Symmetry analysis

MengFanzheng

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1 symmetry analysis

To systematically analyze the thermodynamic properties of high-temperature superconductors, we construct the free energy functional F in terms of the order parameters Δ using group-theoretical methods. The starting point is the **Ginzburg-Landau functional**, which takes the following form:

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

This functional is invariant under the symmetry group:

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

where G_0 represents the point group symmetry, $U(1)$ corresponds to gauge symmetry, and T denotes time-reversal symmetry.

Under a particular representation, the order parameter Δ transforms as:

$$\Delta \to R^{ij}(g_0)e^{i\phi}\Delta_j, \tag{3}$$

where $R^{ij}(g_0)$ is the matrix representation of the group element $g_0 \in G_0$, and ϕ is the phase factor associated with the $U(1)$ symmetry.

The first term in the free energy functional (Equation 1) transforms as:

$$\alpha_{ij}R_{ik}(g)R_{jl}^*(g)\Delta_k^*\Delta_l = R_{ki}^\dagger(g)\alpha_{ij}R_{jl}(g)\Delta_k^*\Delta_l. \tag{4}$$

For the free energy to remain invariant under the symmetry group G, the following condition must be satisfied:

$$R_{ki}^\dagger(g)\alpha_{ij}R_{jl}(g) = \alpha_{kl}. \tag{5}$$

Equivalently, this can be expressed in matrix form as:

$$R(g)\alpha = \alpha R(g). \tag{6}$$

This condition implies that the coefficient matrix α must commute with all group representations $R(g)$. According to **Schur's Lemma**, under an irreducible representation, the matrix α reduces to a constant matrix proportional to the identity, such that:

$$\alpha_{ij} = \alpha\delta_{ij}.$$

For reducible representations, by choosing an appropriate basis, α_{ij} can be block-diagonalized.

The temperature dependence of α_{ij} plays a crucial role in determining the phase behavior of the system. At high temperatures, α_{ij} is positive definite, and the free energy is minimized when all components of the order parameter vanish, i.e., $\Delta_i = 0$. As the temperature decreases, α_{ij} ceases to be positive definite. Suppose α_1 is the first eigenvalue to become non-positive. In this case, we can express the order parameter as:

$$\Delta_i = \sum_{i=1}^{g} \eta_i x_i^{(j)},$$

where $x^{(i)}$ are the eigenfunctions of α_1 corresponding to an irreducible representation, and g is the dimensionality of the representation. Here, we neglect contributions from eigenfunctions of other irreducible representations. This allows us to focus solely on the group-theoretical aspects of the problem.

We identify η_i as the new order parameters and rewrite the free energy functional (Equation 1) in terms of η_i:

$$f[\eta] = \alpha(T - T_c)\eta_i^*\eta_i + \beta_{ijkl}\eta_i^*\eta_j^*\eta_k\eta_l + K_{ijkl}\partial_i\eta_j^*\partial_k\eta_l + \cdots \tag{7}$$

The basis transformation between Δ_i and η_i is given by:

$$\Delta_i = \sum_{i=1}^{g} \eta_i x_i^{(j)} \tag{8}$$

From this, we can express η_i in terms of Δ_j as:

$$\eta_i = \sum_j (x_i^{(j)})^{-1}\Delta_j \tag{9}$$

This transformation simplifies the free energy functional, as the quadratic term now takes the form $\eta_i^*\eta_i$, which is manifestly invariant under symmetry transformations.

This transformation is advantageous because, in the new basis, the free energy functional takes a more convenient form. Specifically, the quadratic term simplifies to $\eta_i^*\eta_i$, which is manifestly invariant under symmetry transformations. We will explore this further in subsequent sections.

