

TSC exercises

① (a) $\hat{H} = \sum_{\underline{k}} (\epsilon_{\underline{k}} - \mu) \underline{C}_{\underline{k}}^+ \underline{C}_{\underline{k}} + \frac{1}{2} \sum_{\underline{k}} (\Delta_{\underline{k}} \underline{C}_{\underline{k}}^+ \underline{C}_{-\underline{k}} + \Delta_{\underline{k}}^* \underline{C}_{-\underline{k}} \underline{C}_{\underline{k}})$

$\psi_{\underline{k}} \equiv \begin{pmatrix} C_{\underline{k}} \\ C_{-\underline{k}}^+ \end{pmatrix} \Rightarrow \hat{H} = \frac{1}{2} \sum_{\underline{k}} \psi_{\underline{k}}^+ H_{\underline{k}}^{\text{BdG}} \psi_{\underline{k}}$

$H_{\underline{k}}^{\text{BdG}} \equiv \begin{pmatrix} P_{\underline{k}} & Q_{\underline{k}} \\ R_{\underline{k}} & S_{\underline{k}} \end{pmatrix} \Rightarrow \hat{H} = \frac{1}{2} \sum_{\underline{k}} (C_{\underline{k}}^+ \ C_{-\underline{k}}) \begin{pmatrix} P & Q \\ R & S \end{pmatrix} \begin{pmatrix} C_{\underline{k}} \\ C_{-\underline{k}}^+ \end{pmatrix} + \text{const} =$
 $= \frac{1}{2} \sum_{\underline{k}} (P_{\underline{k}} \underline{C}_{\underline{k}}^+ \underline{C}_{\underline{k}} + Q_{\underline{k}} \underline{C}_{\underline{k}}^+ \underline{C}_{-\underline{k}} + R_{\underline{k}} \underline{C}_{-\underline{k}} \underline{C}_{\underline{k}} + S_{\underline{k}} \underline{C}_{-\underline{k}} \underline{C}_{-\underline{k}}^+) + \text{const}$

To match wavy-terms, we use $\sum_{\underline{k}} f_{\underline{k}} = \sum_{\underline{k}} f_{-\underline{k}}$, and $\{C_{\underline{k}}, C_{\underline{k}}^+\} = 1$

$\sum_{\underline{k}} (\epsilon_{\underline{k}} - \mu) \underline{C}_{\underline{k}}^+ \underline{C}_{\underline{k}} = \frac{1}{2} \sum_{\underline{k}} [(\epsilon_{\underline{k}} - \mu) \underline{C}_{\underline{k}}^+ \underline{C}_{\underline{k}} + (\epsilon_{-\underline{k}} - \mu) \underline{C}_{-\underline{k}}^+ \underline{C}_{-\underline{k}}] =$
 $= \frac{1}{2} \sum_{\underline{k}} [(\epsilon_{\underline{k}} - \mu) \underline{C}_{\underline{k}}^+ \underline{C}_{\underline{k}} + (\epsilon_{-\underline{k}} - \mu) (1 - \underline{C}_{-\underline{k}} \underline{C}_{-\underline{k}}^+)] =$
 $= \frac{1}{2} \sum_{\underline{k}} [(\epsilon_{\underline{k}} - \mu) \underline{C}_{\underline{k}}^+ \underline{C}_{\underline{k}} - (\epsilon_{-\underline{k}} - \mu) \underline{C}_{-\underline{k}} \underline{C}_{-\underline{k}}^+] + \frac{1}{2} \sum_{\underline{k}} (\epsilon_{\underline{k}} - \mu)$

$\Rightarrow Q_{\underline{k}} = \Delta_{\underline{k}} ; R_{\underline{k}} = \Delta_{\underline{k}}^* ; P_{\underline{k}} = \epsilon_{\underline{k}} - \mu ; S_{\underline{k}} = -(\epsilon_{-\underline{k}} - \mu) ; \text{const} = \frac{1}{2} \sum_{\underline{k}} (\epsilon_{\underline{k}} - \mu)$

