Analytic of VPT in iron-based superconductor

Wei Cheng

From the analysis, we want to understand change the sign of the A_z will cause the topological phase transition from two to one. For simplify we choose vortex along the z direction.

In the basics $|p_z,\uparrow\rangle$, $|p_z,\downarrow\rangle$, $|d_{xz+iyz},\downarrow\rangle$, $|d_{xz-iyz},\uparrow\rangle$, $|d_{xz+iyz},\uparrow\rangle$, $|d_{xz-iyz,\downarrow}\rangle$, we consider the $k_z=0$

$$H = \begin{pmatrix} M(k) & 0 & 0 & -iAk_{-} & -iAk_{+} & 0 \\ 0 & M(k) & -iAk_{+} & 0 & 0 & -iAk_{-} \\ 0 & iAk_{-} & -M(k) & 0 & 0 & 0 \\ iAk_{+} & 0 & 0 & -M(k) & 0 & 0 \\ iAk_{-} & 0 & 0 & 0 & -M(k) + \delta & 0 \\ 0 & iAk_{+} & 0 & 0 & 0 & -M(k) + \delta \end{pmatrix}$$
(1)

 $M(k) = M_0 + M_1(k_x^2 + k_y^2), k_+ = k_x + ik_y, k_- = k_x - ik_y$ we can do a transformation to diagonalization the Hamiliton

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$
 (2)

Finally we can get the block from is

The block from is
$$H_{k} = \begin{pmatrix} M(k) & -iAk_{-} & -iAk_{+} \\ iAk_{+} & -M(k) & 0 \\ iAk_{-} & 0 & -M(k) + \delta \end{pmatrix}$$

$$M(k) & -iAk_{+} & -iAk_{-} \\ iAk_{-} & -M(k) & 0 \\ iAk_{+} & 0 & -M(k) \end{pmatrix}$$

$$(3)$$

we can get the electron in the basics $\{|p_z,\uparrow\rangle_e, |d_{xz-iyz},\uparrow\rangle_e, |d_{xz+iyz},\uparrow\rangle_e\}$, the Hamiliton is

$$H_{e\uparrow}(k) = \begin{pmatrix} M(k) & -iAk_{-} & -iAk_{+} \\ iAk_{+} & -M(k) & 0 \\ iAk_{-} & 0 & -M(k) \end{pmatrix}$$
(4)

In the $\{|p_z,\downarrow\rangle_e$, $|d_{xz+iyz},\downarrow\rangle_e$, $|d_{xz-iyz},\downarrow\rangle_e\}$ the Hamiliton is

$$H_{e\downarrow}(k) = \begin{pmatrix} M(k) & -iAk_{+} & -iAk_{-} \\ iAk_{-} & -M(k) & 0 \\ iAk_{+} & 0 & -M(k) \end{pmatrix}$$
 (5)

The we can do the particle-hole transformation to get the Hamiliton in the hole space $\{|p_z,\downarrow\rangle_h, |d_{xz+iyz},\downarrow\rangle_h, |d_{xz+iyz},\downarrow\rangle_h$

$$H_{h\downarrow}(k) = -H_{e\downarrow}^{*}(-k) = -\begin{pmatrix} M(k) & -iAk_{+} & -iAk_{-} \\ iAk_{-} & -M(k) & 0 \\ iAk_{+} & 0 & -M(k) \end{pmatrix} = -H_{e\uparrow}(k)$$
 (6)

Then we can solve the eigenvalue and eigenwave function for $H_{e\uparrow}(k)$, for simplify, we can write it in the polar coordinate, we can get the $H_{e\uparrow}(k)$ is

$$H_{e\uparrow}(k) = \begin{pmatrix} M(k) & -iAke^{-i\theta} & -iAke^{i\theta} \\ iAke^{i\theta} & -M(k) & 0 \\ iAke^{-i\theta} & 0 & -M(k) \end{pmatrix}$$

$$(7)$$

we can get the three eigenvalue

$$E_{+} = \pm \sqrt{M(k)^{2} + 2A^{2}k^{2}} \qquad E_{0} = -M(k)$$
(8)