Our next objective is to reduce the higher-order terms (quartic and gradient terms) to a similarly convenient form. To guide this process, let us revisit how we simplified the quadratic term:

$$\alpha_{ij}\Delta_i^*\Delta_j \quad \xrightarrow{\eta_i = \sum_j (x_i^{(j)})^{-1}\Delta_j} \quad \alpha(T - T_c)\eta_i^*\eta_i.$$

Here, $\alpha(T - T_c)$ is a temperature-dependent constant, and $\eta_i^*\eta_i$ is invariant under symmetry transformations. The invariance of $\eta_i^*\eta_i$ arises from constructing it as a linear combination of the original terms $\Delta_i^*\Delta_j$. In other words, by forming appropriate linear combinations of $\Delta_i^*\Delta_j$, we obtain the invariant quantity $\eta_i^*\eta_i$.

The transformation properties of Δ_i are governed by the representation matrices $R_{ik}(g)$, where $g \in G_0$. Different representations correspond to different transformation matrices, which may vary in dimensionality and structure. The product $\Delta_i^*\Delta_j$ transforms under the direct product of representations:

$$\Gamma^* \otimes \Gamma = \Gamma_1 \oplus \Gamma_2 \oplus \cdots,$$

where Γ_1 is the identity representation. While the identity representation Γ_1 is not always present in the direct sum, its appearance is crucial for constructing invariant quantities. Only when Γ_1 appears in the decomposition can we form linear combinations of $\Delta_i^*\Delta_j$ that are invariant under symmetry transformations.

To determine the appropriate linear combinations, we require the **Clebsch-Gordan (C-G) coefficients**. For a direct product of irreducible representations $\Gamma^{(\mu)}$ and $\Gamma^{(\nu)}$, the decomposition is given by:

$$\Gamma^{(\mu)} \otimes \Gamma^{(\nu)} = \sum_{\sigma} a_\sigma \Gamma^{(\sigma)}, \tag{10}$$

where a_σ denotes the multiplicity of $\Gamma^{(\sigma)}$ in the decomposition. If the bases of $\Gamma^{(\mu)}$ and $\Gamma^{(\nu)}$ are $|\mu, j\rangle$ and $|\nu, k\rangle$, respectively, then the basis of the direct product representation $\Gamma^{(\mu)} \otimes \Gamma^{(\nu)}$ is:

$$|\mu, \nu; j, k\rangle = |\mu, j\rangle\, |\nu, k\rangle\, .$$

The basis of the decomposed representation $\Gamma^{(\sigma)}$ is denoted by $|\sigma, s; l\rangle$, where σ labels the irreducible representation, and s distinguishes between multiple occurrences of σ. The relationship between these bases is given by:

$$|\sigma, s; l\rangle = \sum_{j,k} \begin{pmatrix} \mu & \nu & | & \sigma & s \\ j & k & | & l & \end{pmatrix} |\mu, \nu; j, k\rangle\, , \tag{11}$$

where the coefficients are the Clebsch-Gordan coefficients.

To simplify the quartic terms in the free energy functional, we employ group-theoretical methods. The quartic term transforms under the direct product representation:

$$\Gamma^* \otimes \Gamma^* \otimes \Gamma \otimes \Gamma = \sum_i n_i \Gamma_i, \tag{12}$$

where n_i denotes the multiplicity of each irreducible representation Γ_i. The independent quartic terms can be extracted from the decomposition of this reducible representation.

1.1 Tetragonal Symmetry

As an illustrative example, consider the case of tetragonal symmetry (see Section 2.3.2 of [2]). The product $\eta_i\eta_j$ transforms according to the decomposition:

$$E_g \otimes E_g = A_{1g} \oplus A_{2g} \oplus B_{1g} \oplus B_{2g}. \tag{13}$$

1.1.1 Orthogonal Method

The orthogonal method provides a systematic approach to determine the Clebsch-Gordan coefficients (CGCs). The orthogonality condition for CGCs is given by:

$$\sum_s \begin{pmatrix} \mu\nu & | & \sigma s \\ ik & | & m \end{pmatrix} \begin{pmatrix} \sigma s & | & \mu\nu \\ n & | & jl \end{pmatrix} = \frac{d_\sigma}{g} \sum_{R\in\mathcal{G}} \Gamma^{(\mu)}_{ij}(R)\Gamma^{(\nu)}_{kl}(R)\Gamma^{(\sigma)*}_{mn}(R), \tag{14}$$

