Dirac fermions

1. Ø Dirac equation in 2D:

$$H_D \Psi = \left(\beta m + \sum_{n=1}^{2} \alpha_n p_n \right) \Psi = i \partial_t \Psi$$

↳ 2 dim. spinor

with

- $*$ $\alpha_1, \alpha_2, \beta$ Hermitian matrices
- $*$ $\alpha_1^2 = \alpha_2^2 = \beta^2 = \mathbb{1}$
- $*$ $\{\alpha_1, \alpha_2\} = \{\beta, \alpha_1\} = \{\beta, \alpha_2\} = 0$

→ Solution: $\alpha_1 = \sigma^x$, $\alpha_2 = \sigma^y$ and $\beta = \sigma^z$

→ Fourier transform of H_D $(\vec{k} \in \mathbb{R}^2)$

$$H_D(\vec{k}) = \overset{\hbar v_F}{k_x} \sigma^x + k_y \sigma^y + m \sigma^z = \vec{d}(\vec{k}) \cdot \vec{\sigma} \quad \text{with } \vec{d}(\vec{k}) = \begin{pmatrix} k_x \\ k_y \\ m \end{pmatrix}$$

Spectrum: $E_\pm(\vec{k}) = \pm |\vec{d}(\vec{k})| = \pm \sqrt{k^2 + m^2}$ → Gapped if $m \neq 0$

2. Time-reversal symmetry:

- $\tilde{T}_0 = K \rightarrow d_x(\vec{k}) \overset{!}{=} d_x(-\vec{k}) \rightarrow H_D$ not TRI!
- $\tilde{T}_{\frac{1}{2}} = \sigma^y K \rightarrow d_z(\vec{k}) \overset{!}{=} -d_z(-\vec{k}) \rightarrow H_D$ not TRI for $m \neq 0$!

→ Non-zero Chern number possible

3. Berry curvature (of the lower band):

$$\tilde{F}_{xy}(\vec{k}) \overset{\circ}{=} \frac{m}{2(\vec{k}^2+m^2)^{3/2}}$$

4. "Chern number":

$$C = -\frac{1}{2\pi}\int_{\mathbb{R}^2} \tilde{F}_{xy}(\vec{k})\, d^2k = -\int_0^\infty \frac{mk}{2(k^2+m^2)^{3/2}}\, dk \overset{\circ}{=} -\frac{\text{sign}(m)}{2}$$

Why $C \notin \mathbb{Z}$? → Stokes' theorem not valid since $\mathbb{R}^2$ not compact!

→ Change from $m<0$ to $m>0$ ⇒ Change of Chern number $\Delta C = -1$

5. ∢ 2-band lattice model $H_\Gamma(\vec{k}) = \varepsilon_\Gamma(\vec{k})\cdot\mathbb{1} + \vec{d}_\Gamma(\vec{k})\cdot\vec{\sigma}$

Γ: parameters of the model

→ $\vec{K}\in T^2$ = Dirac point if

$$H_\Gamma(\vec{K}+\vec{k}) = \underbrace{v_F}_{\text{Fermi velocity}}\left[k_x\sigma^x + k_y\sigma^y + v_F m_\Gamma \sigma^z\right] + O(k^2)$$

$m_\Gamma = 0$ → Band structure at $\vec{K}$: $e_\pm(\vec{K}+\vec{k}) = \pm v_F|\vec{k}|$

1.2.2. The Qi – Wu – Zhang Model

1. Idea: "Regularize" Dirac Hamiltonian on a lattice

$\rightarrow$ $H_{QWZ}(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma}$ with

