Flavor Magnetism and Superconductivity.

Theory of entwined orders in Magic Angle Graphene (s)

Ashvin Vishwanath

Lecture Notes for More Technical Details:
https://scholar.harvard.edu/avishwanath/teaching
Quantum Phases of Matter

• Landau Orders

  - Ferromagnet
  - Superfluid
  - Solid

In many cases the distinguishing feature: *Spontaneous Symmetry Breaking* => Landau order parameter.

• topological Phases

  - Integer Quantum Hall States
    - Different Integers `n' - different phases but same symmetry - topological distinction.

  ![Graph showing Integer Quantum Hall States](image)

Spontaneous symmetry breaking & topology

=> Entwined Landau orders
MAGIC ANGLE ~1.1°: Tunneling time = Lattice Moire time

\[ \theta \sim \frac{1}{60} \text{ radians} \quad L \sim \frac{a}{\theta} \]

From Quantum Magazine

Real Space
Experiments

Pablo Jarillo-Herrero’s group (MIT)

Valley K

$\theta = 1.05^\circ$

$\xi_0, t = \xi_0$

Valley K’

B

Resistance ($\Omega$)

$R_{\mu\nu} - \frac{1}{2}$

\[ R_{\mu\nu} = \frac{1}{2} - \frac{n(\omega)}{S - p_d\omega} \]

D

Displacement field ($\text{V/m}$)

$T = 10 \text{ mK}$

Yankowitz et al. Science
Correlation Effects in Twisted Bilayer Graphene

Gap ~ 30 meV

Energy (meV)

\[ W_{\text{bare}} \sim 8 \text{ meV} \]

Koshino et al

Gap ~ 30 meV

Electron Count

\[ \nu = +4 \]

\[ \nu = -4 \]

\[ \theta \sim 1/60 \text{ radians} \]

\[ V \sim 30 \text{ meV} \]

\[ \nu \sim 8 \text{ meV} \]

Balents et al

Superconductivity

1.06°
1.16°
1.14°
1.10°
1.27° (1.33 GPa)
1. Flat Bands
Graphene band structure

- Time reversal $\mathcal{T}$ and two-fold rotation $C_2$ exchanges $\kappa$ and $K^8$
- $C_2\mathcal{T}$ leaves momentum invariant → no gap at the Dirac points.
Monolayer

Bi-layer

Twisted Bi-layer
Continuum model

- Larger unit cell $\rightarrow$ smaller BZone
- Bistrizer-Macdonald (BM) model (2011)
  \[ \mathcal{H}_K = \begin{pmatrix} -i v_F \sigma_{\theta/2} \cdot \nabla & T(r) \\ T^\dagger(r) & -i v_F \sigma_{-\theta/2} \cdot \nabla \end{pmatrix}_{12}, \]
- Moire “potential”
  \[ T(r) = \begin{pmatrix} w_0 U_0(r) & w_1 U(r) \\ w_1 U^*(-r) & w_0 U_0(r) \end{pmatrix}_{AB} \]
- Lattice relaxation: AB stacking favored to AA stacking (Carr et al. 2019, Nam, Koshino 2017)
  \[ \implies \frac{w_0}{w_1} \approx 0.7 \]
Chiral Model

Tarnopolski, Kruchkov, AV
PRL 2019

Switch off AA coupling. Only AB coupling

\[ T(\mathbf{r}) = \begin{pmatrix} w_{0}(\mathbf{r}) & w_{1}U(\mathbf{r}) \\ w_{1}U^{*}(-\mathbf{r}) & w_{0}(\mathbf{r}) \end{pmatrix} \]

\[ w_{0} = w_{1} \quad \text{and} \quad w_{0} = 0.75w_{1} \]