where d_σ is the dimension of the irreducible representation $\Gamma^{(\sigma)}$, and g is the order of the group $\mathcal{G}$. To determine the CGCs, we set $m = n$, $i = j$, and $k = l$, yielding:

$$\left| \begin{pmatrix} \mu\nu & | & \sigma s \\ ik & | & m \end{pmatrix} \right|^2 = \frac{d_\sigma}{g} \sum_{R\in\mathcal{G}} \Gamma^{(\mu)}_{ii}(R)\Gamma^{(\nu)}_{kk}(R)\Gamma^{(\sigma)*}_{mm}(R).$$

1.1.2 Representation of E_g

The matrix representations of the symmetry operations for the E_g representation are given below. For the identity operation E:

$$^{(5)}\Gamma(E) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

For the C_{2z} rotation:

$$^{(5)}\Gamma(C_{2z}) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}.$$

For the C_{4z} and C_{4z}^{-1} rotations:

$$^{(5)}\Gamma(C_{4z}) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad ^{(5)}\Gamma(C_{4z}^{-1}) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}.$$

For the C_{2x} and C_{2y} rotations:

$$^{(5)}\Gamma(C_{2x}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad ^{(5)}\Gamma(C_{2y}) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

For the C_{2xy} and $C_{2\bar{x}\bar{y}}$ rotations:

$$^{(5)}\Gamma(C_{2xy}) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad ^{(5)}\Gamma(C_{2\bar{x}\bar{y}}) = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}.$$

For the inversion operations:

$$^{(5)}\Gamma(i) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad ^{(5)}\Gamma(iC_{2z}) = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}, \quad ^{(5)}\Gamma(iC_{4z}) = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad ^{(5)}\Gamma(iC_{4z}^{-1}) = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}.$$

For the combined inversion and rotation operations:

$$^{(5)}\Gamma(iC_{2x}) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad ^{(5)}\Gamma(iC_{2y}) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad ^{(5)}\Gamma(iC_{2xy}) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad ^{(5)}\Gamma(iC_{2\bar{x}\bar{y}}) = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}.$$

1.1.3 Application of the Orthogonal Method

Using the orthogonal method, we derive the following Clebsch-Gordan coefficients:

$$\left(\begin{array}{c|c} 55 & 1 \\ ik & 1 \end{array}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \quad \left(\begin{array}{c|c} 55 & 2 \\ ik & 1 \end{array}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},$$
$$\left(\begin{array}{c|c} 55 & 3 \\ ik & 1 \end{array}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}, \quad \left(\begin{array}{c|c} 55 & 4 \\ ik & 1 \end{array}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}.$$

The corresponding basis functions are:

$$\eta_1\eta_1 + \eta_2\eta_2, \quad \eta_1\eta_1 - \eta_2\eta_2, \quad \eta_1\eta_2 + \eta_2\eta_1, \quad \eta_1\eta_2 - \eta_2\eta_1.$$

1.1.4 Quartic Terms in Tetragonal Symmetry

The quartic term transforms under the representation:

$$(E_g \otimes E_g)^* \otimes (E_g \otimes E_g) = (A_{1g} \oplus A_{2g} \oplus B_{1g} \oplus B_{2g})^* \otimes (A_{1g} \oplus A_{2g} \oplus B_{1g} \oplus B_{2g}),$$

which decomposes into:

$$4A_{1g} \oplus \cdots.$$

Noting that:

$$A_{1g} \otimes A_{1g} = A_{1g}, \quad A_{2g} \otimes A_{2g} = A_{1g},$$
$$B_{1g} \otimes B_{1g} = A_{1g}, \quad B_{2g} \otimes B_{2g} = A_{1g},$$

the four invariant quartic terms are:

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

1.1.5 Projection Method

An alternative approach to analyze the problem is through the **projection operator method**. The basis of the representation E_g consists of η_1 and η_2, which transform according to the matrices of E_g. The basis of the representation $E_g \otimes E_g^*$ is given by the set:

$$\{\eta_1\eta_1^*, \eta_1\eta_2^*, \eta_2\eta_1^*, \eta_2\eta_2^*\},$$

which transforms under the direct product of the matrices of E_g and E_g^*. The projection operator method allows us to extract the basis functions of the irreducible representations A_{1g}, A_{2g}, B_{1g}, and B_{2g} as linear combinations of the basis of $E_g \otimes E_g^*$.

