Note for vertex phase transition in iron-based superconductor

Wei Cheng

2023.3.17

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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.

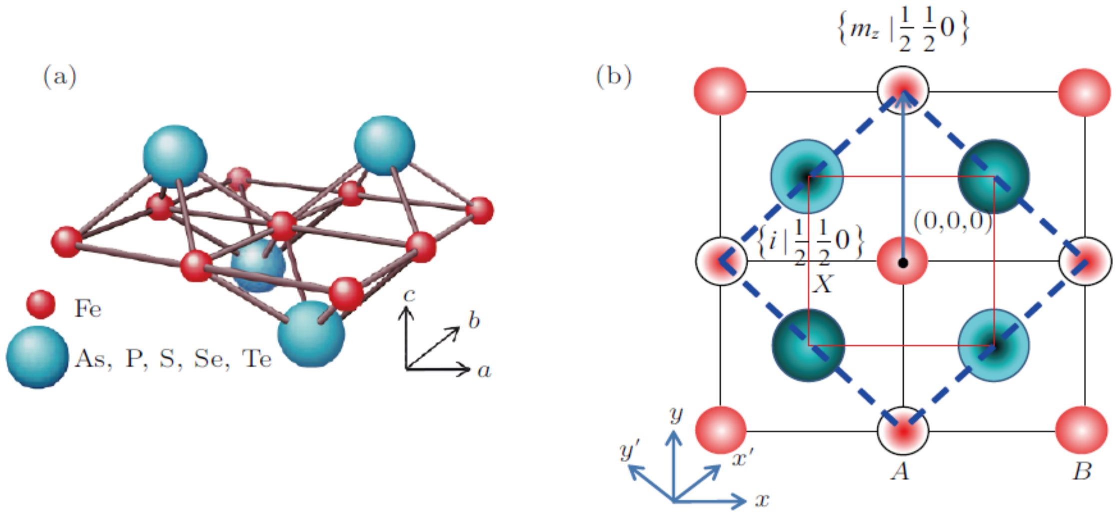

图 1: [1]

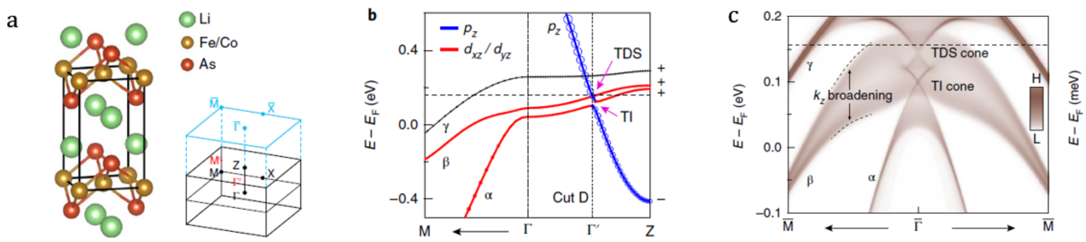

图 2: [2]

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.

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

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

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

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_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.So we can get the Hamiliton of the iron-based superconductor.

$$\begin{aligned} H &= M_1(k)M_{30} + M_2(k)M_{80} + A_1k_xM_{21} + A_1k_yM_{22} + A_2k_xM_{50} + A_2k_yM_{43} \\ &\quad + B_1k_zM_{23} + C_1k_xk_zM_{63} - C_1k_yk_zM_{70} + D_1(k_x^2-k_y^2)M_{61} + D_2k_xk_yM_{62} \\ &= \begin{pmatrix} M_1(k) & 0 & -iB_1k_z & -iA_1k_- & -iA_2k_+ & 0 \\ 0 & M_1(k) & -iA_1k_+ & iB_1k_z & 0 & -iA_2k_- \\ iB_1k_z & iA_1k_- & -M_1(k) & 0 & C_1kzk_+ & D(k_x,k_y) \\ iA_1k_+ & -iB_1k_z & 0 & -M_1(k) & D(k_x,k_y)^* & C_1k_zk_- \\ iA_2k_- & 0 & C_1k_zk_- & D(k_x,k_y) & -M_1(k)+\delta_{so} & 0 \\ 0 & iA_2k_+ & D(k_x,k_y)^* & C_1k_zk_+ & 0 & -M_1(k)+\delta_{so} \end{pmatrix} \end{aligned} \tag{5}$$

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(VPT) 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.we need to consider the interplay of the three band.At the same time,we can consider symmetry breaking effect to it's topological properties.

From the $k \cdot p$ method,we can get the Hamiliton of the iron-based superconductor.So we can do some mumerical calculation and the theory analysis.When we breaking C_{4z} symmetry to C_{2z},the symmetry group will from D_{4h} down to D_{2h},with the same analysis,we can know that it's Hamiliton will add $A_z^{'}M_{41}$,it will open the gap of the DSM.Then we can consider the vortex along the x directation,and calculate it's Energy at $k_x = 0$ change by μ.We can find somethings from the numerical result.First,when $A_z^{'} > 0$,the VPT's eigvalue of the $C_{2x} = -1$ and when the δ_{so} is decrease,the VPT point from 4 change to 1.Second,when change the sign of the $A_z^{'}$,one part of the VPT's eigvalues of the C_{2x} change from -1 to +1.we can understand this phenon from the theory analysis when the $\delta_{so} \to \infty$ and $\delta_{so} = 0$.For theory simpilipy,we consider the vortex along the z direction,and change the parameter of the k_y.

The vortex line is the 1D topological superconductor system,which belong to 1D D class of the Altland-Zirnbauer classification of topological phases.So we can define Z_2 topological invariant at $k_z = 0 or \pi$ to describe it's topological properties.So we can to calculate it's gap close times to know whether it's topological or not.So the following analysis is counting the zero solution of the H_{BdG} at the $k_z = 0$.

2.1 $\delta_{so} \to \infty$, change sign of k_y

In this part,I want to prove that when change the sign of the parameter of k_y,the VPT of the TI(DSM) will change from the $C_{2z} = 1(-1)$ to $C_{2z} = -1(1)$

Reference

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