We can see that the eigenvalue is only relate to the length of k,independent of theta,so we can definit a angular momentum

$$J_{z} = -i\partial_{\theta} + J_{basis} = -i\partial_{\theta} + \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ \frac{3}{2} \end{pmatrix}$$
 (9)

For the orbit angular momentum, we can write it in p appearance

$$L_z = (\vec{r} \times \vec{p})_z = x p_v - y p_x \tag{10}$$

$$=ip_{y}\partial_{p_{x}}-ip_{x}\partial_{p_{y}} \tag{11}$$

In the coordinate of the p

$$\partial_{p_x} = \cos(\theta)\partial_p - \frac{1}{p}\sin(\theta)\partial_\theta \tag{12}$$

$$\partial_{p_{y}} = \sin(\theta)\partial_{p} + \frac{1}{p}\cos(\theta)\partial_{\theta}$$
 (13)

Then we can get

$$L_z = i p_y \partial_{p_x} - i p_x \partial_{p_y} \tag{14}$$

$$= ipsin(\theta)[cos(\theta)\partial_p - \frac{1}{p}sin(\theta)\partial_\theta] - ipcos(\theta)[sin(\theta)\partial_p + \frac{1}{p}cos(\theta)\partial_\theta]$$
 (15)

$$=-i\partial_{\theta} \tag{16}$$

Due to $[H_{e\uparrow}(k), J_z] = 0$, we can get the common eigen states of the $H_{e\uparrow}(k)$ and J_z

$$\psi(k,\theta)^{j} = \begin{pmatrix} e^{i(j-\frac{1}{2})\theta} u_{1}(k) \\ e^{i(j+\frac{1}{2})\theta} u_{2}(k) \\ e^{i(j-\frac{3}{1})\theta} u_{3}(k) \end{pmatrix}$$
(17)

Then we can definite a unitary transformation

$$U = \begin{pmatrix} e^{i(j-\frac{1}{2})\theta} & & & \\ & e^{i(j+\frac{1}{2})\theta} & & \\ & & e^{i(j-\frac{3}{2})\theta} \end{pmatrix}$$
 (18)

The we can get

$$U^{\dagger}H_{e\uparrow}(k)U = \begin{pmatrix} M(k) & -iAk & -iAk \\ iAk & -M(k) & 0 \\ iAk & 0 & -M(k) \end{pmatrix}$$

$$(19)$$

we can solve the eigen states

$$|\psi_0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0\\ -1\\ 1 \end{pmatrix} \qquad |\psi_{\pm}\rangle = \frac{1}{a_{\pm}} \begin{pmatrix} -i(M(k) \pm E)\\ Ak\\ Ak \end{pmatrix} \tag{20}$$

The $E = \sqrt{M(k)^2 + 2A^2k^2}$, a_{\pm} is normalization constant, then we can get the eigen states of angular momentum j is

$$|\psi_{0}^{j}\rangle_{e} = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} 0\\ -e^{i(j+\frac{1}{2})\theta}\\ e^{i(j-\frac{3}{2}\theta)} \end{pmatrix} \qquad |\psi_{\pm}^{j}\rangle_{e} = \frac{1}{a_{\pm}\sqrt{2\pi}} \begin{pmatrix} -i(M(k)\pm E)e^{i(j-\frac{1}{2})\theta}\\ Ake^{i(j+\frac{1}{2})\theta}\\ Ake^{i(j-\frac{3}{2})\theta} \end{pmatrix}$$
(21)

For the hole part, because $H_{h\downarrow}(k) = -H_{e\uparrow}(k)$, use the same way to calculate, we can find it's eigen value is negative to the electronic part, it's eigen states will correspondenced to electronic part.

