1, A_2, B_1, B_2 and E for ${}_{II}D_4$. Thus the order parameter corresponding to the representation Γ is given by

$$\Delta(k) = \sum_j \lambda_j d(\Gamma,j) \qquad (2\cdot 1)$$

where λ_j is a complex number and $d(\Gamma,j)$ is the basis function belonging to the representation Γ. The bases corresponding to degenerate representations are listed in Table I.

Table I Basis functions of degenerate representation of D_6 and D_4

Γ	basis function $d(\Gamma,j)$
D_6 : E_1	(s=0) $(k_zk_y, -k_zk_x)\tau_0$
	(s=1) $(\tau_zk_y, -\tau_zk_x)$, $(\tau_yk_z, -\tau_xk_z)$
E_2	(s=0) $(k_x^2-k_y^2, 2k_xk_y)\ \tau_0$
	(s=1) $(\tau_xk_x-\tau_yk_y, \tau_xk_y+\tau_yk_x)$
D_4 : E	(s=0) $(k_zk_y, -k_zk_x)\tau_0$
	(s=1) $(\tau_zk_y, -\tau_zk_x)$, $(\tau_yk_z, -\tau_xk_z)$

$(\tau_j = i\delta_j\delta_y)$

G_0 action on $\{\lambda_j\}$ is given by

$$pu(p)\mathfrak{d}\lambda_j = \sum_{j} D^{\Gamma}(p)_{jj'}\, e^{i\phi}\lambda_{j'}$$

$$tpu(p)\mathfrak{d}\lambda_j = \sum_{j'} D^{\Gamma}(p)_{jj'} e^{-i\phi}\lambda_j^{*} \qquad (2\cdot 2)$$

where $D^{\Gamma}(p)$ is the representation matrix of Γ.

Now let us define the G_0 action on the lattice configuration R as follows :

$$pu(p)\mathfrak{d}R = pR, \quad tpu(p)\mathfrak{d}R = pR \qquad (2\cdot 3)$$

where pR is the lattice configuration obtained by rotating R by $p\varepsilon P$. Then we consider the lattice configuration which can be obtained from the given symmetrical configuration R_0 ($PR_0 = R_0$) by adding a linear combination of the irreducible normal modes $Q(\gamma;m)$,

$$R = R_0 + \sum_{\gamma}\sum_{m} Q(\gamma;m)\eta(\gamma;m) \qquad (2\cdot 4)$$

where γ denotes the irreducible representation of P and $\eta(\gamma;m)$ is a small real number. Then $\eta(\gamma;m)$ transforms as follows ;

$$pu(p)\mathfrak{d}\eta(\gamma;m) = \sum_{m} D^{\gamma}(p)_{mm'}\, \eta(\gamma;m')$$

$$tpu(p)\mathfrak{d}\eta(\gamma;m) = \sum_{m'} D^{\gamma}(p)_{mm'}\, \eta(\gamma;m') \qquad (2\cdot 5)$$

Let $F(\eta,\lambda)$ be the GL functional at the lattice configuration $R(\eta)$. Then $F(\eta,\lambda)$ is invariant to a simultaneous G_0 action on η and λ ;

$$F(g\eta,g\lambda) = F(\eta,\lambda) \text{ for } g\varepsilon G_0 \qquad (2\cdot 6)$$

From this invariance the expansion of $F(\eta,\lambda)$ up to the fourth order of λ and the second of η has the form

$$F(\eta,\lambda) = F(0,\lambda) + \sum_{\gamma} C(\gamma) \sum_{m} V(\gamma;\lambda)_m \eta(\gamma;m)$$

$$+ \sum_{\gamma} B(\gamma) \sum_{m}\eta(\gamma;m)^2 \qquad (2\cdot 7)$$

where $F(0,\lambda)$ is GL functional at $R = R_0$ (η=0) which is given in reference 1), $V(\gamma;\lambda)_m$ is the irreducible bilinear form of λ and λ^* of the relevant representaion Γ, which are given in Table II, and $C(\gamma)$ and $B(\gamma)$ are real numbers.