$$d_x = \sin(k_x) = k_x + O(k^2)$$

$$d_y = \sin(k_y) = k_y + O(k^2)$$

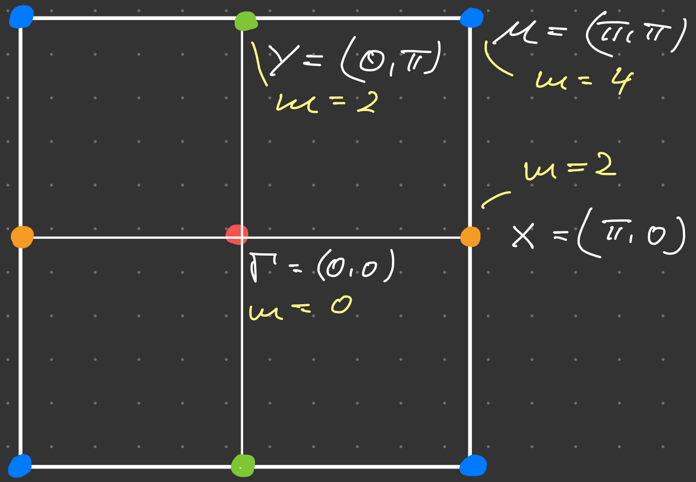
$$d_z = -m + 2 - \cos(k_x) - \cos(k_y) = -m + O(k^2)$$

$m \in \mathbb{R}$: only parameter of the theory

2. Spectrum:

$\varepsilon_\pm(\vec{k}) = \pm|\vec{d}(\vec{k})| \neq 0$ for all $\vec{k} \in T^2 \setminus \{\Gamma, X, Y, M\}$

with



3. Phases

- $m < 0$: $\measuredangle\ m \to -\infty \to \vec{d}(\vec{k}) \approx -m\vec{e}_z \to C(m<0) = 0$

  $\to$ Trivial band insulator

- $m > 4$ $\measuredangle\ m \to +\infty \to \vec{d}(\vec{k}| \approx -m\vec{e}_z \to C(m>4) = 0$

  $\to$ Trivial band insulator

* $\underline{0 < m < 2:}$

$\measuredangle$ Transition from $m < 0$ to $m > 0$ → Gap closing at Γ:

$$H(\vec{\Gamma}+\vec{k}) = k_x \sigma^x + k_y \sigma^y - m \sigma^z + O(k^2)$$

→

$$C(0<m<2) = C(m<0) + \Delta C(m<0 \to m>0)$$

$$= 0 + \left[\underbrace{-\frac{\text{sign}(-m)}{2}\Big|_{m>0}}_{\frac{1}{2}} \underbrace{- \left(-\frac{\text{sign}(-m)}{2}\Big|_{m<0}\right)}_{\frac{1}{2}}\right]$$

$$= +1$$

→ Topological phase (I)

* $\underline{2 < m < 4}$: X Transition from $m > 4$ to $m < 4$ → Gap closes M:

$$H(\vec{M}+\vec{k}) = -k_x\sigma^x - k_y\sigma^y + (4-m)\sigma^z + \mathcal{O}(k^2)$$

→

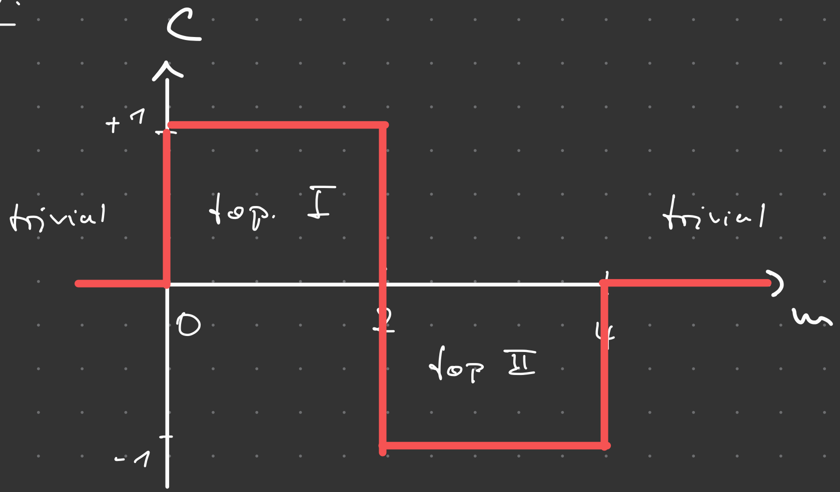
$$C(2<m<4) = C(m>4) + \Delta C(m>4 \to m<4)$$

$$= 0 + \Bigg[\underbrace{-\frac{\text{sign}(4-m)}{2}\Bigg|_{m<4}}_{-\frac{1}{2}} - \underbrace{\left(-\frac{\text{sign}(4-m)}{2}\right|_{m>4}\Bigg]}_{-\frac{1}{2}}\Bigg]$$

$$= \underline{\underline{-1}}$$

→ Topological phase (II)