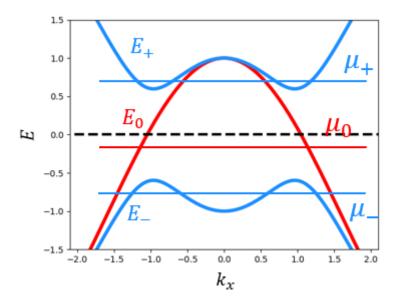
$$|\psi_{0}^{j}\rangle_{h} = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} 0\\ -e^{i(j+\frac{1}{2})\theta}\\ e^{i(j-\frac{3}{2}\theta)} \end{pmatrix} \qquad |\psi_{\pm}^{j}\rangle_{h} = \frac{1}{a_{\pm}\sqrt{2\pi}} \begin{pmatrix} -i(M(k)\pm E)e^{i(j-\frac{1}{2})\theta}\\ Ake^{i(j+\frac{1}{2})\theta}\\ Ake^{i(j-\frac{3}{2})\theta} \end{pmatrix}$$
(22)

For simplify, we can choose $j = \frac{1}{2}$, we can get

$$|\psi_{0}\rangle_{e} = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} 0\\ -e^{i\theta}\\ e^{-i\theta} \end{pmatrix} \qquad |\psi_{\pm}\rangle_{e} = \frac{1}{a_{\pm}\sqrt{2\pi}} \begin{pmatrix} -i(M(k) \pm E)\\ Ake^{i\theta}\\ Ake^{-i\theta} \end{pmatrix}$$
(23)

$$|\psi_{0}\rangle_{h} = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} 0\\ -e^{i\theta}\\ e^{-i\theta} \end{pmatrix} \qquad |\psi_{\pm}\rangle_{h} = \frac{1}{a_{\pm}\sqrt{2\pi}} \begin{pmatrix} -i(M(k)\pm E)\\ Ake^{i\theta}\\ Ake^{-i\theta} \end{pmatrix}$$
(24)

We can choose the parameter $M_0 = -1$, $M_1 = 1$, A = 0.5, we can plot the band structure along the k_x direction(because we consider the system has circle rotation symmetry, so along the any direction of the $k_x - k_y$ plane, we will get the same band structure.) When the Fermi surface near the μ_0 , Only one



band near Fermi surace, so we can project H_{BdG} to this band, it means that we can write H_{BdG} on the $\{|\psi_0\rangle_e, |\psi_0\rangle_h\}$ basics.

$$H_{BdG}^{00} = \begin{pmatrix} E - \mu & i\Delta_e e^{-i\theta} \left(\partial_k - \frac{i\partial_\theta + A_\theta^{00}}{k}\right) \\ i\Delta_e e^{i\theta} \left(\partial_k + \frac{i\partial_\theta + A_\theta^{00}}{k}\right) & \mu - E \end{pmatrix}$$
 (25)

The vortex will not break the rotation symmetry on the x - y plane, so we can define the angular

momentum

$$J_{z} = L_{z} + J_{basis} + J_{vortex} = -i\partial_{\theta} + \frac{1}{2} + \frac{1}{2}\tau_{z}$$
 (26)

The eigne wave function is

$$\psi(k,\theta) = \frac{1}{\sqrt{k}} \begin{pmatrix} e^{i(j-1)\theta} u_1(k) \\ -ie^{ij\theta} u_2(k) \end{pmatrix}$$
 (27)

so we can do the unitary transformation

$$U = \begin{pmatrix} e^{i(j-1)\theta} & \\ -ie^{ij\theta} \end{pmatrix}$$
 (28)

Then we can get

$$(H_{BdG}^{00})^{j} = U^{\dagger} H_{BdG}^{00} U = \begin{pmatrix} E - \mu & \Delta_{e} (\frac{j - \frac{1}{2} - A_{\theta}^{00}}{k} + \partial_{k}) \\ \Delta_{e} (\frac{j - \frac{1}{2} - A_{\theta}^{00}}{k} - \partial_{k}) & \mu - E \end{pmatrix}$$
(29)

$$= (E - \mu)\sigma_z + i\Delta_e\partial_k + \frac{\Delta_e}{k}(j - \frac{1}{2} - A_\theta^{00})$$
 (30)

The resulting Hamiltonian is equivalent to the Jackiw-Rebbi model, so we can get

$$E_{j} = \frac{\Delta_{e}}{k} (j - \frac{1}{2} - A_{\theta}^{00}) \tag{31}$$

we can calculate $A_{\theta}^{00} = i_e \langle \psi_0 | \partial_{\theta} | \psi_0 \rangle_h = -1$, so E_j is impossible to be zero, so we can conclude that it's will not have vortex transition point near the μ_0