$\Rightarrow H_{\underline{k}}^{\text{BdG}} = \begin{vmatrix} \epsilon_{\underline{k}} - \mu & \Delta_{\underline{k}} \\ \Delta_{\underline{k}}^* & -(\epsilon_{-\underline{k}} - \mu) \end{vmatrix}$

⑥ $H_{\underline{k}}^{\text{BdG}} \equiv \vec{D}_{\underline{k}} \cdot \vec{\sigma} = D_{\underline{k},1} \sigma_x + D_{\underline{k},2} \sigma_y + D_{\underline{k},3} \sigma_z = \begin{pmatrix} D_{\underline{k},3} & D_{\underline{k},1} - i D_{\underline{k},2} \\ D_{\underline{k},1} + i D_{\underline{k},2} & -D_{\underline{k},3} \end{pmatrix}$
 $\Rightarrow D_{\underline{k},1} = \text{Re} \Delta_{\underline{k}} ; D_{\underline{k},2} = -\text{Im} \Delta_{\underline{k}} ;$

while $D_{\underline{k},3} = \epsilon_{\underline{k}} - \mu$ if $\epsilon_{-\underline{k}} = \epsilon_{\underline{k}}$ is even.

NOTE: IF $\epsilon_{-\underline{k}} \neq \epsilon_{\underline{k}}$, we separate $\epsilon_{\underline{k}} = \frac{\epsilon_{\underline{k}} + \epsilon_{-\underline{k}}}{2} + \frac{\epsilon_{\underline{k}} - \epsilon_{-\underline{k}}}{2} \equiv \epsilon_{\underline{k}}^{\text{even}} + \epsilon_{\underline{k}}^{\text{odd}}$
 Then, $D_{\underline{k},3} = \epsilon_{\underline{k}}^{\text{even}} - \mu$, while $H_{\underline{k}}^{\text{BdG}} = \vec{D}_{\underline{k}} \cdot \vec{\sigma} + \epsilon_{\underline{k}}^{\text{odd}} \cdot \mathbb{1}$. The last term cannot cause a band crossing and preserves wavefunctions, hence we can simply discard $\epsilon_{\underline{k}}^{\text{odd}}$.

$$\vec{D}_k = (\text{Re}\Delta_k, -\text{Im}\Delta_k, \epsilon_k - \mu)$$

$$\text{BdG bands: } E_{\pm} = \pm |\vec{D}_k| = \pm \sqrt{(\epsilon_k - \mu)^2 + (\text{Re}\Delta_k)^2 + (\text{Im}\Delta_k)^2} = \pm \sqrt{(\epsilon_k - \mu)^2 + |\Delta_k|^2}$$

③ GAP CLOSES WHEN $\exists \underline{k}_0, E_{\pm} = 0$

$$E_{\pm} = 0 \Rightarrow \epsilon_{\underline{k}_0} - \mu \stackrel{(1)}{=} 0 \wedge |\Delta_{\underline{k}_0}| \stackrel{(2)}{=} 0$$

$$\text{OUR MODELS: } \epsilon_k \equiv -t[\cos(k_x) + \cos(k_y)]; \text{ BZ: } \begin{array}{c} k_y \\ \uparrow \\ -\pi \quad \pi \\ \hline -\pi \quad \pi \\ \hline \downarrow \\ k_x \end{array}$$

$$\textcircled{1} \Rightarrow -t[\cos k_x + \cos k_y] \equiv \mu$$

$$\textcircled{1A} \quad |\mu| > 2t \Rightarrow \text{NO SOLUTION FOR } \underline{k}_0$$

$$\textcircled{1B} \quad \mu = 2t \Rightarrow \cos k_x \equiv -1 \wedge \cos k_y \equiv -1 \Rightarrow \underline{k}_0 = (\pi, \pi) = M$$

$$\textcircled{1C} \quad \mu = -2t \Rightarrow \cos k_x \equiv +1 \wedge \cos k_y \equiv +1 \Rightarrow \underline{k}_0 = (0, 0) = \Gamma$$

