Spin-Orbit Coupled Dirac Fermions On Honeycomb Lattice

Basudeb Mondal APS Satellite Meeting International Center for Theoretical Sciences, Bengaluru March 17, 2022

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Symmetry realization in low-energy sector and SOC

 SOC and interactions can give rise to interesting phases of matter.



(Ref : Witczak-Krempa, Chen, Kim, Balents, 2014)

Figure: Schematic phase diagram in presence of $SOC(\lambda)$ and Coulomb interaction(U)

 Symmetries can act non-trivially on the low-energy degrees of freedom.

Outline

- Implementation of symmetries on the low-energy degrees of freedom
- Different phases in presence of interactions.

d^1 Honeycomb Materials





$$H = -\frac{t}{\sqrt{3}} \sum_{\langle \mathbf{rr}' \rangle} \psi^{\dagger}(\mathbf{r}) U_{\mathbf{rr}'} \psi(\mathbf{r}') + \frac{U}{2} \sum_{\mathbf{r}} \psi^{\dagger} \psi(\psi^{\dagger} \psi - 1)$$
(1)

Has emergent global SU(4) symmetry.

Candidate materials are : α -ZrCl₃, α -HfCl₃, $A_2M'O_3$ (A = Na, Li and $M' = Nb, Ta \ etc.$)

Low-energy theory

• Low energy DOF are Dirac fermions.



$$S_0 = \int d^3x \, \bar{\chi} \left[-i \left(\mathbb{I}_4 \otimes \gamma_\mu \right) \partial_\mu \right] \chi \tag{2}$$

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Symmetry transformations
 Effect of interactions

$$H_{\rm int} = \int d^2 \mathbf{x} d^2 \mathbf{x}' \ V_{ijkl}(\mathbf{x} - \mathbf{x}') \chi_i(\mathbf{x})^{\dagger} \chi_j(\mathbf{x}')^{\dagger} \chi_k(\mathbf{x}) \chi_l(\mathbf{x}')$$

Symmetries

Lattice symmetries :

$$S: \chi(\mathbf{x}) \xrightarrow{S} \Omega^f_S \otimes \Omega^c_S \ \chi(S^{-1}\mathbf{x})$$
(3)

$$E.g., \qquad \mathcal{I}: \chi(\mathbf{x}) \xrightarrow{\mathcal{I}} (i\Sigma_{45}) \otimes (i\gamma_0) \ \chi(-\mathbf{x})$$
 (4)

Time reversal :

$$\mathcal{T}: \chi(\mathbf{x}) \xrightarrow{\mathcal{T}} \Omega^f_{\mathcal{T}} \otimes \Omega^c_{\mathcal{T}} K \ \chi(\mathbf{x})$$
(5)

Emergent SU(8) :

$$\chi(\mathbf{x}) \to \exp\left(-i\lambda_a \mathcal{P}_a\right) \chi(\mathbf{x}),$$
 (6)

with

$$\mathcal{P}_{a} = \left\{ \underbrace{\zeta_{i}}_{chiral \ space \ flavor \ space}, \Sigma_{i}\zeta_{j} \right\}$$
(7)

Mean-field phases

The semi-metal phase

$$S_0 = \int d^2 \mathbf{x} d\tau \, \bar{\chi} \left[-i\gamma_\mu \partial_\mu \right] \chi \tag{8}$$

is stable in presence of weak interactions

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(9)

In case of strong interaction, a fermion bilinear

$$\Delta_a = \langle -i\bar{\chi}\mathcal{P}_a\chi\rangle \tag{10}$$

can condense and gap out the fermions.