When the Fermi surface near the μ_- , there will have two band E_0, E_- near the Fermi surface, we can project H_{BdG} to this two band. For simipilify calculte, we can do a transformation from $(k,\theta)to(E,\theta)$, Then we can write H_{BdG} in the basics $\{|\psi_0(E,\theta)\rangle_e, |\psi_-(E,\theta)\rangle_e, |\psi_0(E,\theta)\rangle_h, |\psi_-\rangle(E,\theta)_h\}$

$$\begin{pmatrix}
E - \mu & \Delta_{11} & \Delta_{12} \\
E - \mu & \Delta_{21} & \Delta_{22} \\
\Delta_{11}^{\dagger} & \Delta_{12}^{\dagger} & \mu - E \\
\Delta_{21}^{\dagger} & \Delta_{22}^{\dagger} & \mu - E
\end{pmatrix}$$
(32)

The elements is

$$\Delta_{11} = i\Delta_e e^{-i\theta} \left(\frac{dE}{dk_-}\partial_E - \frac{i\partial_\theta + A_\theta^{00}}{k_-(E)}\right)$$
(33)

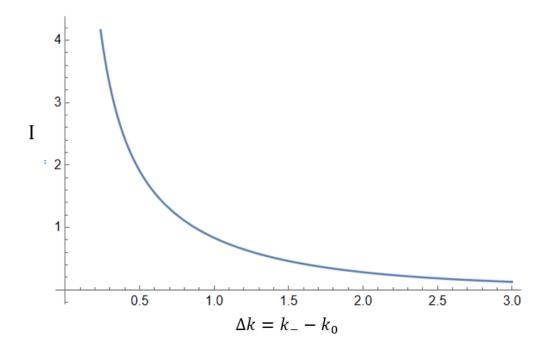
$$= i\Delta_e e^{-i\theta} (\hbar \nu_{k_-} \partial_E - \frac{i\partial_\theta + A_\theta^{00}}{k_-(E)})$$
(34)

$$\Delta_{12} =_{e} \langle \psi_{0}(k_{0}, \theta) | \Delta_{0} \tanh(\frac{r}{\xi}) e^{-i\theta} | \psi_{-}(k_{-}, \theta) \rangle_{h}$$
(35)

$$=_{e} \langle \psi_{0}(k_{0}, \theta) | \Delta_{e} r e^{-i\theta} \frac{\tanh(\frac{r}{\xi})}{\frac{r}{\xi}} | \psi_{-}(k_{-}, \theta) \rangle_{h}$$
 (36)

$$= -\frac{\Delta_e}{k_-} A_{\theta e}^{12} \langle \psi_0(k_0, \theta) | \frac{\tanh(\frac{r}{\xi})}{\frac{r}{\xi}} | \psi_-(k_-, \theta) \rangle_h$$
 (37)

The right integral can be calculate by numeral calculations, we can get



The horizontal axis representation the difference of the k_0 and k_- ,we can see that the more difference,the little integral. So we can only consider the interaction of the nearst k. For simplify we can treat this integral as a correction on k_- , we can change k_- to $k_m = \frac{k_0 + k_-}{2}$, Then we can get

$$\Delta_{12} = -\frac{\Delta_e}{k_m} A_\theta^{12} \tag{38}$$

At the same time

$$\Delta_{22} = i\Delta_e e^{-i\theta} (\hbar \nu_{k_-} \partial_E - iA_E^{22} - \frac{i\partial_{\theta + A_\theta^{22}}}{k})$$
(39)

we can do the gauge transfomation $|\psi_{-}(E,\theta)\rangle \to e^{i\int_{E'}^{E}A_{E'}^{22}}dE'$ to eliminate A_{E}^{22} , The we can get the form of

the project H_{BdG} , For easy to calculate, we can write the H_{BdG} in the basics $\{|\psi_0(E,\theta)\rangle_e$, $|\psi_0(E,\theta)\rangle_h$, $|\psi_-(E,\theta)\rangle_e$,