$$\textcircled{1D} \quad |\mu| < 2t \Rightarrow \cos k_x + \cos k_y \equiv -\frac{\mu}{t} \Rightarrow \underline{k}_0 \in \text{Fermi surface (FS)}, \Gamma, M \notin \text{FS}$$

$$\Delta_k^{1\pm} \equiv \sin k_x \pm i \sin k_y \quad ("p_x \pm i p_y")$$

$$\Delta_k^{2\pm} \equiv \cos k_x - \cos k_y \pm i \sin k_x \cdot \sin k_y \quad ("d_{x^2-y^2} \pm i d_{xy}")$$

$$\textcircled{2} \Rightarrow |\Delta_{\underline{k}_0}| = 0 \Rightarrow \text{Re}\Delta_{\underline{k}_0} = 0 \wedge \text{Im}\Delta_{\underline{k}_0} = 0$$

$$\Rightarrow \text{FOR } \Delta^{1\pm}: \sin k_x = 0 \wedge \sin k_y = 0 \Rightarrow \left. \begin{array}{l} k_x = 0, \pi \\ k_y = 0, \pi \end{array} \right\} \Rightarrow \underline{k}_0 \in \{\Gamma, X, Y, M\}$$

$$\text{FOR } \Delta^{2\pm}: \cos k_x = \cos k_y \wedge (\sin k_x = 0 \vee \sin k_y = 0) \Rightarrow \underline{k}_0 \in \{\Gamma, M\}$$

$$\text{Combine } \textcircled{1} \& \textcircled{2}: \Delta^{1\pm}: \begin{array}{l} \mu = 2t \quad (\underline{k}_0 = M) \\ \mu = -2t \quad (\underline{k}_0 = \Gamma) \end{array}$$

$$\left. \begin{array}{l} \underline{k}_0 = X \Rightarrow \cos \pi + \cos 0 = -\frac{\mu}{t} \Rightarrow \mu = 0 \\ \underline{k}_0 = Y \Rightarrow \cos 0 + \cos \pi = -\frac{\mu}{t} \Rightarrow \mu = 0 \end{array} \right\} (\underline{k}_0 = X, Y \text{ simultaneously})$$

$$\Delta^{2\pm}: \begin{array}{l} \mu = 2t \quad (\underline{k}_0 = M) \\ \mu = -2t \quad (\underline{k}_0 = \Gamma) \end{array}$$

NOTE: $\Delta_k^{1\pm} = -\Delta_{-k}^{1\pm}$ is odd, allowing a gap closing @ TRIM inside the band.

GAPPED PHASES:

$\Delta^{1\pm}$: 

$\Delta^{2\pm}$: 

$$\textcircled{d} \quad \text{Ch}_1(H^{\text{Bdg}}) = \int_{B\mathbb{Z}} \hat{\vec{D}}_1 \cdot (\partial_{k_x} \hat{\vec{D}}_1 \times \partial_{k_y} \hat{\vec{D}}_1) = \int_{B\mathbb{Z}} \frac{1}{|\vec{D}_1|^3} \vec{D}_1 \cdot (\partial_{k_x} \vec{D}_1 \times \partial_{k_y} \vec{D}_1)$$

$$p^{(n)} = \text{sgn}[\vec{D}_k \cdot (\partial_{k_x} \vec{D}_k \times \partial_{k_y} \vec{D}_k)]|_{k=k^{(n)}}; \quad \vec{D}_k^{(n)} = (a, 0, 0), a \in [0, +\infty)$$

$$\vec{D}_k = (\text{Re} \Delta_k, -\text{Im} \Delta_k, \varepsilon_k - \mu)$$

$n=1, 2, \dots$ solution counter

→ Solve $\Delta_{\frac{1}{2}}^{\pm}$ case:

