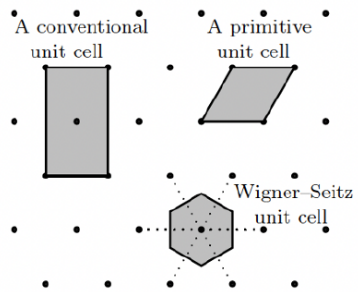
Twisted Bilayer Graphene

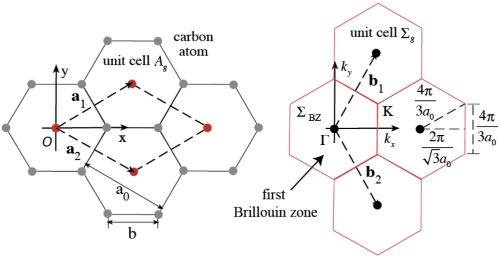
Amir Shapour Mohammadi

Fall 2022 Junior Paper
Advisor: Duncan Haldane, Second Reader: Shinsei Ryu
Princeton University

March 2023

Lattices





(a) Bravais lattice (b) Reciprocal lattice

Electrons in a lattice

Bloch theorem (eigenstates of periodic potential)

$$H(\mathbf{r}) = \frac{-\hbar^2\nabla^2}{2m} + U_{ion}(\mathbf{r}) \implies f_{n,\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} e^{i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r}) \tag{1}$$

Tight-binding model (electrons hopping around lattice)

$$H = \sum_{n,n'} \sum_{\langle \mathbf{R},\mathbf{R}' \rangle} t_{nn';\mathbf{R}-\mathbf{R}'} c^\dagger_{n,\mathbf{R}} c_{n',\mathbf{R}'}, \tag{2}$$

simplified model of electron dynamics.

Graphene

Low-energy expansion about corners (Dirac points)

$$h(\mathbf{k}) = \hbar v_F(\tau_z \sigma_x k_x + \sigma_y k_y) + m\sigma_z, \qquad E = \pm v_F \sqrt{|\hbar \mathbf{k}|^2 + (m/v_F)^2} \quad (3)$$

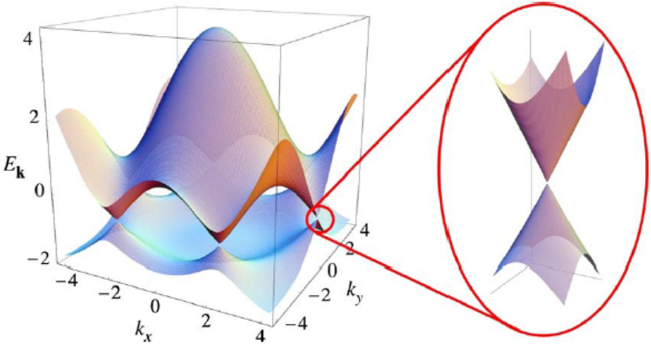
Dirac equation (relativistic Schrodinger equation)

$$(i\hbar\gamma^\mu \partial_\mu - Mc)\psi(\mathbf{r}) = 0, \qquad \{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu} \quad (4)$$

$$H = \pm c\boldsymbol{\sigma} \cdot \mathbf{p}, \qquad E = \pm c\sqrt{|\mathbf{p}|^2 + M^2 c^2} \quad (5)$$

Electrons in graphene are ultra-relativistic! The $\pm$ energy solutions of the Dirac equation correspond to valence, conduction bands in graphene.

Graphene Band Structure



Twisted Bilayer Graphene

Periodic structure with much larger characteristic length (more atoms per unit cell) $\implies$ tight-binding model computationally intensive

$$\mathcal{H}^{\alpha\beta}_{\mathbf{kp}'} = \sum_{\mathbf{G}_1,\mathbf{G}_2'} \frac{t^{\alpha\beta}_{\mathbf{k}+\mathbf{G}_1}}{\mathcal{B}} e^{i(\mathbf{G}_1\cdot\boldsymbol{\tau}_\alpha - \mathbf{G}_2'\cdot(\boldsymbol{\tau}'_\beta - \boldsymbol{\tau}))} \delta_{\mathbf{k}+\mathbf{G}_1,\mathbf{p}'+\mathbf{G}_2'} \tag{6}$$