$$\begin{pmatrix}
E - \mu & i\Delta_{e}e^{-i\theta}(\hbar\nu_{k_{-}}\partial_{E} - \frac{i\partial_{\theta} + A_{\theta}^{00}}{k_{-}(E)}) & 0 & -\frac{\Delta_{e}}{k_{m}}e^{-i\theta}A_{\theta}^{0-} \\
i\Delta_{e}e^{i\theta}(\hbar\nu_{k_{-}}\partial_{E} + \frac{i\partial_{\theta} + A_{\theta}^{00}}{k}) & \mu - E & -\frac{\Delta_{e}}{k_{m}}e^{i\theta}A_{\theta}^{-0} & 0 \\
0 & -\frac{\Delta_{e}}{k_{m}}e^{-i\theta}A_{\theta}^{0-} & E - \mu & i\Delta_{e}e^{-i\theta}(\hbar\nu_{k_{-}}\partial_{E} - \frac{i\partial_{\theta} + A_{\theta}^{--}}{k_{-}(E)}) \\
-\frac{\Delta_{e}}{k_{m}}e^{i\theta}A_{\theta}^{-0} & 0 & i\Delta_{e}e^{i\theta}(\hbar\nu_{k_{-}}\partial_{E} + \frac{i\partial_{\theta} + A_{\theta}^{--}}{k}) & E - \mu
\end{pmatrix}$$
(40)

The \mathcal{H}_{BdG} has the rotation symmetry, so we can definite the angular momentum

$$J_z = -i\partial_\theta + \frac{1}{2} + \frac{1}{2}\tau_z \tag{41}$$

The egie wave function is

$$\psi(E,\theta) = \frac{1}{\sqrt{k_{-}(E)}} \begin{pmatrix} e^{i(j-1)\theta} u_1(k) \\ -ie^{ij\theta} u_2(k) \\ e^{i(j-1)\theta} u_3(k) \\ -ie^{ij\theta} u_4(k) \end{pmatrix}$$
(42)

So we can do a unitary transformation

$$U = \frac{1}{\sqrt{k_{-}(E)}} \begin{pmatrix} e^{i(j-1)\theta} & & & \\ & -ie^{ij\theta} & & \\ & & e^{i(j-1)\theta} & \\ & & & -ie^{ij\theta} \end{pmatrix}$$
(43)

Then we can get

$$\begin{pmatrix}
E - \mu & \Delta_{e}(\hbar \nu_{k_{-}} \partial_{E} + \frac{j - \frac{1}{2} - A_{\theta}^{00}}{k}) & 0 & -\Delta_{e} \frac{A_{\theta}^{0-}}{k} \\
-\Delta_{e}(\frac{j - \frac{1}{2} - A_{\theta}^{00}}{k} - \hbar \nu_{k_{-}} \partial_{E}) & \mu - E & -\Delta_{e} \frac{A_{\theta}^{0-}}{k} & 0 \\
0 & -\Delta_{e} \frac{A_{\theta}^{-0}}{k} & E - \mu & \Delta_{e}(\hbar \nu_{k_{-}} \partial_{E} + \frac{j - \frac{1}{2} - A_{\theta}^{--}}{k}) \\
-\Delta_{e} \frac{A_{\theta}^{-0}}{k} & 0 & \Delta_{e}(\frac{j - \frac{1}{2} - A_{\theta}^{--}}{k} - \hbar \nu_{k_{-}} \partial_{E}) & \mu - E
\end{pmatrix} (44)$$

$$= (E - \mu)s_{0}\tau_{z} + i\Delta_{e}\hbar\nu_{k_{-}}\partial_{E}s_{0}\tau_{y} + \frac{\Delta_{e}}{k_{-}(E)}(j - \frac{1}{2})s_{0}\tau_{x} - \begin{pmatrix} 0 & \frac{\Delta_{e}}{k_{-}(E)}A_{\theta}^{00} & 0 & \frac{\Delta_{e}}{k_{m}}A_{\theta}^{0-} \\ \frac{\Delta_{e}}{k_{-}(E)}A_{\theta}^{00} & 0 & \frac{\Delta_{e}}{k_{m}}A_{\theta}^{0-} & 0 \\ 0 & \frac{\Delta_{e}}{k_{m}}A_{\theta}^{-0} & 0 & \frac{\Delta_{e}}{k_{-}(E)}A_{\theta}^{--} \\ \frac{\Delta_{e}}{k_{m}}A_{\theta}^{-0} & 0 & \frac{\Delta_{e}}{k_{-}(E)}A_{\theta}^{--} & 0 \end{pmatrix}$$

