Note for vortex phase transition in iron-based superconductor

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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. The structure of the iron-based superconductor and the band structure as follows.

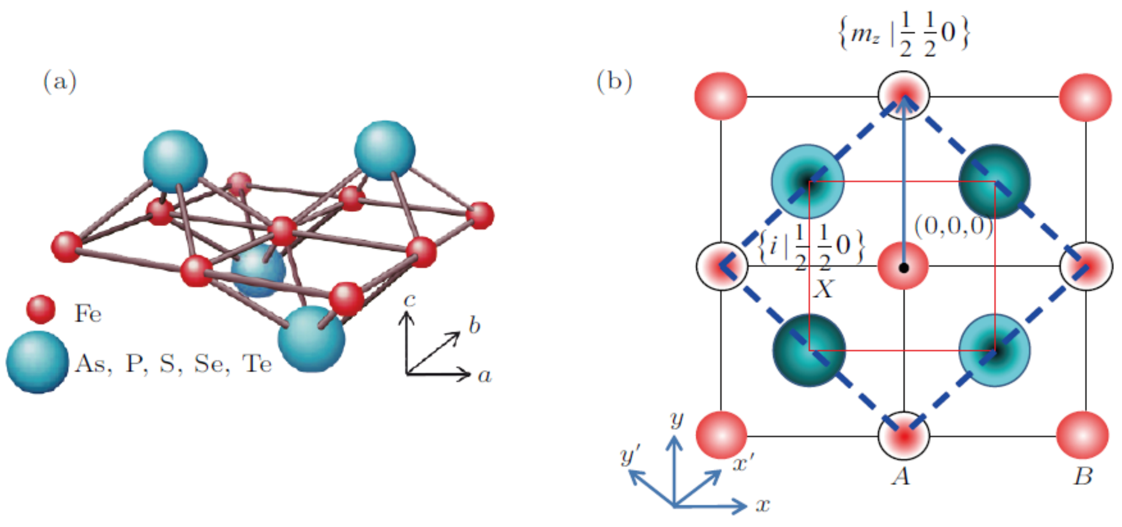

图 1: [1]

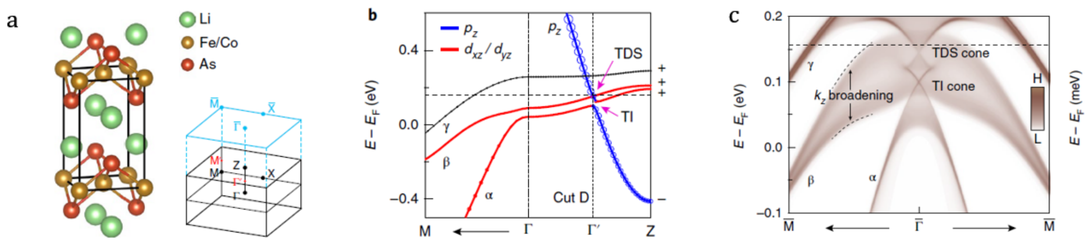

图 2: [2]

For any 6·6matrix,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 3:

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.So we can get the Hamiliton for the iron-based superconductor.

$$H = M_1(k)M_{30} + M_2(k)M_{80} + A_1k_xM_{21} + A_1k_yM_{22} + A_2k_xM_{50} + A_2k_yM_{43} + B_1k_zM_{23} + C_1k_xk_zM_{63} - C_1k_yk_zM_{70} + D_1(k_x^2-k_y^2)M_{61} + D_2k_xk_yM_{62}$$

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

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

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^+	+
$k_x k_y$	Γ_4^+	+
$k_x^2 - k_y^2$	Γ_3^+	+
$\{k_x k_z, k_y k_z\}$	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.So we can get the Hamiliton of the iron-based superconductor.

$$\begin{aligned} H &= M_1(k)M_{30} + M_2(k)M_{80} + A_1 k_x M_{21} + A_1 k_y M_{22} + A_2 k_x M_{50} + A_2 k_y M_{43} \\ &\quad + B_1 k_z M_{23} + C_1 k_x k_z M_{63} - C_1 k_y k_z M_{70} + D_1(k_x^2 - k_y^2)M_{61} + D_2 k_x k_y M_{62} \\ &= \begin{pmatrix} M_1(k) & 0 & -iB_1k_z & -iA_1k_- & -iA_2k_+ & 0 \\ 0 & M_1(k) & -iA_1k_+ & iB_1k_z & 0 & -iA_2k_- \\ iB_1k_z & iA_1k_- & -M_1(k) & 0 & C_1kzk_+ & D(k_x,k_y) \\ iA_1k_+ & -iB_1k_z & 0 & -M_1(k) & D(k_x,k_y)^* & C_1k_zk_- \\ iA_2k_- & 0 & C_1k_zk_- & D(k_x,k_y) & -M_1(k)+\delta_{so} & 0 \\ 0 & iA_2k_+ & D(k_x,k_y)^* & C_1k_zk_+ & 0 & -M_1(k)+\delta_{so} \end{pmatrix} \end{aligned} \tag{5}$$

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 4:

2 Vortex Phase Transition

As we were know,when the δ_{so} is very big,the three band can be seen the independent of the TI and DSM.At this time,the topological vortex phase transition can be seen the independent of TI and DSM use the Berry phase crition by Vishwanath.[3].But when the δ_{so} become very small,the situation become complex.

Reference

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[3] P. Hosur, P. Ghaemi, R. S. K. Mong, and A. Vishwanath, “Majorana modes at the ends of superconductor vortices in doped topological insulators,” *Phys. Rev. Lett.*, vol. 107, p. 097001, Aug 2011. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevLett.107.097001