Chiral Symmetry
\[ \{\sigma_{z} \otimes 1, \mathcal{H}\} = 0 \]
Perfectly Flat Bands in the Chiral Model

\[ \alpha = \frac{w_1}{2v_0 k_D \sin(\theta/2)} \]
Chiral Model

\[
\mathcal{H} = \begin{pmatrix}
0 & \mathcal{D}^*(-r) \\
\mathcal{D}(r) & 0
\end{pmatrix}, \quad \mathcal{D}(r) = \begin{pmatrix}
-2i\bar{\partial} & \alpha U(r) \\
\alpha U(-r) & -2i\bar{\partial}
\end{pmatrix}
\]

\[\bar{\partial} = \frac{1}{2}(\partial_x + i\partial_y)\]

\[
\begin{pmatrix}
0 & \mathcal{D}^*(-r) \\
\mathcal{D}(r) & 0
\end{pmatrix}
\begin{pmatrix}
0 \\
\psi_B(r)
\end{pmatrix} = 0
\]

Perturbation Theory:

\[
\psi_K(r) = \begin{pmatrix}
\psi_{K,1} \\
\psi_{K,2}
\end{pmatrix} = \begin{pmatrix}
1 + \alpha^2 u_2 + \alpha^4 u_4 + \ldots \\
\alpha u_1 + \alpha^3 u_3 + \ldots
\end{pmatrix}
\]

\[
v_F(\alpha) = \frac{1 - 3\alpha^2 + \alpha^4 - \frac{111\alpha^6}{49} + \frac{143\alpha^8}{294} + \ldots}{1 + 3\alpha^2 + 2\alpha^4 + \frac{6\alpha^6}{7} + \frac{107\alpha^8}{98} + \ldots}
\]

Gives: perfectly flat bands at a series of magic angles.
Chiral Limit Wavefunctions

Many special properties:

(i) Chern number + sublattice polarized

(ii) nearly uniform Berry curvature

(iii) Ideal droplet condition - quantum metric is

\[ \psi_A(x, y) = \left( \frac{\psi_K(x, y)}{\theta_1(\frac{z - z_0}{a_1})} \right) f(x + iy) \]

\[ \eta(k) = \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} \Omega(k) \]

Linear combination of bands

Valley K

\[ |A\rangle + |B\rangle \]

\[ |A\rangle - |B\rangle \]

Chern = ±1;
Sublattice polarized

Ledwith, Tarnopolsky, Khalaf, AV `20
Wang, Zheng, Millis, Cano `20
Becker, Embree, Wittsten, Zworski `20
Interactions

\[ \rho(q) = \sum_{k \in BZ} c_k^\dagger \Lambda q(k) c_{k+q} \]

Form factor - wave functions of flat bands - plays a key role

\[ \mathcal{H} = \sum_k c_k^\dagger h_k c_k + \frac{1}{2A} \sum_q V_q \delta \rho_q \delta \rho_{-q}, \quad \delta \rho_q = \rho_q - \bar{\rho}_q, \]

\[ \rho = \sum_k \Lambda q(k) c_{k+q} \]

Screened Coulomb

Kang, Vafek PRL 2019: SU(4)
Bultnick, Khalaf et al. arXiv:1911.02045
2. Flavor Ordered Insulator

[Image: Ground State and Hidden Symmetry of Magic Angle Graphene at Even Integer Filling]

arXiv:1911.02045 (PRX 2020)
Correlated Insulators - Ideal Limit

\[ \rho \approx \rho_{C=+1} + \rho_{C=-1} \]
Generalized Flavor Ferromagnets

\[ Q_+ = 4 - \sum |z_{\text{filled}}^+ \rangle \langle z_{\text{filled}}^+ | \]
\[ Q_- = 4 - \sum |z_{\text{filled}}^- \rangle \langle z_{\text{filled}}^- | \]

Kumar, Xie, MacDonald arXiv:2010.05946
Bernevig, Lian, Cowsik; Xie, Regnault, Song
Simplified Model - Spinless TBG

\[ \mathcal{H}_{\text{int}} = \frac{1}{2A} \sum_q V_q \delta \rho_q \delta \rho_{-q}. \]

Density: \( \rho \approx \rho_{C=+1} + \rho_{C=-1} \)

No Dispersion & Chiral limit:

- Family of exact ground states - generalized ferromagnets. Fill Chern Bands.