→ Phase diagram:



4. Real-space Hamiltonian:

SP Hilbert space : $|\psi_{i\alpha}\rangle \longrightarrow \underbrace{|x,y\rangle}_{\text{external}} \otimes \underbrace{|\sigma\rangle}_{\text{internal}}$

$x = 1, \ldots, N_x$: x-position

$y = 1, \ldots, N_y$: y-position

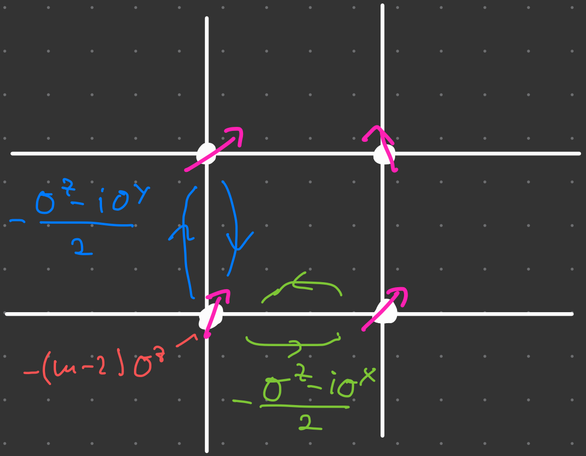
$\sigma = \pm 1$: spin

SP Hamiltonian:

$$H_{QWZ} \overset{\circ}{=} -\sum_{x,y}{}' \left\{ |x+1,y\rangle\langle x,y| \otimes \frac{\sigma^z - i\sigma^x}{2} + h.c. \right\}$$

$$-\sum_{x,y}{}' \left\{ |x,y+1\rangle\langle x,y| \otimes \frac{\sigma^z - i\sigma^y}{2} + h.c. \right\}$$

$$-(u-2)\sum_{x,y}{}' |x,y\rangle\langle x,y| \otimes \sigma^z$$



→ Example of Spin-Orbit-Coupling

1.2.3. The Haldane Model

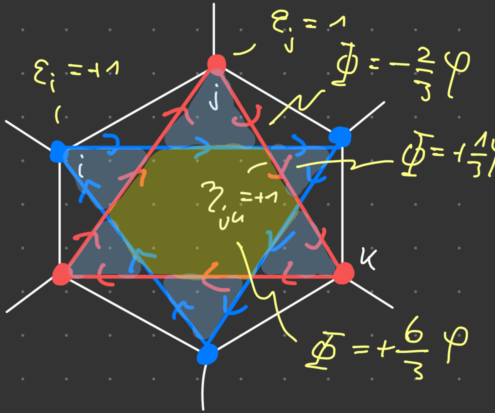
1. a) & Graphene → 2 Dirac cones (gapless)

   b) Staggered chemical potentials^{m} → Gap but not TRS breaking → Trivial

   c) Complex NNN hopping^{t} → Gap with Chern bands !

   d) Keep m and t, map phase diagram in m-t-plane

2. Real space MB Hamiltonian on the honeycomb lattice:

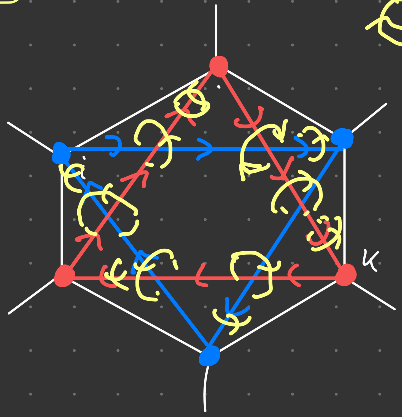


$$\hat{H}_H = \underbrace{\sum_{\underset{\text{nearest neighbours}}{\langle i,j \rangle}} c_i^\dagger c_j}_{\text{Graphene}} + \underbrace{m \sum_i \overset{\text{sublattice dependent sign}}{\varepsilon_i} c_i^\dagger c_i}_{\text{Staggered potential}} + \underbrace{t \sum_{\underset{\text{next-nearest neighbours}}{\langle\langle i,j \rangle\rangle}} e^{i\underset{\text{direction-dependent sign}}{\eta_{ij}} \overset{\text{hopping phase}}{\varphi}} c_i^\dagger c_j}_{\text{Complex NNN hopping}}$$

$$\Phi_{tot} = \frac{6}{3}\varphi + 6 \cdot \frac{1}{3}\varphi - 6 \cdot \frac{2}{3}\varphi$$

$$= 0$$

Note:



$\circlearrowleft = \frac{1}{3} \varphi$

Phases due to

"curled up" magnetic field,

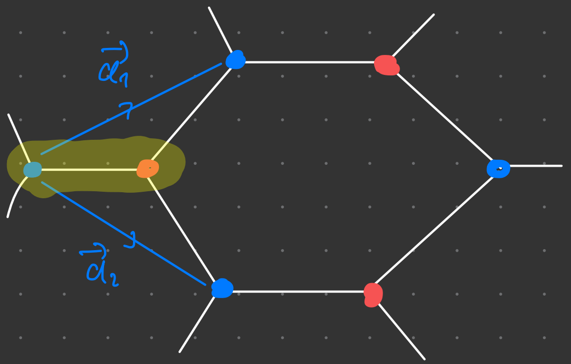
→ no net magnetic field

3. a) Brillouin zone

Honeycomb lattice = Hexagonal lattice + 2-atom basis

→ Brillouin zone → 2 bands

Hexagonal lattice: $\vec{a}_1 = \frac{1}{2}(\sqrt{3},1)^T$, $\vec{a}_2 = \frac{1}{2}(\sqrt{3},-1)^T$

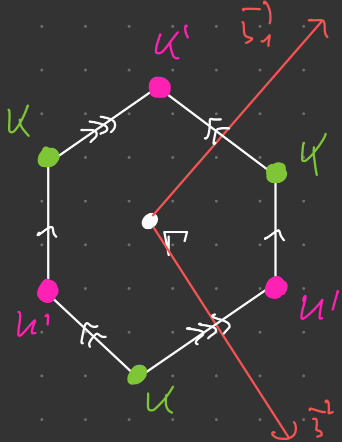


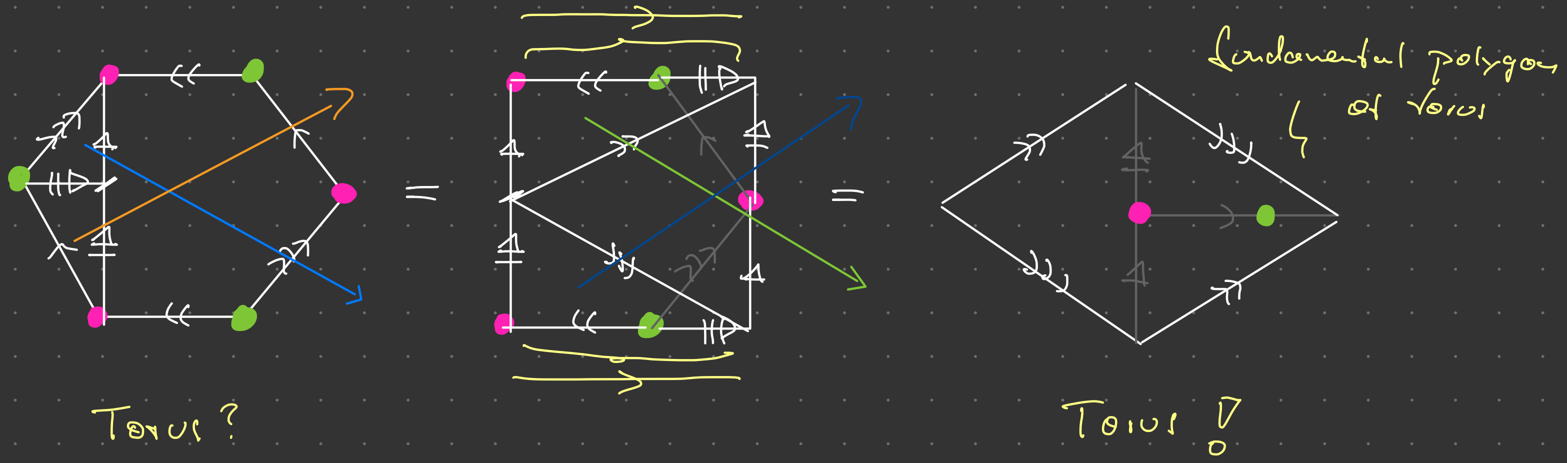
Reciprocal lattice (= Hexagonal lattice):

$$\vec{b}_1 = 2\pi\left(\frac{1}{\sqrt{3}},1\right)^T, \quad \vec{b}_2 = 2\pi\left(\frac{1}{\sqrt{3}},-1\right)^T$$

$$\ulcorner \vec{b} : \vec{b}\cdot\vec{a} \in 2\pi\mathbb{Z}, \quad \vec{a} \in \mathbb{Z}\vec{a}_1 + \mathbb{Z}\vec{a}_2 \lrcorner$$