Solve $\Delta_{\underline{k}}^{1\pm}$ case:

$$\Rightarrow \left. \begin{aligned} \vec{D}_{\underline{k}}^{1\pm} &= (\sin k_x, \mp \sin k_y, -t(\cos k_x + \cos k_y) - \mu) \\ 2_{k_x} \vec{D}_{\underline{k}}^{1\pm} &= (\cos k_x, 0, +t \sin k_x) \\ 2_{k_y} \vec{D}_{\underline{k}}^{1\pm} &= (0, \mp \cos k_y, +t \sin k_y) \end{aligned} \right\} \vec{D}_{\underline{k}}^{(m)} = (1, 0, 0) \sim \hat{x} \Rightarrow$$

$$\vec{D}_{\underline{k}}^{1\pm} \cdot \{2_{k_x} \vec{D}^{1\pm} \times 2_{k_y} \vec{D}^{1\pm}\} \Big|_{\underline{k}=\underline{k}^{(m)}} =$$

$$= D_{\underline{k}^{(m)}}^{1\pm} \cdot \left(2_{k_x} D_y^{1\pm} 2_{k_y} D_z^{1\pm} - 2_{k_x} D_z^{1\pm} 2_{k_y} D_y^{1\pm} \right) \Big|_{\underline{k}=\underline{k}^{(m)}}$$

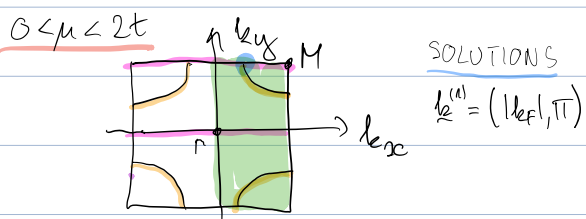
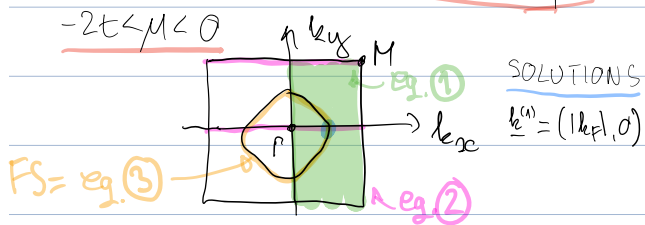
$$\Rightarrow P_{1\pm}^{(n)} = \text{sgn} \left\{ \sin k_x^{(n)} (\pm t \sin k_x^{(n)} \cos k_y^{(n)}) \right\} = \pm \text{sgn} \{ \cos k_y^{(n)} \} \quad \text{NOTE: } t > 0 \text{ by definition}$$

NEED $\underline{h}^{(n)}$: $\vec{D}_{\underline{h}^{(n)}}^{1\pm} \equiv (1, 0, 0) \Rightarrow \sin h_{xz}^{(n)} \equiv 1 \wedge \sin h_{yz}^{(n)} \equiv 0 \wedge -(\cos h_{xz}^{(n)} + \cos h_{yz}^{(n)}) \mu = 0$

- IN GAPPED PHASES $|u| > 2t$, there is NO solution to (3) equation.

So no $\underline{h}_2^{(n)}$ exists $\Rightarrow \text{Chern}[H_{1\pm}^{\text{BdG}}(|\mu| > 2t)] = 0$.

GRAPHICAL SOLUTION FOR $I_2^{(n)}$



- Evaluate $p^{(1)}(\Delta_{\frac{1}{2}}^{\frac{1}{2}})$, for $-2t < \mu < 0$; $\underline{b}^{(1)} = (|k_p|, 0)$

$$p_{\pm}^{(1)} = \pm \operatorname{sgn}\{\cos k_y^{(1)}\} = \pm 1.$$

$$\text{Chern} \left(H_{\frac{1}{2}}^{\text{BdG}} \left(\Delta_{\frac{1}{2}}^{\pm} \right) \right) = \pm 1 \text{ for } -2t < \mu < 0.$$

- Evaluate $p_{1\pm}^{(n)}$ for $0 < \mu < 2t$, $\underline{k}^{(n)} = (|k_F|, \pi)$.

$$p_{1\pm}^{(n)} = \pm \text{sgn}\{\cos k_y\} = \mp 1$$

$$\text{Chern}(H_{\underline{k}}^{\text{BdG}}(\Delta_{\underline{k}}^{1\pm})) = \mp 1 \text{ for } 0 < \mu < 2t.$$