Table II The irreducible bilinear form $V(\gamma,\lambda)_m$ for degenerate instability of D_6 and D_4

the representation of the instability	$V(\gamma,\lambda)$
D_6 : E_1	$V(A_1;\lambda) = \lambda_1{}^*\lambda_1 + \lambda_2{}^*\lambda_2$ $V(E_2;\lambda)_1 = \lambda_1{}^*\lambda_1 - \lambda_2{}^*\lambda_2$ $V(E_2;\lambda)_2 = \lambda_1{}^*\lambda_2 + \lambda_2{}^*\lambda_1$
E_2	$V(A_1;\lambda) = \lambda_1{}^*\lambda_1 + \lambda_2{}^*\lambda_2$ $V(E_2:\lambda)_1 = -\lambda_1{}^*\lambda_1 +\lambda_2{}^*\lambda_2$ $V(E_2;\lambda)_2 = \lambda_1{}^*\lambda_2+ \lambda_2{}^*\lambda_1$
D_4 : E	$V(A_1;\lambda) = \lambda_1{}^*\lambda_1 + \lambda_2{}^*\lambda_2$ $V(B_1;\lambda)_1 = \lambda_1{}^*\lambda_1 - \lambda_2{}^*\lambda_2$ $V(B_2;\lambda)_2 = \lambda_1{}^*\lambda_2 + \lambda_2{}^*\lambda_1$

§3 The Possible lattice distortion

Using the generalized Hellmann-Feynman theorem[6], we have the free energy $E(\eta)$ up to the first order of $\eta(\gamma;m)$

$$E(\eta) = E(0) + \sum_{\gamma} C\,(\gamma) \sum_{m} V\,(\gamma;\lambda_0)\;\eta(\gamma;m) \tag{3·1}$$

where $E(0)$ is the free energy at $\eta = 0$, λ_0 is the minimum point λ at $\eta = 0$ and the normalized value of λ_0 is given in the second column of Table III. If $V(\gamma;\lambda_0)_m \neq 0$ for some (γ,λ_0), the lattice distortion $\eta(\gamma;m)$ proportional to $V(\gamma;\lambda_0)_m$ must occur. For example in the $D_2(C_{2x})\times R$ state (in the notation of Volovik and Gor'kov[1]) of E_1

transition of D_6 system, $\lambda_0 = (1.0)$. Thus we have from Table II, $V(A_1;\lambda_0) = 1$, $V(E_2;\lambda_0)_1 = 1$ and $V(E_2;\lambda_0)_2 = 0$.

Table III Classes of singlet or triplet superconductivity derived by degenerate instability, their possible lattice distortion and the residual point symmetry for D_6 and D_4

class	order parameter λ_0	lattice distortion	residual point symmetry
D_6:E_1			
$D_6(E)$[a]	$(1/\sqrt{2})(1,i)$	..... b)	D_6
$D_2(C_{2x})$[c]$\times R$[d]	$(1,0)$	$\eta(E_2;1)$	D_2
$C_2(E)\times R$	$(1/\sqrt{2})(1,1)$	$\eta(E_2;2)$	C_2
D_6:E_2			
$D_6(C_2)$	$(1/\sqrt{2})(1,i)$	.....	D_6
$D_2\times R$	$(1,0)$	$\eta(E_2;1)$	D_2
$D_2(C_2)\times R$	$(0,1)$	$\eta(E_2;2)$	D_2
D_4:(E)			
$D_4(E)$	$(1/\sqrt{2})(1,i)$	.....	D_4
$D_2(C_{2x})\times R$	$(1,0)$	$\eta(B_1)$	D_2
$D_2(C_{2y})\times R$	$(0,1)$	$\eta(B_1)$	D_2

notes to Table III

a) For class we use Volovik and Gor'kov notation.

b) All states have non-zero $\eta(A_1)$ and it is not listed in this Table.

c) $D_2(C_{2x}) = (E, C_{2x}, C_{2y}e^{i\pi}, C_{2z}e^{i\pi})$

d) R : time reversal operation

Then we can expect the lattice distortion to the direction $\eta(E_2;1)$. The distorted lattice has the residual point symmetry D_2. In Table III, I list the type of the possible lattice distortion and its residual point symmetry. Note that the residual point symmetry P' of the distorted lattice has the form

$$P' = \{p \varepsilon P \mid pu(p)\phi \text{ or } tpu(p)\phi \varepsilon G_1\} \tag{3·2}$$

where G_1 is the invariance group of λ_0.

References

1) G.E. Volovik and L.P. Gor'kov, JETP 61 843 (1985)

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3) E.I. Blount, Phys. Rev. B32 2935 (1985)

4) M. Ozaki, K. Machida and T. Ohmi, Prog. Theor. Phys. 74 221 (1986) 75 422 (1986)

5) R. Joynt and T.M. Rice, Phys. Rev. B32 6074 (1985)

6) M. Ozaki, Prog. Theor. Phys. 76 1008 (1986)