Brillouin zone = Wigner-Seitz cell of reciprocal lattice





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b) Bloch Hamiltonian: $\mathcal{H}_H(\vec{k}) = \varepsilon(\vec{k})\,\mathbb{1} + \vec{d}(\vec{k})\cdot\vec{\sigma}$ with

$$\boxed{\begin{aligned}
d_x &\overset{\circ}{=} \cos(\vec{k}\cdot\vec{a}_1) + \cos(\vec{k}\vec{a}_2) + 1\\
d_y &\overset{\circ}{=} \sin(\vec{k}\cdot\vec{a}_1) + \sin(\vec{k}\vec{a}_2)\\
d_z &\overset{\circ}{=} m + 2t\sin(\varphi)\left\{\sin(\vec{k}\vec{a}_1) - \sin(\vec{k}\vec{a}_2) - \sin[k(\vec{a}_1-\vec{a}_2)]\right\}
\end{aligned}}$$

→ Gap can only close at the corners of the BZ

$$\vec{K} = \frac{2\pi}{3}(\sqrt{3},1)^T \quad \text{and} \quad \vec{K}' = \frac{2\pi}{3}(\sqrt{3},-1)$$

→ Dirac Hamiltonians: $i,j = 1,2$

$$* \; \mathcal{H}_H(\vec{K}+\vec{k}) \overset{\circ}{=} k_i h_{ij} \sigma^j + \overbrace{[m - 3\sqrt{3}\, t \sin\varphi]}^{h_z} \sigma^z + O(k^2)$$

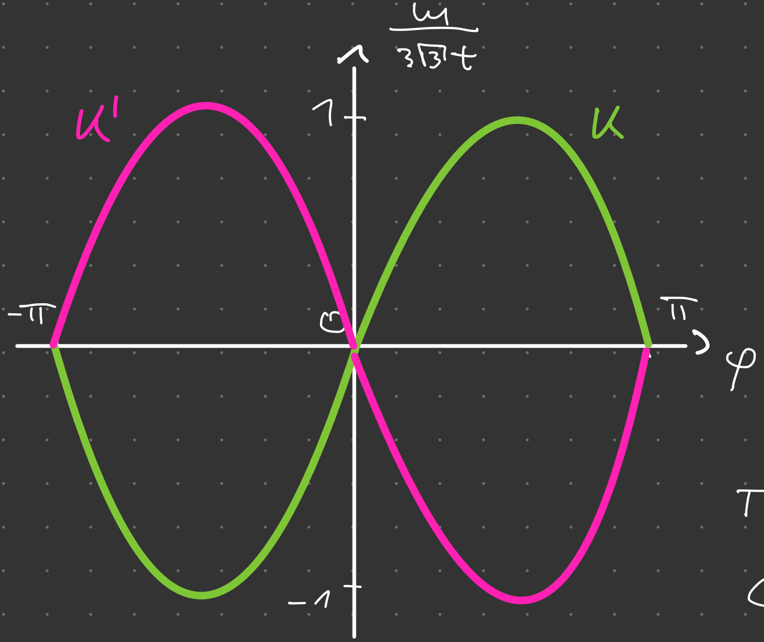
$$\text{with} \quad h = \frac{\sqrt{3}}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$* \; \mathcal{H}_H(\vec{K}'+\vec{k}) \overset{\circ}{=} k_i h'_{ij} \sigma^j + \overbrace{[m + 3\sqrt{3}\, t \sin\varphi]}^{h'_z} \sigma^z + O(k^2)$$

$$\text{with} \quad h' = \frac{\sqrt{3}}{2}\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