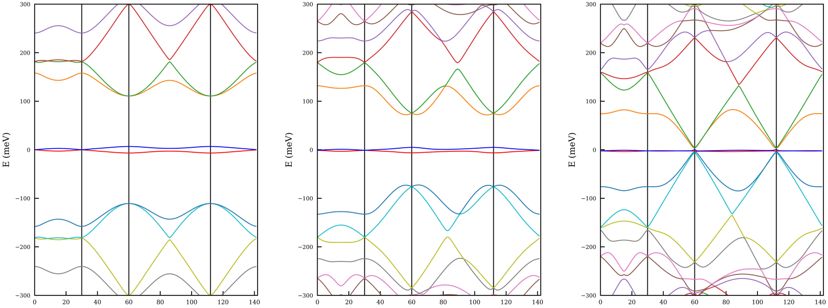
Game-changing BM continuum model

$$\mathcal{H}_{BM}(\mathbf{k}) = \begin{pmatrix} h_{\theta/2}(\mathbf{k}) & T_1 & T_2 & T_3 \\ T_1^\dagger & h_{-\theta/2}(\mathbf{k}+\mathbf{q_1}) & 0 & 0 \\ T_2^\dagger & 0 & h_{-\theta/2}(\mathbf{k}+\mathbf{q_2}) & 0 \\ T_3^\dagger & 0 & 0 & h_{-\theta/2}(\mathbf{k}+\mathbf{q_3}) \end{pmatrix} \tag{7}$$

Low-energy expansion about Dirac points

$$\mathcal{H}^L_{BM}(\mathbf{k}) = \tilde{v}_F \boldsymbol{\sigma}\cdot\mathbf{k}, \qquad \theta = 1.05^\circ \implies \tilde{v_F} = 0 \tag{8}$$

Kinetic energy is quenched at magic angles!



Large band gap is incredibly important for wavefunction manipulations (vis-a-vis Adiabatic theorem).

Berry Phase

Adiabatic theorem (start in eigenstate then vary parameter over time)

$$|\psi_n(t)\rangle = e^{i\Phi_n(t)} |\psi_n(\boldsymbol{\lambda})\rangle , \qquad \Phi_n(t) = -\frac{1}{\hbar}\int_0^t dt' E_n(\boldsymbol{\lambda}(t')) + \Phi_B^n \tag{9}$$

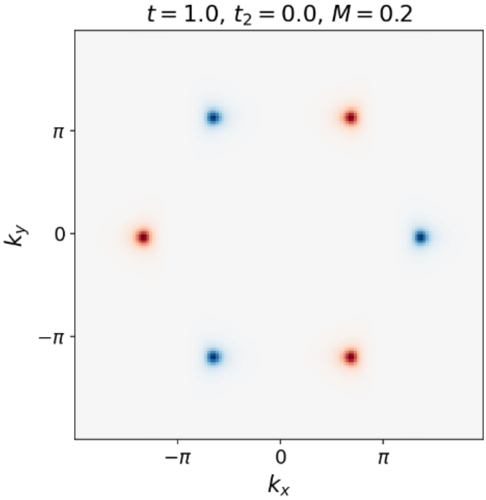
Berry (geometric) phase

$$\Phi_B^n = \int_C d\lambda^\mu \mathcal{A}_\mu^n = \int_S d\lambda^\mu d\lambda^\nu \mathcal{B}_{\mu\nu}^n \tag{10}$$

$$\mathcal{B}_{\mu\nu}^n = \partial_\mu \mathcal{A}_\nu^n - \partial_\nu \mathcal{A}_\mu^n = -2\mathrm{Im}\,\langle \partial_\mu \psi_n(\boldsymbol{\lambda}) | \partial_\nu \psi_n(\boldsymbol{\lambda})\rangle \tag{11}$$

Time-independent! Depends only on the path you take in parameter space. Take $\boldsymbol{\lambda} = \mathbf{k}$ and apply to Bloch states.

Graphene Berry Curvature



Quantum Anamolous Hall Effect

Electron equation of motion

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \frac{1}{\hbar}\nabla_{\mathbf{k}} E_{\mathbf{k}} - \frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t} \times \mathcal{B}(\mathbf{k}), \qquad \frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t} = -\frac{e}{\hbar}\mathbf{E} \tag{12}$$

Current density

$$\mathbf{j} = \sigma \mathbf{E} + \sigma_{AH} \hat{\mathbf{n}} \times \mathbf{E} \tag{13}$$

Quantized anomalous Hall current (for band insulator)

$$\sigma_{AH}^{n} \hat{\mathbf{n}} = \frac{\sigma_0}{2\pi} \int_{BZ} d^2\mathbf{k}\ \mathcal{B}_n(\mathbf{k}) := \sigma_0 C_n \hat{\mathbf{n}}. \tag{14}$$

Remarkably, $C_n \in \mathbb{Z}$!