Argument:

- \( V_q \geq 0 \) and \( \delta \rho_q \left| \Psi \right\rangle = 0 \)

(Spinless Model) Or \( \nu = \pm 2 \)
Ground States of Ideal Model

\[ Q_+ = 1 - |z_+\rangle\langle z_+| = \sigma \cdot \hat{n}_+ \]
\[ Q_- = 1 - |z_-\rangle\langle z_-| = \sigma \cdot \hat{n}_- \]

Psuedo-Spin

Valley polarized

\[ K, A \]
\[ C = +1 \]
\[ \sigma_z \tau_z = +1 \]
\[ \hat{n}_+ = \hat{n}_- = -\hat{\tau}_z \]

Psuedo-Spin

Valley Hall

\[ K, A \]
\[ C = +1 \]
\[ \sigma_z \tau_z = +1 \]
\[ \hat{n}_+ = -\hat{n}_- = -\hat{\tau}_z \]
Ground States of Ideal Model

- Intervalley coherent (IVC) states break valley U(1): translation symmetry at graphene scale.

\[
\hat{n}_+ = \hat{n}_- = -\hat{x}
\]
Effect of Dispersion & $W_0$

$J_n + \cdots n - \frac{J^2}{U} \approx 1 \text{ meV}$

Antiferro-pseudospin coupling

$\lambda (n_+ \cdot n_- - 2n_z n_z)$

anisotropy - moving from chiral limit

$K$, $A$

$K'$, $B$

$C = +1$

$C = -1$

$K$, $B$

$K'$, $A$

Band Dispersion

Ideal

$U(4) \times U(4)$

Realistic

$\frac{w_0}{w_1}$

$K\text{-IVC}$

Bultnick et al. arXiv:1911.02045
Kang and Vafek `19

$J \sim 4t^2/U$

Superexchange
Hartree Fock & DMRG Numerics
-Confirms This Picture

\[ \theta = 1.05^\circ \ w_0 = 80\text{meV}; \ w_1 = 110\text{meV}; \ e = 7 \]

\[ Q = \sigma_y \left( \Delta_R \tau_x + \Delta_I \tau_y \right) \]

Bultnick et al. arXiv:1911.02045
Kang and Vafek `19

Competing state - *nematic* semimetal.

Shang Liu et al. arXiv:1905.07409
Kang & Vafek `19
Kramers IVC - Properties

\( \text{U}(1)_{\text{valley}} \) spontaneously broken -
Goldstone modes (lattice translation)

- Spontaneously breaks \( \mathcal{T} \), but
  preserves a combination of \( \mathcal{T} \) and \( \pi \)
  valley rotation \( \mathcal{T}' = \tau_z \mathcal{T} = \tau_y \mathcal{K} \).

\[ \mathcal{T}'^2 = -1 \]

Same symmetries as topological insulator
Involves opposite Chern number band
**Nontrivial \( \mathbb{Z}_2 \) topology!**

"Spontaneous" topological insulator
(Topological "Mott" Insulator - Raghu, Qi, Honerkamp, Zhang)

Edge states? Requires `smooth' edge

\[ Q = \sigma_y \left( \Delta_R \tau_x + \Delta_I \tau_y \right) \]

\( \text{Current pattern}^* \)

\( \nu \sim 10^4 \text{m/sec} \)

Acknowledgements

• Flat Band Topology and Geometry
  • Hoi Chun (Adrian) Po, Liujun Zou, T. Senthil,
  • Grisha Tarnopolski, Alex Kruchkov, Patrick Ledwith

• Correlated Insulators and Nematic Semimetal
  • (Harvard) Eslam Khalaf, Shang Liu, Jong Yeon Lee
  • (Berkeley) Nick Bultnick, Shubhayu Chatterjee, Mike Zaletel

Lecture Notes for More Technical Details:
https://scholar.harvard.edu/avishwanath/teaching