The projection operator for an irreducible representation $\Gamma^{(\sigma)}$ is defined as:

$$
{}^{(\sigma)}P_{ii} = \frac{d_\sigma}{g} \sum_{R \in G} {}^{(\sigma)}\Gamma_{ii}(R^{-1}) \hat{\mathbf{R}}_{\text{outer}}, \tag{15}
$$

where d_σ is the dimension of $\Gamma^{(\sigma)}$, g is the order of the group G, and $\hat{\mathbf{R}}_{\text{outer}}$ is the outer product of the matrix representations of E_g and E_g^*. In this case, the projection operator is a 4×4 matrix.

To apply the projection operator, we act on an arbitrary 4-dimensional column vector constructed from the basis $\{\eta_1\eta_1^*, \eta_1\eta_2^*, \eta_2\eta_1^*, \eta_2\eta_2^*\}$. The resulting column vector provides the correct linear combination of the basis functions corresponding to the irreducible representation $\Gamma^{(\sigma)}$.

1.1.6 Computational Implementation

To illustrate the projection operator method explicitly, we provide a Python implementation for the computation. The code performs the following steps:

1. Defines the matrix representations of the symmetry operations for E_g.
2. Constructs the outer product matrices for $E_g \otimes E_g^*$.
3. Computes the projection operators for the irreducible representations A_{1g}, A_{2g}, B_{1g}, and B_{2g}.
4. Applies the projection operators to extract the basis functions.

