Note for vortex phase transition in iron-based superconductor

Wei Cheng

2023.3.17

Content

Abstract

Iron-based superconductor is a very good platform to search Majorana zero model due to it's topological band and high temperature superconductor.Here we search the vortex phase transition in iron-based superconductor.First we can use the $k \cdot p$ method to construct the Hamiliton.Then use the Hamiliton we can do some numerical calculation and theory analysis.

1 $k \cdot p$ construct Hamiliton

The space group of iron-based superconductor is P4/nmm,it include the frational translate,so it can't can be seen the the direct product of the translate group and the point group.But along the $\Gamma - Z$,it can be seen the $D4h$ group。At the same time,we can know the band near the fermi surface of the iron-based superconductor are p_z, d_{xz}, d_{yz} orbit.So we can choose the basics $|p_z, \uparrow\rangle$, $|p_z, \downarrow\rangle$, $|d_{xz+iyz}, \downarrow\rangle$, $|d_{xz-iyz}, \uparrow\rangle$, $|d_{xz+iyz}, \uparrow\rangle$, $|d_{xz-iyz}, \downarrow\rangle$ to construct our Hamiliton.For any $6 \cdot 6$matrix,we can break down to the linear superposition of 36 basics matrix.

$$H(\vec{k}) = \sum_{ij} f_{ij}(\vec{k}) M_{ij} \tag{1}$$

we can construct the 36 basics Hermitian matrix from the direct product of the Pauli matrix and the Gellman matrix.

$$M_{ij} = G_i \otimes \sigma_j \tag{2}$$

The G_i means the Gell-Man matrix,it's range is from 0 to 8.The σ_j means the Pauli matrix,it's range is from 0 to 3. At the same time,because we need to consider the spin orbit coupling,so we neend sonsider the double group,we can find the character table of the D4h.

D_{4h}	E	$\bar{E}$	$2C_4$	$2\bar{C}_4$	C_2 $\bar{C}_2$	$2C_2'$ $2\bar{C}_2'$	$2C_2''$ $2\bar{C}_2''$	I	$\bar{I}$	$2S_4$	$2\bar{S}_4$	σ_h $\bar{\sigma}_h$	$2\sigma_v$ $2\bar{\sigma}_v$	$2\sigma_d$ $2\bar{\sigma}_d$	Time Inv.	Bases
Γ_1^+	1	1	1	1	1	1	1	1	1	1	1	1	1	1	a	R
Γ_2^+	1	1	1	1	1	−1	−1	1	1	1	1	1	−1	−1	a	S_z
Γ_3^+	1	1	−1	−1	1	1	−1	1	1	−1	−1	1	1	−1	a	(x^2-y^2)
Γ_4^+	1	1	−1	−1	1	−1	1	1	1	−1	−1	1	−1	1	a	xy
Γ_5^+	2	2	0	0	−2	0	0	2	2	0	0	−2	0	0	a	S_x, S_y
Γ_1^-	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	a	$(x^2-y^2)xyz$
Γ_2^-	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	1	1	a	z
Γ_3^-	1	1	−1	−1	1	1	−1	−1	−1	1	1	−1	−1	1	a	xyz
Γ_4^-	1	1	−1	−1	1	−1	1	−1	−1	1	1	−1	1	−1	a	$(x^2-y^2)z$
Γ_5^-	2	2	0	0	−2	0	0	−2	−2	0	0	2	0	0	a	x,y
Γ_6^+	2	−2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	2	−2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	c	$\phi(1/2,-1/2)$, $\phi(1/2, 1/2)$
Γ_7^+	2	−2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	2	−2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	c	$\Gamma_6^+ \times \Gamma_3^+$
Γ_6^-	2	−2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	−2	2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	c	$\Gamma_6^+ \times \Gamma_1^-$
Γ_7^-	2	−2	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	−2	2	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	c	$\Gamma_6^+ \times \Gamma_3^-$

图 1:

We can get the generator of D4h group is $C_{4z}, C_{2x}^{'}, Inversion$.At the same time,the system has the time reversal symmetry.We can get the transformation matrix in the basics before we mentioned.

$$C_{4z} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1-i & & & & & \\ & 1+i & & & & \\ & & 1-i & & & \\ & & & 1+i & & \\ & & & & -1-i & \\ & & & & & -1+i \end{pmatrix} \quad C_{2x} = \begin{pmatrix} & i & & & & \\ i & & & & & \\ & & & i & & \\ & & i & & & \\ & & & & & i \\ & & & & i & \end{pmatrix} \tag{3}$$

$$I = \begin{pmatrix} -1 & & & & & \\ & -1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & 1 \end{pmatrix} \quad T = \begin{pmatrix} & -1 & & & & \\ 1 & & & & & \\ & & & -1 & & \\ & & 1 & & & \\ & & & & & -1 \\ & & & & 1 & \end{pmatrix}\mathcal{K} \tag{4}$$

we can get the character table of the polynomials of the momentum k

k polynomial	representation	time reversal
$1,k_x^2+k_y^2,k_z^2$	Γ_1^+	+
k_xk_y	Γ_4^+	+
$k_x^2-k_y^2$	Γ_3^+	+
$\{k_xk_z, k_yk_z\}$	Γ_5^+	+
$\{k_x, k_y\}$	Γ_5^-	-
k_z	Γ_2^-	-

we can get the character table of M_{ij},Then we can multiple the same representation of the k polynomials and the M_{ij} matrix.

Matrix	representation	time reverse
M_{03}	Γ_2^+	-
M_{10}	Γ_1^-	-
$\{M_{11}, M_{12}\}$	Γ_5^-	+
M_{13}	Γ_2^-	+
M_{20}	Γ_1^-	+
$\{M_{21}, M_{22}\}$	Γ_5^-	-
M_{23}	Γ_2^-	-
M_{30}, M_{80}	Γ_1^+	+
$\{M_{31}, M_{32}\}$	Γ_5^+	-
M_{33}	Γ_2^+	-
$\{M_{40}, M_{53}\}$	Γ_5^-	+
M_{41}	Γ_3^-	-
M_{42}	Γ_4^-	-
$\{M_{43}, M_{50}\}$	Γ_5^-	-
M_{51}	Γ_3^-	+
M_{52}	Γ_4^-	-
$\{M_{60}, M_{73}\}$	Γ_5^+	-
M_{61}	Γ_3^+	+
M_{62}	Γ_4^+	+
$\{M_{63}, M_{70}\}$	Γ_5^+	+
M_{71}	Γ_3^+	-
M_{72}	Γ_4^+	-
M_{83}	Γ_2^+	-

图 2:

2 Vortex Phase Transition