Symmetry of the order parameter for high-temperature superconductivity

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January 21, 2025

Outline

Introduction

Ginzburg-Landau equation:

$$f[\Delta] = \alpha_{ij}\Delta_i^*\Delta_j + \beta_{ijkl}\Delta_i^*\Delta_j^*\Delta_k\Delta_l + K_{ijkl}\partial_i\Delta_j^*\partial_k\Delta_l \tag{1}$$

$$G = G_0 \times U(1) \times T \tag{2}$$

$\Delta \rightarrow R^{ij}(g_0)exp(i\phi)\Delta_j$, then the first term of 1 will be:

$$\alpha_{ij}R_{ik}(g)R_{jl}^*(g)\Delta_k^*\Delta_l = R_{ki}^\dagger(g)\alpha_{ij}R_{jl}(g)\Delta_k^*\Delta_l$$

To be invariant we should have:

$$R_{ki}^\dagger(g)\alpha_{ij}R_{jl}(g) = \alpha_{kl}$$

or in another form:

$$R(g)\alpha = \alpha R(g)$$

Schur's Lemma

Have the form

$$[\alpha_{ij}] = \begin{bmatrix} \begin{bmatrix} \alpha^1 & 0 \\ 0 & \alpha^1 \end{bmatrix} & 0 & \cdots \\ 0 & \begin{bmatrix} \alpha^2 & \cdots \\ \vdots & \ddots \end{bmatrix} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \tag{3}$$

$$\Delta_i = \sum_{j=1}^{g} \eta_j x_i^{(j)} \tag{4}$$

What is $\mathbf{x}^{(j)}$:
Matrix that diagonalizes α_{ij}.
${x^{(j)}}_i$, A matrix.

$$\Delta_j \to \sum_i \Gamma_{ij}(g)\Delta_i = \sum_{l,k} \Gamma'_{lk}\eta_l x_j^{(k)} \tag{5}$$

Left $=$ Right, we have:

$$\sum_{i,l} \Gamma_{ij} x_i^{(l)} \eta_l = \sum_{l,k} \Gamma'_{lk} x_j^{(k)} \eta_l \tag{6}$$

Comparing term of η_l

$$\Gamma'_{lk} {x^{(k)}}_j = {x^{(l)}}_i \gamma_{ij} \tag{7}$$

$$\Gamma' = X\Gamma X^{-1} \tag{8}$$

η_i and Δ_i transform according to the same representation.

$$f[\eta] = \alpha(T - T_c)\eta_i^*\eta_i + \beta_{ijkl}\eta_i^*\eta_j^*\eta_k\eta_l + K_{ijkl}\partial_i\eta_j^*\partial_k\eta_l + \cdot \tag{9}$$

$$G = SO(3) \times G_c \times U(1) \times T \tag{10}$$

For $SO(3)$: singlet and triplet.
For G_c: determined by crystal structure.Here we consider Orthorhombic symmetry and Tetragonal symmetry.(table)

$\Delta_i^* \Delta_j$ transform under the direct product of representations $\Gamma^* \otimes \Gamma = \Gamma_1 \oplus \cdots$, which can be rewrite as a direct sum of irreducible representations.

To get the appropriate linear combination, we should get the **C-G coefficients**.

Projection Method

Example:

The basis of representation $E_g \otimes E_g^*$ is $\{\eta_1\eta_1^*, \eta_1\eta_2^*, \eta_2\eta_1^*, \eta_2\eta_2^*\}$, which transform like the direct product matrices of E_g and E_g^*.

Table 2. Group character tables for the (*a*) D_{2h} point group and (*b*) the D_{4h} point group.

D_{2h} basis	Representation	E	C_2^z	C_2^y	C_2^x	i	iC_2^z	iC_2^y	iC_2^x
1	A_{1g}	1	1	1	1	1	1	1	1
XY	B_{1g}	1	1	−1	−1	1	1	−1	−1
XZ	B_{2g}	1	−1	1	−1	1	−1	1	−1
YZ	B_{3g}	1	−1	−1	1	1	−1	−1	1
XYZ	A_{1u}	1	1	1	1	−1	−1	−1	−1
Z	B_{1u}	1	1	−1	−1	−1	−1	1	1
Y	B_{2u}	1	−1	1	−1	−1	1	−1	1
X	B_{3u}	1	−1	−1	1	−1	1	1	−1