The Python code is provided as below:

```python
import sympy as sp
import numpy as np
# Define all 16 symmetry operations for E_g
symmetry_operations_Eg = {
     "E": np.array([[1, 0], [0, 1]]),
    "C2z": np.array([[-1, 0], [0, -1]]),
    "C4z": np.array([[0, 1], [-1, 0]]),
    "C4z_inv": np.array([[0, -1], [1, 0]]),
    "C2x": np.array([[-1, 0], [0, 1]]),
    "C2y": np.array([[1, 0], [0, -1]]),
    "C2xy": np.array([[0, 1], [1, 0]]),
    "C2x_y": np.array([[0, -1], [-1, 0]]),
    "i": np.array([[1, 0], [0, 1]]),
    "iC2z": np.array([[-1, 0], [0, -1]]),
    "iC4z": np.array([[0, 1], [-1, 0]]),
    "iC4z_inv": np.array([[0, -1], [1, 0]]),
    "iC2x": np.array([[-1, 0], [0, 1]]),
    "iC2y": np.array([[1, 0], [0, -1]]),
    "iC2xy": np.array([[0, 1], [1, 0]]),
    "iC2x_y": np.array([[0, -1], [-1, 0]]),
}

character_table = {
    "A1g": [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1],
    "A2g": [1, 1, 1, 1, -1, -1, -1, -1, 1, 1, 1, 1, -1, -1, -1, -1],
    "B1g": [1, 1, -1, -1, 1, 1, -1, -1, 1, 1, -1, -1, 1, 1, -1, -1],
```

```
    "B2g": [1,1]+[-1]*4+[1]*4+[-1]*4+[1,1],
    "A1u": [1]*8+[-1]*8,
    "A2u": [1]*4+[-1]*8+[1]*4,
    "B1u": [1,1,-1,-1,1,1]+[-1]*4+[1]*2+[-1]*2+[1]*2,
    "B2u": [1,1]+[-1]*4+[1,1]+[-1]*2+[1]*4+[-1]*2
}

# Group order
order_of_group = 16

# Function to calculate the projection matrix
def calculate_projection_matrix(irrep, character_table, symmetry_operations_1, symmetry_operations_2):
    projection_matrix = sp.zeros(4, 4)
    for i, op in enumerate(symmetry_operations_1.keys()):
        char = character_table[irrep][i]
        T1 = symmetry_operations_1[op]
        T2 = symmetry_operations_2[op]
        direct_product = sp.Matrix([
            [T1[0, 0] * T2[0, 0], T1[0, 0] * T2[0, 1], T1[0, 1] * T2[0, 0], T1[0, 1] * T2[0, 1]],
            [T1[0, 0] * T2[1, 0], T1[0, 0] * T2[1, 1], T1[0, 1] * T2[1, 0], T1[0, 1] * T2[1, 1]],
            [T1[1, 0] * T2[0, 0], T1[1, 0] * T2[0, 1], T1[1, 1] * T2[0, 0], T1[1, 1] * T2[0, 1]],
            [T1[1, 0] * T2[1, 0], T1[1, 0] * T2[1, 1], T1[1, 1] * T2[1, 0], T1[1, 1] * T2[1, 1]],
    ])
        projection_matrix += char * direct_product
    projection_matrix /= order_of_group
    return projection_matrix


projection_matrix_A1g = calculate_projection_matrix("A1g", character_table, symmetry_operations_Eg, symmetry_operations_Eg)
projection_matrix_A2g = calculate_projection_matrix("A2g", character_table, symmetry_operations_Eg, symmetry_operations_Eg)
projection_matrix_B1g = calculate_projection_matrix("B1g", character_table, symmetry_operations_Eg, symmetry_operations_Eg)
projection_matrix_B2g = calculate_projection_matrix("B2g", character_table, symmetry_operations_Eg, symmetry_operations_Eg)
print("Projection Matrix for A1g,A2g,B1g,B2g:")
# 2* is just for normalization
sp.pprint(2*projection_matrix_A1g)
print('\n')
sp.pprint(2*projection_matrix_A2g)
print('\n')
sp.pprint(2*projection_matrix_B1g)
print('\n')
sp.pprint(2*projection_matrix_B2g)
```

The output of the program is as follows:
Projection Matrices for A_{1g}, A_{2g}, B_{1g}, and B_{2g}:

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

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

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

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

The corresponding basis functions are:

$$\eta_1\eta_1 + \eta_2\eta_2, \quad \eta_1\eta_1 - \eta_2\eta_2, \quad \eta_1\eta_2 + \eta_2\eta_1, \quad \eta_1\eta_2 - \eta_2\eta_1.$$

Subsequent analysis proceeds analogously to the orthogonal method.

1.1.7 Gradient Terms

The gradient operator ∂_i transforms under the representation $E_u \oplus A_{2\mu}$, where the basis of E_u is (x, y) and the basis of $A_{2\mu}$ is z. Consequently, the term $\partial_i\eta_j$ transforms under the representation:

$$(E_u \oplus A_{2\mu}) \otimes E_g = A_{1\mu} \oplus A_{2\mu} \oplus B_{1\mu} \oplus B_{2\mu} \oplus E_\mu. \tag{16}$$

The product $\partial_i\eta_j\partial_k\eta_l^*$ transforms as:

$$(A_{1\mu} \oplus A_{2\mu} \oplus B_{1\mu} \oplus B_{2\mu} \oplus E_\mu) \otimes (A_{1\mu} \oplus A_{2\mu} \oplus B_{1\mu} \oplus B_{2\mu} \oplus E_\mu)^* = (4+1)A_{1g} \oplus \cdots. \tag{17}$$

The first four A_{1g} invariants arise from:

$$A_{1u} \otimes A_{1u} = A_{2u} \otimes A_{2u} = B_{1u} \otimes B_{1u} = B_{2u} \otimes B_{2u} = A_{1g}. \tag{18}$$