→ Solve the $\Delta_{\underline{k}}^{2\pm}$ case: [NOTATION: $\cos k_x \equiv cx$; $\sin k_x \equiv sx$; $\cos k_y \equiv cy$; $\sin k_y \equiv sy$]

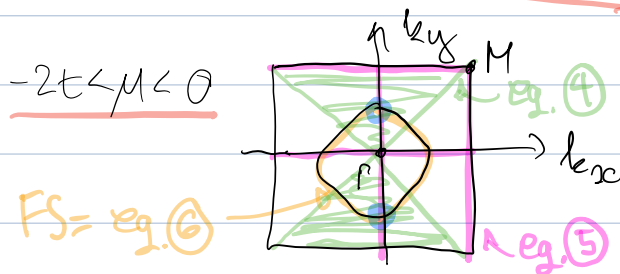
$$\begin{aligned} \vec{D}_{\underline{k}}^{2\pm} &= (cx - cy, \mp sx sy, t(cx + cy) - \mu) \\ \partial_{k_x} \vec{D}_{\underline{k}}^{2\pm} &= (-sx, \mp cx sy, +tsx) \\ \partial_{k_y} \vec{D}_{\underline{k}}^{2\pm} &= (sy, \mp sx cy, +tsy) \end{aligned} \quad \left\{ \begin{aligned} \vec{D}_{\underline{k}}^{(n)} &\equiv (|a|, 0, 0) \sim \hat{x} \Rightarrow \\ \vec{D}_{\underline{k}}^{2\pm} \cdot (\partial_{k_x} \vec{D}_{\underline{k}}^{2\pm} \times \partial_{k_y} \vec{D}_{\underline{k}}^{2\pm}) \Big|_{\underline{k}=\underline{k}^{(n)}} &= \\ &= D_{\underline{k}}^{2\pm} \cdot \partial_{k_x} \partial_{k_y} \vec{D}_{\underline{k}}^{2\pm} \Big|_{\underline{k}=\underline{k}^{(n)}} = D_{\underline{k}}^{2\pm} \cdot (2sx sy, 2sy sx, 0) \Big|_{\underline{k}=\underline{k}^{(n)}} \end{aligned} \right.$$

$$p_{2\pm}^{(n)} = \text{sgn}\{(cx - cy) \cdot t(\mp cx sy \pm sx cy)\} = \mp \text{sgn}\{(cx - cy)(cx sy - sx cy)\}$$

NEED $\underline{k}^{(n)}$: $\vec{D}_{\underline{k}^{(n)}}^{2\pm} \equiv (|a|, 0, 0) \Rightarrow cx - cy \stackrel{(4)}{=} |a| \wedge sx sy \stackrel{(5)}{=} 0 \wedge -t(\cos k_x + \cos k_y) \stackrel{(6)}{\mu} \equiv 0$

- Again for $|\mu| > 2t$, $\text{Ch}(\Delta_{\underline{k}}^{2\pm}; |\mu| > 2t) = 0$

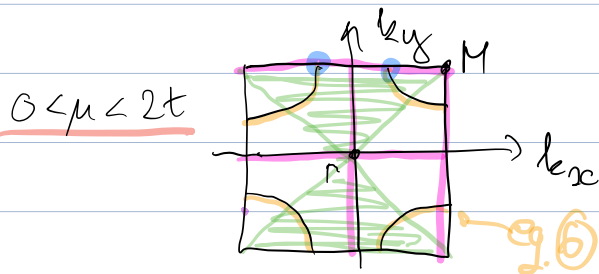
GRAPHICAL SOLUTION FOR $\underline{k}^{(n)}$ eg. (4): $\cos k_x \geq \cos k_y$



SOLUTIONS

$$\underline{k}^{(n)} = (0, |k_F|)$$

$$\underline{k}^{(2)} = (0, -|k_F|)$$



SOLUTIONS

$$\underline{k}^{(n)} = (|k_F|, \pi)$$

$$\underline{k}^{(2)} = (-|k_F|, \pi)$$

$$P_{2\pm}^{(m)} = \mp \text{sgn}\{(cx - cy)(cxs^2y - s^2xcy)\}$$

$$\Rightarrow P_{2\pm}^{(2)} = P_{2\pm}^{(1)} (|k_A \rightarrow -k_A) = P_{2\pm}^{(1)} = \mp 1$$