(*a*)

D_{4h} basis	Representation	E	C_2	$2C_4$	$2C'_2$	$2C''_2$	i	iC_2	$2iC_4$	$2iC'_2$	$2iC''_2$
1	A_{1g}	1	1	1	1	1	1	1	1	1	1
$XY(X^2-Y^2)$	A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1
(X^2-Y^2)	B_{1g}	1	1	−1	1	−1	1	1	−1	1	−1
XY	B_{2g}	1	1	−1	−1	1	1	1	−1	−1	1
(XZ,YZ)	E_g	2	−2	0	0	0	2	−2	0	0	0
$XYZ(X^2-Y^2)$	A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1
Z	A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1
XYZ	B_{1u}	1	1	−1	1	−1	−1	−1	1	−1	1
$Z(X^2-Y^2)$	B_{2u}	1	1	−1	−1	1	−1	−1	1	1	−1
(X,Y)	E_u	2	−2	0	0	0	−2	2	0	0	0

(*b*)

Table 3. The four possible order parameters which can occur for the high-temperature superconductors. The equation number of the free energy for each is also given.

Order parameter	Space representations	Spin representations	Free energy
η	orthorhombic tetragonal A_1,A_2, B_1,B_2	singlet triplet (strong spin–orbit)	2.9
(η_1,η_2)	tetragonal E	singlet triplet (strong spin–orbit)	2.10
(η_1,η_2,η_3)	orthorhombic tetragonal A_1,A_2, B_1,B_2	triplet (weak spin–orbit)	2.11
$\begin{bmatrix} \eta_{11} & \eta_{21} & \eta_{31} \\ \eta_{21} & \eta_{22} & \eta_{32} \end{bmatrix}$	tetragonal E	triplet (weak spin–orbit)	2.12

Take section (2.3.2. Tetragonal symmetry)[**?**] as an example.
the product like $\eta_i \eta_j$ transform according to :

$$E_g \otimes E_g = A_{1g} \oplus A_{2g} \oplus B_{1g} \oplus B_{2g} \tag{11}$$

And the quartic term is $(E_g \otimes E_g)^* \otimes (E_g \otimes E_g)$ such that:

$$(A_{1g} \oplus A_{2g} \oplus B_{1g} \oplus B_{2g})^* \otimes (A_{1g} \oplus A_{2g} \oplus B_{1g} \oplus B_{2g}) = 4A_{1g} \oplus \cdots \quad (12)$$

Note that

$$A_{1g} \otimes A_{1g} = A_{1g} \qquad A_{2g} \otimes A_{2g} = A_{1g}$$
$$B_{1g} \otimes B_{1g} = A_{1g} \qquad B_{2g} \otimes B_{2g} = A_{1g}$$

Then the four invariants are:

$$|\eta_1\eta_1 + \eta_2\eta_2|^2, \quad |\eta_1\eta_1 - \eta_2\eta_2|^2, \quad |\eta_1\eta_2 + \eta_2\eta_1|^2 \quad |\eta_1\eta_2 - \eta_2\eta_1|^2 = 0$$

Note that ∂_i transforms like $E_u \oplus A_{2\mu}$ because the basis of E_u and $A_{2\mu}$ is (x, y) and z.Thus $\partial_i \eta_j$ transforms like $(E_\mu \oplus A_{2\mu}) \otimes E_g$.

$$(E_\mu \oplus A_{2\mu}) \otimes E_g = A_{1\mu} \oplus A_{2\mu} \oplus B_{1\mu} \oplus B_{2\mu} \oplus E_\mu \tag{13}$$

Thus $\partial_i \eta_j \partial_k \eta_l^*$ transform like:

$$(A_{1\mu} \oplus A_{2\mu} \oplus B_{1\mu} \oplus B_{2\mu} \oplus E_\mu) \otimes (A_{1\mu} \oplus A_{2\mu} \oplus B_{1\mu} \oplus B_{2\mu} \oplus E_\mu)^* = (4+1) A_{1g} \oplus \cdots \tag{14}$$