The fifth A_{1g} invariant originates from:

$$E_u \otimes E_u = A_{1g} \oplus A_{2g} \oplus B_{1g} \oplus B_{2g}. \tag{19}$$

Starting from Equation 16, we note that:

$$A_{2u} \otimes E_g = E_u.$$

The basis of E_u is $(\partial_z \eta_1, \partial_z \eta_2)$. Using Equation 19 and the projection matrix for A_{1g}, we obtain the first invariant combination:

$$|\partial_z \eta_1|^2 + |\partial_z \eta_2|^2.$$

The projection matrix for A_{1g} is:

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

From Equation 16, we have:

$$E_u \otimes E_g = A_{1\mu} \oplus A_{2\mu} \oplus B_{1\mu} \oplus B_{2\mu}. \tag{20}$$

The basis of $E_u \otimes E_g$ is $(\partial_x \eta_1, \partial_x \eta_2, \partial_y \eta_1, \partial_y \eta_2)$. Applying the projection operators for A_{1u}, A_{2u}, B_{1u}, and B_{2u}, we obtain the following basis functions:

$$\begin{aligned} &\partial_x \eta_2 - \partial_y \eta_1, \quad \partial_x \eta_1 + \partial_y \eta_2, \\ &\partial_x \eta_2 + \partial_y \eta_1, \quad \partial_x \eta_1 - \partial_y \eta_2. \end{aligned} \tag{21}$$

The corresponding invariant combinations are:

$$\begin{aligned} &|\partial_x \eta_2 - \partial_y \eta_1|^2, \quad |\partial_x \eta_1 + \partial_y \eta_2|^2, \\ &|\partial_x \eta_2 + \partial_y \eta_1|^2, \quad |\partial_x \eta_1 - \partial_y \eta_2|^2. \end{aligned} \tag{22}$$

Expanding these terms, we obtain:

$$|\partial_x \eta_2 - \partial_y \eta_1|^2 = |\partial_x \eta_2|^2 + |\partial_y \eta_1|^2 - (\partial_x \eta_2 \partial_y \eta_1^* + \text{c.c.}), \tag{23}$$

$$|\partial_x \eta_1 + \partial_y \eta_2|^2 = |\partial_x \eta_1|^2 + |\partial_y \eta_2|^2 + (\partial_x \eta_1 \partial_y \eta_2^* + \text{c.c.}), \tag{24}$$

$$|\partial_x \eta_2 + \partial_y \eta_1|^2 = |\partial_x \eta_2|^2 + |\partial_y \eta_1|^2 + (\partial_x \eta_2 \partial_y \eta_1^* + \text{c.c.}), \tag{25}$$

$$|\partial_x \eta_1 - \partial_y \eta_2|^2 = |\partial_x \eta_1|^2 + |\partial_y \eta_2|^2 - (\partial_x \eta_1 \partial_y \eta_2^* + \text{c.c.}). \tag{26}$$

We select the following linear combinations of the invariant components:

$$\begin{aligned} &|\partial_x \eta_2|^2 + |\partial_y \eta_1|^2, \quad |\partial_x \eta_1|^2 + |\partial_y \eta_2|^2, \\ &(\partial_x \eta_2 \partial_y \eta_1^* + \text{c.c.}), \quad (\partial_x \eta_1 \partial_y \eta_2^* + \text{c.c.}). \end{aligned} \tag{27}$$

1.1.8 Ginzburg-Landau Free Energy

The final form of the **Ginzburg-Landau free energy** is given by:

$$
\begin{aligned}
f[\eta_1, \eta_2] = {} & \alpha(T - T_c)\eta_i^* \eta_i + \beta_1(\eta_i \eta_i)^2 + \beta_2 |\eta_i \eta_i|^2 + \beta_3(|\eta_1|^4 + |\eta_2|^4) \\
& + \frac{\hbar^2}{2m_1'}(|\partial_x \eta_1|^2 + |\partial_y \eta_2|^2) + \frac{\hbar^2}{2m_1''}(|\partial_y \eta_1|^2 + |\partial_x \eta_2|^2) \\
& + \frac{\hbar^2}{2m_2}(|\partial_x \eta_1|^2 + |\partial_z \eta_2|^2) \\
& + \frac{\hbar^2}{2m_3'}(\partial_x \eta_2^* \partial_y \eta_1 + \text{c.c.}) + \frac{\hbar^2}{2m_3''}(\partial_x \eta_1^* \partial_y \eta_2 + \text{c.c.}).
\end{aligned}
\tag{28}
$$