$$(45)$$

$$= (E - \mu)s_0\tau_z + i\Delta_e \hbar \nu_{k_-} \partial_E s_0\tau_y + \frac{\Delta_e}{k_-(E)} [(j - \frac{1}{2})s_0 - \begin{pmatrix} A_\theta^{00} & \frac{k_-(E)}{k_m} A_\theta^{0-} \\ \frac{k_-(E)}{k_m} A_\theta^{-0} & A_\theta^{--} \end{pmatrix}] \tau_x$$
 (46)

The resulting Hamiltonian is equivalent to the 4*4Jackiw-Rebbi model, we can solve the zero solution of the first two items

$$\psi_0^1(E) = \frac{1}{2} e^{\int_{\frac{\mu - E'}{\Delta_e \hbar \nu_{k_-}}}^{E} dE'} \begin{pmatrix} 1\\1\\1\\1\\1 \end{pmatrix}$$
(47)

$$\psi_0^2(E) = \frac{1}{2} e^{\int_{-\frac{\mu - E'}{\Delta_e \hbar \nu_{k_-}} dE'}} \begin{pmatrix} 1\\1\\-1\\-1 \end{pmatrix}$$
(48)

we can calculate that

$$A_{\theta}^{00} = 0$$
 $A_{\theta}^{--} = 0$ $A_{\theta}^{0-} = \frac{\sqrt{2}Ak_{-}(E)}{a}$ (49)

The energy can be determined by

$$H_{j} = \frac{\Delta_{e}}{k_{-}(E)} (j - \frac{1}{2}) s_{0} \tau_{x} - \frac{\Delta_{e}}{k_{m}} A_{\theta}^{0-} s_{x} \tau_{x}$$
 (50)

Then we can get the eigen value

$$E_{j} = \frac{\Delta_{e}}{k_{-}(E)} (j - \frac{1}{2} \pm \frac{k_{-}(E)}{k_{m}} A_{\theta}^{0-})$$
 (51)

It's eigen value is $(1,1,1,1)^T$ and $(1,1,-1,-1)^T$ corresponed to the zero solution of the Jackiw-Rebbi model. If we want to get the zero solution, we need to require $\frac{k_-(E)}{k_m}A_\theta^{0-}$ be a half integer, we can easily to analysis that $\frac{k_-(E)}{k_m}A_\theta^{0-}$ more than zero and less than 1, so the only possible is to be $\frac{1}{2}$, Then we can get the zero solution's angular must be 0 or 1, Then we can get the zero solution

$$\psi_0^{j=0}(E,\theta) = \frac{1}{2\sqrt{k_{-}(E)}} e^{\int_{-\frac{\mu-E'}{\Delta_e \hbar \nu_{k_{-}}} dE'} \begin{pmatrix} e^{-i\theta} \\ -i \\ e^{-i\theta} \\ -i \end{pmatrix}$$
(52)

$$\psi_0^{j=1}(E,\theta) = \frac{1}{2\sqrt{k_-(E)}} e^{\int_{\frac{\mu-E'}{\Delta_e\hbar\nu_{k_-}}}^{E} dE'} \begin{pmatrix} 1\\ -ie^{i\theta}\\ -1\\ ie^{i\theta} \end{pmatrix}$$
(53)

At the same time, we can calculate the vortex phase transition energy, we can get

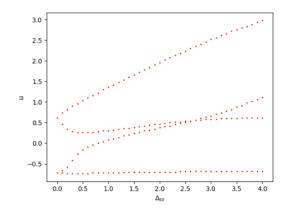
$$\frac{k_{-}(E)}{k_{m}}A_{\theta}^{0-} = \frac{k_{-}(E)}{\frac{k_{0}(E) + k_{-}(E)}{2}} \frac{\sqrt{2}Ak_{-}(E)}{a_{-}} = \frac{1}{2}$$
(54)

we can bring the parameter into equation, it's the M0 = -1, M1 = 1, A = 0.5, for simplify, we can estimate $\frac{k_-(E)}{\frac{k_-(E)+k_-(E)}{2}}$ to be a constant 0.81, Finally we can get it's vortex phase transition at E=-0.79, At the same time, we can get When the Fermi surface near the μ_+ , it's vortex phase transition point at E=0.66.