- Evaluate $P_{2\pm}^{(1)}, P_{2\pm}^{(2)}$ for $\Delta_{\underline{k}}^{2\pm}$ for $-2t < \mu < 0$; $\underline{k}^{(1)} = (0, |k_F|)$; $\underline{k}^{(2)} = (0, -|k_F|)$

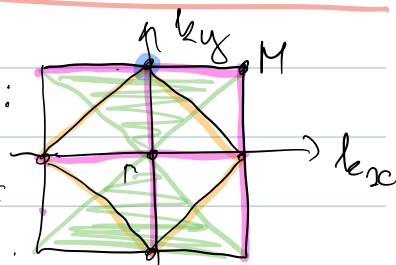
$$\Rightarrow P_{2+}^{(1)} = \mp \operatorname{sgn}\{(1 - c|k_F|) \cdot s^2|k_F|\} = \mp 1$$

$$\Rightarrow P_{2\pm}^{(2)} = P_{2\pm}^{(1)} (|l_2\rangle \rightarrow -|l_2\rangle) = P_{2\pm}^{(1)} = \mp 1$$

SUMMARY

$\triangle^{1t}$: $Ch = 0 \quad \pm 1 \quad \mp 1 \quad 0$

Δ^{2+} : $Ch = 0$  $M/2t$

$$\underline{b}^{(1)} = (0, \pi) \Leftarrow$$

$$P_{2\pm}^{(n)} = \pm \operatorname{sgn}\{2 \cdot 0\} = \operatorname{sgn}\{0\} \quad \text{⚡}$$

$P_{2\pm}^{(1)} = 0$ means that $\vec{D} \parallel \partial_x \vec{D} \times \partial_y \vec{D}$, it is a critical point of the $\vec{D}_x$ surface,

We should choose another ray instead of $\underline{e} = (1, 0, 0)$, e.g., $(0, 0, 1)$.

The critical point is anticipated also from $\underline{h}^{(1)}$ being on a corner of FS, where two solutions $\underline{h}^{(1)}, \underline{h}^{(2)}$ merged. Exercise for the reader...

© WINDING OF Δ : $W(\mu/t)$

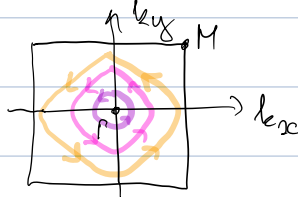
- BY DEFINITION, FOR $|\mu| > 2t$ THE $W(\mu) = 0$ AS THERE IS NO FS.

- GAPPED PHASE $\Rightarrow |\Delta_k| \neq 0 \Rightarrow \Delta_k = e^{i\varphi_k} \cdot |\Delta_k|$ and φ_k is well-defined.

$$W(\mu) = \oint_{FS} \frac{d\mathbf{k}}{L_{FS}} \cdot \frac{\Delta_k^*}{|\Delta_k|} \left(\nabla_k \frac{\Delta_k}{|\Delta_k|} \right) = \oint_{FS} \frac{d\mathbf{k}}{L_{FS}} \cdot e^{-i\varphi_k} (\nabla_k e^{i\varphi_k}) = \oint_{FS} d\mathbf{k} \cdot \nabla_k \varphi_k =$$

= ACCUMULATED PHASE φ on traversing the closed FS.

- FS: for $-2t < \mu < 0$



Since $W(\mu)$ is a topological number, we can deform the FS to a circle around Γ . So, FS: $\{ \mathbf{k} \equiv k_F (\cos \theta_k, \sin \theta_k); k_F \text{ is const} < \pi \}$, we can take $k_F \ll 1$.