The program that calculates the projection matrix:

2 Triplet States in Weak Spin-Orbit Coupling

Once the singlet states are established, the generalization to triplet states follows naturally. Below, we discuss the triplet states for both orthorhombic and tetragonal symmetries.

2.1 Orthorhombic Symmetry

For orthorhombic symmetry, the singlet state is of the form $\eta\eta\eta^*\eta^*$. The corresponding triplet states take the forms:

$$\eta_u \eta_u \eta_v^* \eta_v^* \quad \text{and} \quad \eta_u \eta_v \eta_u^* \eta_v^*.$$

The gradient term in the triplet state is given by:

$$\partial_i \eta_u \partial_j \eta_u^*.$$

2.2 Tetragonal Symmetry

For tetragonal symmetry, the singlet terms include:

$$\eta_i^* \eta_i \eta_j^* \eta_j, \quad \eta_i \eta_i \eta_j^* \eta_j^*, \quad \epsilon_{ijk} \eta_i \eta_i \eta_j^* \eta_j^*, \quad \epsilon_{ijk} \eta_i \eta_i^* \eta_j \eta_j^*, \tag{29}$$

where the second and third terms should be understood as $\epsilon_{ij3} \cdots$.

The triplet states for tetragonal symmetry are given by:

$$
\begin{aligned}
&\eta_{ui}^* \eta_{ui} \eta_{vj}^* \eta_{vj}, \quad \eta_{ui} \eta_{ui} \eta_{vj}^* \eta_{vj}^*, \quad \epsilon_{ijk} \eta_{ui} \eta_{ui} \eta_{vj}^* \eta_{vj}^*, \quad \epsilon_{ijk} \eta_{ui}^* \eta_{ui} \eta_{vj}^* \eta_{vj}, \\
&\eta_{ui}^* \eta_{vi} \eta_{vj}^* \eta_{uj}, \quad \eta_{ui} \eta_{vi} \eta_{uj}^* \eta_{vj}^*, \quad \epsilon_{ijk} \eta_{ui} \eta_{vi} \eta_{uj}^* \eta_{vj}^*, \quad \epsilon_{ijk} \eta_{ui}^* \eta_{vi} \eta_{vj}^* \eta_{uj}.
\end{aligned}
\tag{30}
$$

Note that the fourth term in the triplet states vanishes.

3 Open Questions

Matrix Representation Uncertainty

There is some uncertainty regarding the matrix representation of the group. I constructed matrices for two representations and applied the projection method, which resulted in an error. Subsequently, I used an alternative derivation method, which yielded a correct result.

Computational Generation of Representation Matrices

How can the matrices of group representations be computed systematically? Are there established algorithms or software tools for this purpose?

Triplet States and $SO(3)$ Group

Further study of the $SO(3)$ group is necessary to fully understand the triplet states. Specifically, how do the representations of $SO(3)$ relate to the symmetry properties of the triplet states?

Spin-Orbit Coupling Effects

What is the role of spin-orbit coupling in this problem? How does it influence the symmetry properties and the resulting free energy functional?

Gap Function and Residual Group

What is the gap function in this context, and how is it related to the residual symmetry group? How does the residual group constrain the form of the gap function?