- There are 64 of such bilinears.
- These have the slowest decaying correlations (Hermele, Senthil, Fisher, 2005)

Mean field phases

- Now, we look at how these bilinears(∆_a) transform under the action of lattice symmetries.
- Space group has 1,2 and 3-dimensional representations

64 bilinears

 $= 2 \cdot A_{1g} \oplus 2 \cdot A_{2g} \oplus 1 \cdot A_{1u} \oplus 1 \cdot A_{2u} \oplus 2 \cdot E_g \oplus 3 \cdot E_u$ $\oplus 4 \cdot T_{1g} \oplus 4 \cdot T_{2g} \oplus 4 \cdot T_{1u} \oplus 4 \cdot T_{2u}$

$$= 2 \cdot A_{1g}^{e} \oplus 2 \cdot A_{2g}^{o} \oplus 1 \cdot A_{1u}^{o} \oplus 1 \cdot A_{2u}^{o}$$

$$\oplus 1 \cdot E_{g}^{e} \oplus 1 \cdot E_{g}^{o} \oplus 2 \cdot E_{u}^{o}$$

$$\oplus 3 \cdot T_{1g}^{e} \oplus 1 \cdot T_{1g}^{o} \oplus 1 \cdot T_{2g}^{e} \oplus 3 \cdot T_{2g}^{o}$$

$$\oplus 2 \cdot T_{1u}^{e} \oplus 2 \cdot T_{1u}^{o} \oplus 2 \cdot T_{2u}^{e} \oplus 2 \cdot T_{2u}^{o}$$
(11)

SU(4) symmetric phases Four SU(4) symmetric masses:

$$4 = 1 \oplus 3 \tag{12}$$

$$\underbrace{-i\bar{\chi}\chi}_{QH}, \underbrace{-i\bar{\chi}\zeta_1\chi, -i\bar{\chi}\zeta_2\chi, -i\bar{\chi}\zeta_3\chi}_{Stripy\ CDW}$$
(13)

► The quantum Hall mass produces a Chern-Simons term :

$$\mathcal{L}_{CS} = \pm i \frac{N_f}{4\pi} \epsilon_{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda, \quad (N_f = 4)$$
(14)

► CDW :



$\mathsf{SU}(2)$ symmetric phases in graphene with electrons are

$$4 = 1 \oplus 1 \oplus 2 \tag{15}$$

► QH

- Staggered charge density wave
- Kekulé

SU(4) breaking phases

Consider the mass

$$-i\bar{\chi}\Sigma_{45}\chi,\tag{16}$$

•
$$\Sigma_{45} \sim (J_x J_y J_z + J_y J_z J_x + J_z J_x J_y) - 15i/8.$$

Does not break break lattice symmetries.

• Breaks
$$SU(4)_F \rightarrow U(1)_{45} \times SO(4).$$

Develops mutual CS terms in the action

$$\mathcal{S}[A_c, A_o] = -i \int d^2 \mathbf{r} d\tau \ \overline{\chi}(\mathbf{r}) \left[\not D - m_0 \Sigma_{45} \right] \chi(\mathbf{r})$$
(17)

$$S_{CS} = i \frac{N_f}{2\pi} \, sgn(m_0) \, \int d^3x \, \epsilon^{\mu\nu\lambda} (A_c)_{\mu} \partial_{\nu} (A_o)_{\lambda} \qquad (18)$$

SU(4) breaking phases

• Density waves :



Stripy density wave in $\boldsymbol{\Sigma}_{12}$



Zig-zag density wave in $\boldsymbol{\Sigma}_{35}$

Here,

$$\Sigma_{12} = \frac{7}{3} \left(S_z - \frac{4}{7} S_z^3 \right)$$

$$\Sigma_{35} = \frac{2}{3\sqrt{3}} \left[\left(S_x^2 S_z + S_x S_z S_x + S_z S_x^2 \right) - \left(S_y^2 S_z + S_y S_z S_y + S_z S_y^2 \right) \right]$$

- \bullet 15 topological phases corresponding to different ways of breaking flavor space symmetry SU(4).
- Partially gapless phases.

Partially Gapless Phases

Some masses have partially gapless spectrum.



- ► These are density waves with semi-metal character.
- Need to understand the gaplessness, symmetry protection and phase transitions between gapless phases.

Summary

- Due to SOC, lattice symmetries act non-trivially on flavor space.
- Emergent SU(8) symmetry in low-energy theory.
- Because of large symmetry, we have different density waves and different QH phases.
- Because of non-trivial symmetry implementation, there are masses with partially gapless spectrum.

Future Directions

- Study the phase transitions.
- Study the superconducting instabilities.

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Thank You

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