$$k_F \ll 1 \Rightarrow \begin{cases} \sin k_x = \sin(k_F \cos \theta_k) \approx k_F \cos \theta_k \\ \sin k_y = \sin(k_F \sin \theta_k) \approx k_F \sin \theta_k \\ \cos k_x = \cos(k_F \cos \theta_k) \approx 1 - \frac{k_F^2}{2} \cos^2 \theta_k \\ \cos k_y \approx 1 - \frac{k_F^2}{2} \sin^2 \theta_k \end{cases} \quad \left| \begin{array}{l} \text{NOTE: } \theta_k \text{ is} \\ \text{polar angle of } \mathbf{k}. \end{array} \right.$$

$$\Rightarrow \Delta_k^{1\pm} = k_F e^{\pm i\theta_k} \Rightarrow \varphi_k^{1\pm} = \pm \theta_k$$

$$\Rightarrow \Delta_k^{2\pm} = \frac{k_F^2}{2} (-\cos^2 \theta_k + \sin^2 \theta_k) \pm i k_F^2 \sin \theta_k \cos \theta_k = \frac{k_F^2}{2} (\cos(2\theta_k) \pm i \sin(2\theta_k)) = -\frac{k_F^2}{2} e^{\mp i 2\theta_k}$$

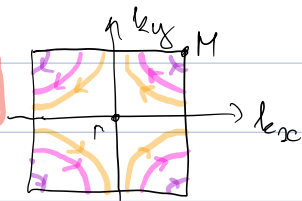
$$\Rightarrow \varphi_k^{2\pm} = \mp 2\theta_k$$

$$\Rightarrow W^{1\pm} = \oint_{FS} \frac{d\mathbf{k}}{L_{FS}} \cdot \nabla_k \varphi_k = \int_0^{2\pi} \frac{k_F d\theta}{2\pi k_F} \partial_\theta \varphi(\theta) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \cdot (\pm 1) = \pm 1$$

$$\Rightarrow W^{2\pm} = \mp 2$$

NOTE: length of FS:
 $L_{FS} = 2\pi k_F$

- FS: for $0 < \mu < 2\pi$



NOTE: We preserve FS loop orientation, so now the loop is clockwise around M-point.

NOW FS: $\underline{k} = (\pi, \pi) + k_F (\cos \theta_k, -\sin \theta_k)$ ← clockwise around M

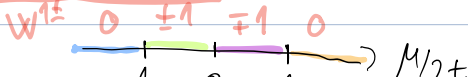
$$k_F \ll 1 \Rightarrow \begin{cases} \sin k_x = \sin(\pi + k_F \cos \theta_k) \approx -k_F \cos \theta_k \\ \sin k_y = \sin(\pi - k_F \sin \theta_k) \approx -k_F \sin \theta_k \\ \cos k_x = \cos(\pi + k_F \cos \theta_k) = -\cos(k_F \cos \theta_k) \approx -1 + \frac{k_F^2}{2} \cos^2 \theta_k \\ \cos k_y = \cos(\pi - k_F \sin \theta_k) = -\cos(k_F \sin \theta_k) \approx -1 + \frac{k_F^2}{2} \sin^2 \theta_k \end{cases}$$

$$\Rightarrow \Delta_k^{1\pm} = -k_F (\cos \theta_k \mp i \sin \theta_k) = -k_F e^{\mp i \theta_k}$$

$$\Delta_k^{2\pm} = \frac{k_F^2}{2} (\cos^2 \theta_k - \sin^2 \theta_k \mp i 2 \sin \theta_k \cos \theta_k) = \frac{k_F^2}{2} e^{\mp i 2 \theta_k}$$

$$\Rightarrow \left. \begin{aligned} \varphi_k^{1\pm} &= \mp \theta_k \\ \varphi_k^{2\pm} &= \mp 2 \theta_k \end{aligned} \right\} \begin{aligned} W^{1\pm} &= \mp 1 \\ W^{2\pm} &= \mp 2 \end{aligned}$$

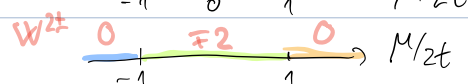
SUMMARY: $\Delta^{1\pm}$:



$M/2\pi$

$$\Delta^{2\pm}: W = Ch$$

$\Delta^{2\pm}$:



$M/2\pi$

NOTE: The sign of W is tied to choosing counter-clockwise loop orientation.