So from the analysis,we can get there will have four vortex phase transition point,two of them have the 0 angular momentum, other have +1 angular momentum, and the vortex phase transition energy at $E_+ = 0.66$, $E_- = -0.79$, there are all correspondence to numerical calculation.

Solve
$$\left[0.81*Sqrt[2]*0.5*\frac{x}{Sqrt[\left(\left(-1+x^2+Sqrt\left[\left(-1+x^2\right)^2+0.5*x^2\right)\right)^2+0.5*x^2\right)\right]}=0.5, x\right]$$
 $\left\{\left\{x\to1.09035\right\}\right\}$ $x2=1.090347871187568$ 、 1.09035 $-Sqrt\left[\left(-1+x2^2\right)^2+0.5*x2^2\right]$ -0.793786

Solve $\left[0.81*Sqrt[2]*0.5*\frac{x}{Sqrt\left[\left(\left(1-x^2+Sqrt\left[\left(-1+x^2\right)^2+0.5*x^2\right)\right)^2+0.5*x^2\right)\right]}=0.5, x\right]$ $\left\{\left\{x\to0.9171384898572194\right\}$ $x1=0.9171384898572194$ 、 $Sqrt\left[\left(-1+x1^2\right)^2+0.5*x1^2\right]$ -0.917138 -0.917138 -0.917138 -0.917138 -0.917138 -0.917138 -0.917138 -0.917138 -0.917138



When change the sign of parameter of the k_y , the Hamiliton change to When we change the sign of ky's parameter in Dirac semimetal, the electron Hamiliton become

$$H_{e\uparrow}(k) = \begin{pmatrix} M(k) & -iAke^{-i\theta} & -iAke^{-i\theta} \\ iAke^{i\theta} & -M(k) & 0 \\ iAke^{i\theta} & 0 & -M(k) \end{pmatrix}$$
(55)

We can definite the angular momentum Now the angular momentum become

$$J_{z} = -i\partial_{\theta} + \begin{pmatrix} \frac{1}{2} & & \\ & -\frac{1}{2} & \\ & & -\frac{1}{2} \end{pmatrix}$$
 (56)

We can use the same way to get the eige states of the $H_{e\uparrow}(k)$ Use the same way,we can solve the eigen states of the $H_{e\uparrow}(k)$

$$|\psi_{0}^{j}\rangle_{e} = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} 0\\ -e^{i(j+\frac{1}{2})\theta}\\ e^{i(j+\frac{1}{2}\theta)} \end{pmatrix} \qquad |\psi_{\pm}^{j}\rangle_{e} = \frac{1}{a_{\pm}\sqrt{2\pi}} \begin{pmatrix} -i(M(k)\pm E)e^{i(j-\frac{1}{2})\theta}\\ Ake^{i(j+\frac{1}{2})\theta}\\ Ake^{i(j+\frac{3}{2})\theta} \end{pmatrix}$$
(57)

For the hole part

$$|\psi_{0}^{j}\rangle_{h} = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} 0\\ -e^{i(j+\frac{1}{2})\theta}\\ e^{i(j+\frac{1}{2}\theta)} \end{pmatrix} \qquad |\psi_{\pm}^{j}\rangle_{h} = \frac{1}{a_{\pm}\sqrt{2\pi}} \begin{pmatrix} -i(M(k)\pm E)e^{i(j-\frac{1}{2})\theta}\\ Ake^{i(j+\frac{1}{2})\theta}\\ Ake^{i(j+\frac{1}{2})\theta} \end{pmatrix}$$
(58)