Symmetries of Chern Number

Time-reversal ($\mathbf{k} \mapsto -\mathbf{k}$) symmetry $\implies$

$$\mathcal{B}(\mathbf{k}) = \Theta^{\dagger}\mathcal{B}(\mathbf{k})\Theta = -\mathcal{B}(-\mathbf{k}) \text{ (odd)} \implies C = 0. \tag{15}$$

Inversion ($\mathbf{r} \mapsto -\mathbf{r}, \mathbf{k} \mapsto -\mathbf{k}$) symmetry $\implies$

$$\mathcal{B}(\mathbf{k}) = \mathcal{I}^{\dagger}\mathcal{B}(\mathbf{k})\mathcal{I} = \mathcal{B}(-\mathbf{k}) \text{ (even)}. \tag{16}$$

Both symmetries $\implies$ $\mathcal{B}$ vanishes identically.
Graphene Dirac cones ($\mathbf{m} = \mathbf{0}$) are topologically protected!

Graphene as Chern insulator?

Continuum model for graphene

$$H = \hbar v_F(\tau_z\sigma_x k_x + \sigma_y k_y) \tag{17}$$

We must break Θ and/or sublattice $\mathcal{C}$ symmetry to open a band gap.

$$m_R\sigma_z \qquad (\mathcal{C}\text{ broken, }\Theta\text{ obeyed}) \tag{18}$$

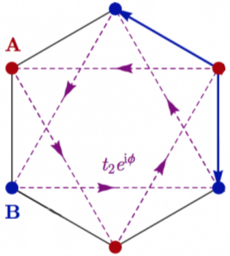
To obtain $C \neq 0$, we must break Θ symmetry (i.e. make the Berry curvature have the same sign at both Dirac points)

$$\boxed{m_H\tau_z\sigma_z \qquad (\mathcal{C},\Theta\text{ broken})} \tag{19}$$

Haldane Model (1988)

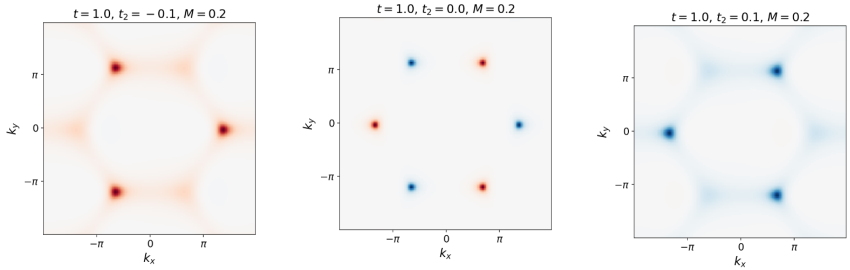
Haldane did this by adding an imaginary next-to-nearest neighbor hopping induced by a magnetic field (Aharanov-Bohm phase)

$$H_{NNN} = -t_2 \sum_{NNN} (e^{i\phi} c_i^\dagger c_j + h.c.), \qquad 3\phi = \frac{e}{\hbar} \int_S d\mathbf{S} \cdot \mathbf{B} \tag{20}$$



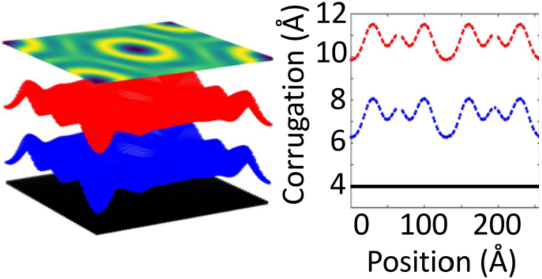
We have a Chern insulator by modifying the graphene model!

Haldane Model Berry Curvature



So graphene is once again pretty cool, but what about TBG?