4. Gap closings:

$$\begin{array}{lll} @K: & h_z \overset{!}{=} 0 & \iff \\[1em] @K': & h'_z \overset{!}{=} 0 & \iff \end{array} \boxed{\begin{array}{l} \dfrac{m}{3\sqrt{3}\, t} = + \sin(\varphi) \\[1em] \dfrac{m}{3\sqrt{3}\, t} = - \sin(\varphi) \end{array}}$$



5. $$\boxed{\begin{gathered} H(\vec{u}) = \sum_{i,j=1}^{2} u_i h_{ij} \sigma^j + h_z \sigma^z \\ \Rightarrow C = -\frac{\text{sign}(h_z)\,\text{sign}[\det(h)]}{2} \end{gathered}}$$

Proof: P-Set 4

Thus

$$C_K = -\frac{1}{2}\,\text{sign}[m - 3\sqrt{3} + \sin(\varphi)]$$

$$C_{K'} = +\frac{1}{2}\,\text{sign}[m + 3\sqrt{3} + \sin(\varphi)]$$

6. Phase diagram:

a) $m \longrightarrow +\infty$: $\vec{d}(\vec{k}) \approx m\vec{e}_z$ $\longrightarrow$ Trivial phase with $C=0$

b) $m \longrightarrow -\infty$: $\vec{d}(\vec{k}) \approx m\vec{e}_z$ $\longrightarrow$ —"—

c) Let $0<\varphi<\pi$ and (1) $m > 3\sqrt{3}t\sin(\varphi)$
to (2) $m < 3\sqrt{3}t\sin(\varphi)$ $\Bigg\}$ $\rightarrow$ Gap closes at K

$$C = 0 + C_K(2) - C_K(1)$$

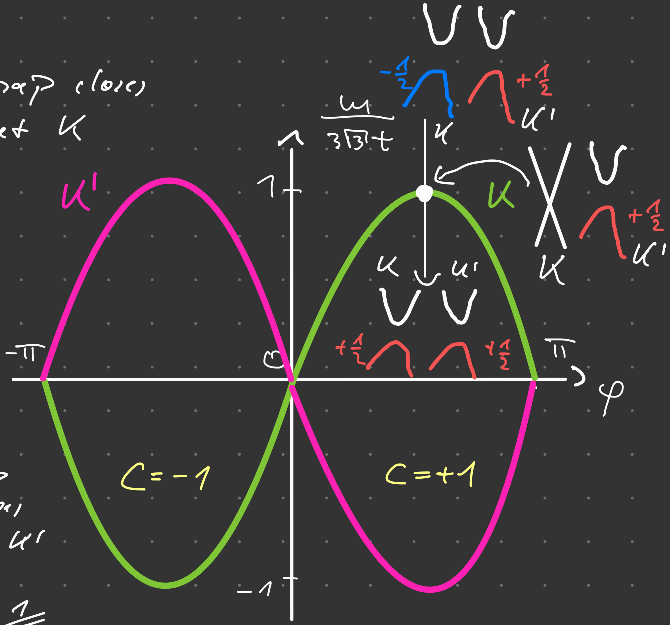
$$= -\frac{1}{2}(-1) - \left[-\frac{1}{2}(+1)\right] = \underline{\underline{+1}}$$

→ Topological phase (I)

d) $-\pi<\varphi<0$ and (1) $m > -3\sqrt{3}t\sin(\varphi)$
(2) $m < -3\sqrt{3}t\sin(\varphi)$ $\Bigg\}$ Gap closes at K'

$$C = 0 + C_{K'}(2) - C_{K'}(1) = \left[+\frac{1}{2}(-1)\right] - \left[+\frac{1}{2}(+1)\right] = \underline{\underline{-1}}$$

→ Topological phase (II)



7. Time-reversal symmetry: $\measuredangle$ $\tilde{T}_0 = K$

$$d_x(k) \overset{?}{=} d_x(-k) \quad ✓$$

$$d_y(k) \overset{?}{=} -d_y(-k) \quad ✓$$

$$d_z(k) \overset{?}{=} d_z(-k) \quad ✓ \text{ for } \varphi = 0, \pi \pmod{2\pi} \quad ✗ \text{ otherwise}$$

$(t \neq 0)$

$\rightarrow$ $C = 0$ for $\varphi = 0, \pi$