The first four A_{1g} are derived from:

$$A_{1u} \otimes A_{1u} = A_{2u} \otimes A_{2u} = B_{1u} \otimes B_{1u} = B_{2u} \otimes B_{2u} = A_{1g} \tag{15}$$

the fifth A_{1g} derived from:

$$E_u \otimes E_u = A_{1g} \oplus A_{2g} \oplus B_{1g} \oplus B_{2g} \tag{16}$$

Then the basis of E_u is $(\partial_z\eta_1, \partial_z\eta_2)$.Given equation (16) and the projection matrix of A_{1g} (I will give the prgram calculate this matrx later) we can get the first invariant combination: $|\partial_z\eta_1|^2+|\partial_z\eta_2|^2$.
In case you want to know, the projection matrix of A_{1g} is:

$$\begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

$$E_u \otimes E_g = A_{1\mu} \oplus A_{2\mu} \oplus B_{1\mu} \oplus B_{2\mu} \tag{17}$$

The basis of $E_u \otimes E_g$ is $(\partial_x \eta_1, \partial_x \eta_2, \partial_y \eta_1, \partial_y \eta_2)$. We calculate the projection matrix of $A_{1u}, A_{2u}, B_{1u}, B_{2u}$ and get the basis are separately:

$$\partial_x \eta_2 - \partial_y \eta_1 \qquad \partial_x \eta_1 + \partial_y \eta_2 \tag{18}$$

$$\partial_x \eta_2 + \partial_y \eta_1 \qquad \partial_x \eta_1 - \partial_y \eta_2 \tag{19}$$

Finally the **Ginzburg-Landau** free energy is therefore of the following form:

$$
\begin{aligned}
f[\eta_1,\eta_2] =& \alpha(T-T_c)\eta_i^*\eta_i + \beta_1(\eta_i\eta_i)^2 + \beta_2|\eta_i\eta_i|^2 + \beta_3(|\eta_1|^4+|\eta_2|^4) && (20)\\
&+ \frac{\hbar^2}{2m_1'}(|\partial_x\eta_1|^2+|\partial_y\eta_2|^2) + \frac{\hbar^2}{2m_1''}(|\partial_y\eta_1|^2+|\partial_x\eta_2|^2) && (21)\\
&+ \frac{\hbar^2}{2m_2}(|\partial_x\eta_1|^2+|\partial_z\eta_2|^2) && (22)\\
&+ \frac{\hbar^2}{2m_3'}(\partial_x\eta_2^*\partial_y\eta_1 + c.c) + \frac{\hbar^2}{2m_3''}(\partial_x\eta_1^*\partial_y\eta_2 + c.c) && (23)
\end{aligned}
$$

Once we get the singlet states, it's easy to generalize singlet states to triplet states as below:
The singlet state of Orthorhombic symmetry is $\eta\eta\eta^*\eta^*$.The triplet states take the form $\eta_u\eta_u\eta_v^*\eta_v^*$ and $\eta_u\eta_v\eta_u^*\eta_v^*$.The gradient term takes the form $\partial_i\eta_u\partial_j\eta_u^*$.
For singlet term, we have:

$$\eta_i^*\eta_i\eta_j^*\eta_j \qquad \eta_i\eta_i\eta_j^*\eta_j^* \qquad \epsilon_{ijk}\eta_i\eta_i\eta_j^*\eta_j^* \qquad \epsilon_{ijk}\eta_i\eta_i^*\eta_j\eta_j^* \tag{24}$$

where the second and third term should be understood as $\epsilon_{ij3}\cdot\cdots$.
The triplet states take the form:

$$\eta_{ui}^*\eta_{ui}\eta_{vj}^*\eta_{vj} \qquad \eta_{ui}\eta_{ui}\eta_{vj}^*\eta_{vj}^* \qquad \epsilon_{ijk}\eta_{ui}\eta_{ui}\eta_{vj}^*\eta_{vj}^* \qquad \epsilon_{ijk}\eta_{ui}^*\eta_{ui}\eta_{vj}^*\eta_{vj} \tag{25}$$

$$\eta_{ui}^*\eta_{vi}\eta_{vj}^*\eta_{uj} \qquad \eta_{ui}\eta_{vi}\eta_{uj}^*\eta_{vj}^* \qquad \epsilon_{ijk}\eta_{ui}\eta_{vi}\eta_{uj}^*\eta_{vj}^* \qquad \epsilon_{ijk}\eta_{ui}^*\eta_{vi}\eta_{vj}^*\eta_{uj} \tag{26}$$

Note that the forth term is zero.

References

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Thank You!

Questions?