For simplify to calculate, we can choose $j = -\frac{1}{2}$

$$|\psi_0\rangle_e = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} 0\\ -1\\ 1 \end{pmatrix} \qquad |\psi_\pm\rangle_e = \frac{1}{a_\pm\sqrt{2\pi}} \begin{pmatrix} -i(M(k)\pm E)e^{-i\theta}\\ Ak\\ Ak \end{pmatrix}$$
(59)

$$|\psi_0\rangle_h = \frac{1}{2\sqrt{\pi}} \begin{pmatrix} 0\\ -1\\ 1 \end{pmatrix} \qquad |\psi_\pm\rangle_h = \frac{1}{a_\pm\sqrt{2\pi}} \begin{pmatrix} -i(M(k)\pm E)e^{-i\theta}\\ Ak\\ Ak \end{pmatrix} \tag{60}$$

We can notice that $|\psi_0\rangle_e$ is independent of the k and θ , so the it's connection of the other band must zero, so we just to consider one band model. For example, When Fermi energy near the μ_- , the eigne

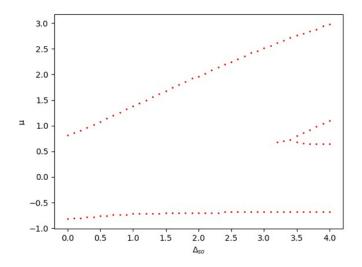
energy is

$$E_{j} = \frac{\Delta_{e}}{k} (j - \frac{1}{2} - A_{\theta}^{-}) \tag{61}$$

If we want to get the zero solution,we need the A_{θ}^{--} is the half of integer,we can get

$$A_{\theta}^{--} = \frac{(-M(k) + E)^2}{(-M(k) + E)^2 + 2A^2k^2}$$
 (62)

From easily analysis, if the A_{θ}^{--} is the half of integer, it must be $\frac{1}{2}$ we can get when M(k)=0, the $A_{\theta}^{--}=\frac{1}{2}$. We can take the parameter into this equation, we can get the vortex phase transition energy is ± 0.707 , and the angular momentum is j=1, so the C_{2z} is -1. This result is corresponding the numerical result too.



When change the parameter of k_y to zero, it says that the Hamiliton change to

$$H_{e\uparrow}(k) = \begin{pmatrix} M(k) & -iAk_{-} & -iAk_{x} \\ iAk_{+} & -M(k) & 0 \\ iAk_{x} & 0 & -M(k) \end{pmatrix}$$

$$(63)$$

we can solve it's eigenvalue and eigenstates

$$E_0 = -M(k) E_{\pm} = \pm \sqrt{M(k)^2 + 2A^2k_x^2 + A^2k_y^2} (64)$$

$$\psi_{0} = \frac{1}{\sqrt{3\pi}} \begin{pmatrix} 0 \\ -\cos\theta \\ e^{-i\theta} \end{pmatrix} \qquad \psi_{\pm} = \frac{1}{a_{\pm}} \begin{pmatrix} -i(M(k) \pm E) \\ Ake^{i\theta} \\ Ak\cos\theta \end{pmatrix}$$
(65)

The normalization coefficient is

$$a_{\pm} = \int_{0}^{2\pi} A^{2}k^{2}\cos\theta^{2} + A^{2}k^{2} + (M(k) \pm E)^{2}d\theta$$
 (66)

$$=3\pi A^{2}k^{2}+2\pi M(k)+\int_{0}^{2\pi}\sqrt{M(k)^{2}+A^{2}k^{2}+A^{2}k^{2}cos\theta^{2}}$$
(67)

At this time,we can find the E_0 is isotropic,but the E_\pm is anisotropy. For simplify to estimate, we can just think E_\pm is isotropic. The we can use the same way of the calculation, we assume that the fermi surface is near the μ_0 we can get the

$$A_{\theta}^{00} = i \langle \psi_0 | \partial_{\theta} | \psi_0 \rangle = \frac{2}{3}$$
 (68)

so it can't be a half of integer, so the middle band can't have a vortex phase transition point.

we next assume that the fermi surface is near the μ_- ,we can get if the vortex phase transition happened,we need $\frac{k_-(E)}{k_m}A_\theta^{0-}$ to be $\frac{1}{2}$