Chiral MATBG



Chiral limit is extreme corrugation. Real space low-energy Hamiltonian

$$H = \begin{pmatrix} 0 & D^*(-\mathbf{r}) \\ D(\mathbf{r}) & 0 \end{pmatrix}, \qquad D(\mathbf{r}) = \begin{pmatrix} -2i\bar{\partial} & \alpha U(\mathbf{r}) \\ \alpha U(-\mathbf{r}) & -2i\bar{\partial} \end{pmatrix} \tag{21}$$

Antiholomorphic operator $\implies$ **holomorphic wavefunction**.

Electron in Magnetic Field: Landau Levels

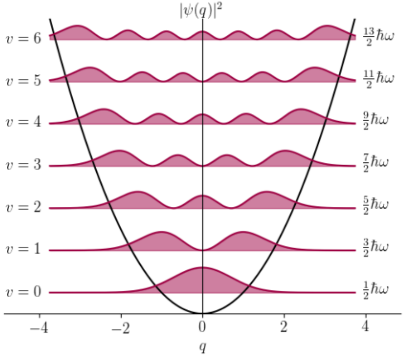
Harmonic-oscillator-like Hamiltonian

$$H = \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 = \hbar\omega_B \left(a^\dagger a + \frac{1}{2} \right) \tag{22}$$

$$a\,|0, m\rangle = 0, \qquad a = -\sqrt{2}i \left(l_B \overline{\partial} + \frac{z}{4l_B} \right), \qquad [a, a^\dagger] = 1 \tag{23}$$

Antiholomorphic operator $\implies$ **LLL has holomorphic wavefunction**.
Lots of interesting physics including IQHE, FQHE, Wigner crystals intuitively because kinectic energy is quenched and interactions play a more central role (for the latter two).

Landau Level Energy Levels



Comparison of Geometries

Quantum geometric tensor captures entire geometry of energy bands

$$\eta_{\mu\nu} = \langle \partial_\mu \psi | (\mathbf{1} - |\psi\rangle \langle \psi|) |\partial_\nu \psi\rangle \tag{24}$$

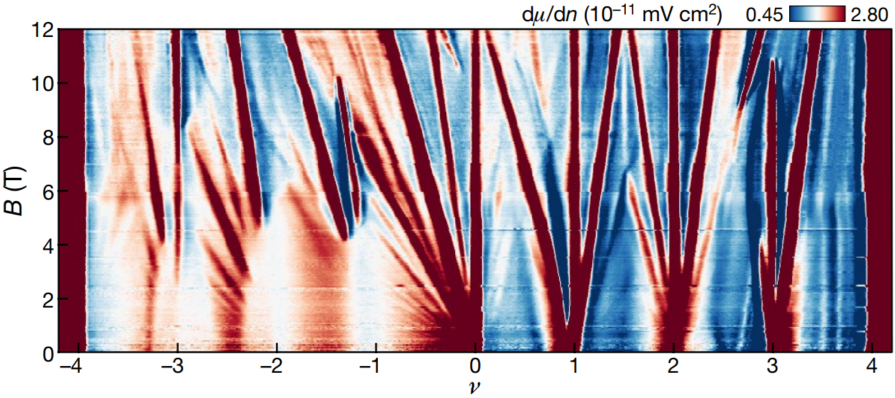
$$g_{\mu\nu} = \mathrm{Re}\eta_{\mu\nu}, \qquad \mathcal{B}_{\mu\nu} = -2\mathrm{Im}\eta_{\mu\nu} \tag{25}$$

Holomorphicity immensely simplifies the geometry of the Hilbert space

$$\text{Holomorphic} \implies \eta(\mathbf{k}) \propto \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} \tag{26}$$

Luckily both Chiral MATBG and LLL wavefunctions are holomorphic. It turns out Chiral MATBG is equivalent to Dirac particle in generalized LL (inhomogenous field). Their bands have very similar geometries; perhaps they share interesting physics.

Experimental Evidence for Fractional Chern Insulator in MATBG



Works Cited

S. M. Girvin and K. Yang, Modern Condensed Matter Physics (Cambridge University press, 2019).

R. Bistritzer and A. H. MacDonald, Moire bands in twisted double-layer graphene, Proceedings of the National Academy of Sciences 108, 12233–12237 (2011).

K. Sun, Topological insulators, University of Michigan (2013).

P. J. Ledwith, G. Tarnopolsky, E. Khalaf, and A. Vishwanath, Fractional Chern insulator states in twisted bilayer graphene: An analytical approach, Physical Review Research 2 (2020).

Code/JP: `https://github.com/amirsm02/mohammadi_haldane_JPI`