4 D_6 symmetry

We begin with the tensor product decomposition of the representation E_2:

$$E_2 \otimes E_2 = A_1 \oplus A_2 \oplus E_1. \tag{31}$$

Let $\{\psi_1, \psi_2\}$ denote the basis of E_2. The basis functions for the irreducible representations A_1, A_2, and E_1 are given by:

$$\begin{align} &\psi_1\psi_1 + \psi_2\psi_2, \quad \text{(basis of } A_1) \tag{32}\\ &\psi_1\psi_2 - \psi_2\psi_1, \quad \text{(basis of } A_2) \tag{33}\\ &\psi_1\psi_1 - \psi_2\psi_2, \quad \text{(basis of } E_1) \tag{34}\\ &\psi_1\psi_2 + \psi_2\psi_1. \quad \text{(basis of } E_1) \tag{35}\end{align}$$

The tensor product of the decomposed representations satisfies:

$$(A_1 \oplus A_2 \oplus E_1) \otimes (A_1 \oplus A_2 \oplus E_1)^* = 3A_1 \oplus \cdots, \tag{36}$$

where the individual products are:

$$A_1 \otimes A_1 = A_1, \tag{37}$$
$$A_2 \otimes A_2 = A_1, \tag{38}$$
$$E_2 \otimes E_2 = A_1 \oplus \cdots. \tag{39}$$

The invariant basis functions derived from these decompositions are:

$$|\psi_1\psi_1 + \psi_2\psi_2|^2, \tag{40}$$
$$|\psi_1\psi_1 - \psi_2\psi_2|^2 + |\psi_1\psi_2 + \psi_2\psi_1|^2. \tag{41}$$

4.1 Alternative Basis from $E_2 \otimes E_2^* \otimes E_2 \otimes E_2^*$

From the perspective of the representation $E_2 \otimes E_2^* \otimes E_2 \otimes E_2^*$, we obtain an alternative set of basis functions:

$$(|\psi_1|^2 + |\psi_2|^2)^2, \tag{42}$$
$$(\psi_1\psi_2^* - \psi_2\psi_1^*)^2. \tag{43}$$

4.2 Derivative Terms

Next, we analyze the derivative terms. The tensor product of E_1 and E_2 decomposes as:

$$E_1 \otimes E_2 = B_1 \oplus B_2 \oplus E_1. \tag{44}$$

Consider the transformation matrix U that maps the basis (x_1, x_2) to $(x_1 + ix_2, x_1 - ix_2)$:

$$U \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1 + ix_2 \\ x_1 - ix_2 \end{pmatrix}, \tag{45}$$

where:

$$U = \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix}, \quad U^\dagger = \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}. \tag{46}$$

The matrix U satisfies:

$$UU^\dagger = 2E, \tag{47}$$

where E is the identity matrix. The derivatives (∂_x, ∂_y) form the basis of E_1, as do (∂_+, ∂_-), where $\partial_\pm = \partial_x \pm i\partial_y$.

The basis functions for B_1, B_2, and E_1 are:

$$\partial_+\psi_1 - \partial_-\psi_2, \quad \text{(basis of } B_1\text{)} \tag{48}$$
$$\partial_+\psi_2 + \partial_-\psi_1, \quad \text{(basis of } B_2\text{)} \tag{49}$$
$$\partial_+\psi_1 + \partial_-\psi_2, \quad \text{(basis of } E_1\text{)} \tag{50}$$
$$\partial_+\psi_2 - \partial_-\psi_1. \quad \text{(basis of } E_1\text{)} \tag{51}$$

The tensor product of these representations satisfies:

$$(B_1 \oplus B_2 \oplus E_1) \otimes (B_1 \oplus B_2 \oplus E_1)^* = 3A_1 \oplus \cdots. \tag{52}$$

The corresponding invariant basis functions are:

$$|\partial_+\psi_1 - \partial_-\psi_2|^2, \tag{53}$$
$$|\partial_+\psi_2 + \partial_-\psi_1|^2, \tag{54}$$
$$|\partial_+\psi_1 + \partial_-\psi_2|^2 + |\partial_+\psi_2 - \partial_-\psi_1|^2. \tag{55}$$

References

[1] M. El-Batanouny, F. Wooten; *Symmetry and Condensed Matter Physics* .

[2] James F. Annett *Symmetry of the order parameter for high- temperature superconductivity*