Insulating phases in twisted bilayer graphene

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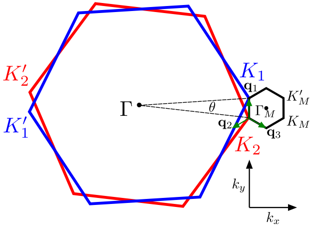
Quantum Fluids of Light and Matter
July 2022

BM in real space

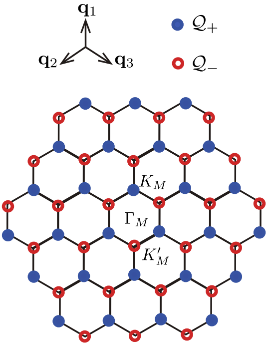
$$H = \begin{pmatrix} iv_F\left(\partial\cdot\sigma + \frac{\theta}{2}\partial\wedge\sigma\right) & T(\mathbf{r}) \\ T^\dagger(\mathbf{r}) & iv_F\left(\partial\cdot\sigma - \frac{\theta}{2}\partial\wedge\sigma\right) \end{pmatrix}$$



$$T(\mathbf{r}) = \sum_{j=1}^{3} T_j e^{i\mathbf{q}_j\cdot\mathbf{r}}$$

$$T_j = w_0\sigma_0 + w_1\left[\sigma_x\cos\left(\frac{2\pi(j-1)}{3}\right) + \sigma_y\sin\left(\frac{2\pi(j-1)}{3}\right)\right]$$

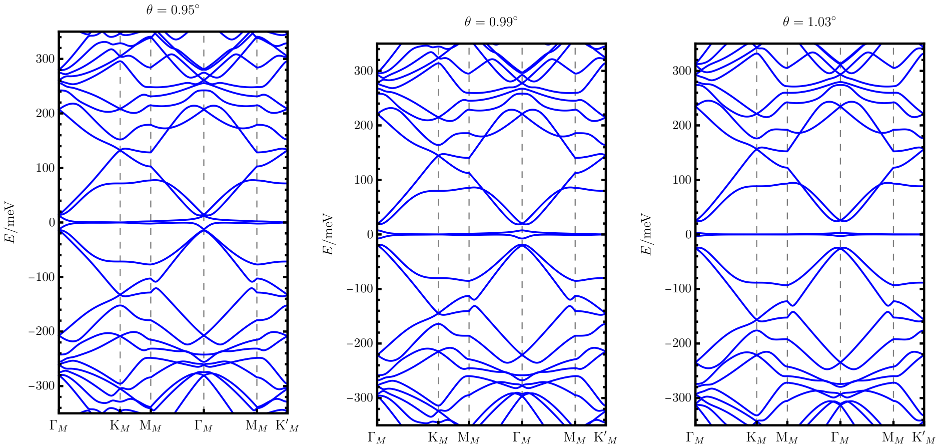
BM in momentum space



$$\hat{H}_0 = \sum_{\mathbf{k}\in \mathrm{MBZ}} \sum_{\eta\alpha\beta s} \sum_{\mathbf{Q}\mathbf{Q}'\in\mathcal{Q}_\pm} \left[h_{\mathbf{Q},\mathbf{Q}'}(\mathbf{k})\right]_{\alpha\beta} c^\dagger_{\mathbf{k},\mathbf{Q},\alpha} c_{\mathbf{k},\mathbf{Q}',\beta}$$

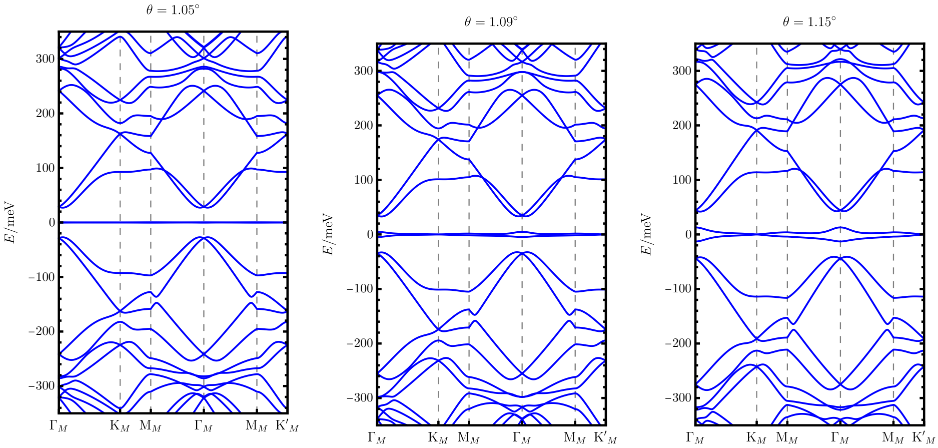
$$h_{\mathbf{Q},\mathbf{Q}'}(\mathbf{k}) = v_F(\mathbf{k}-\mathbf{Q})\cdot\sigma\delta_{\mathbf{Q},\mathbf{Q}'} - \lambda v_F \frac{\theta}{2}\xi_Q \delta_{\mathbf{Q},\mathbf{Q}'}(\mathbf{k}-Q)\wedge\sigma + \sum_{j=1}^{3} T_j \delta_{\mathbf{Q},\mathbf{Q}'\pm\mathbf{q}_j}$$

TBG band structure: effect of θ



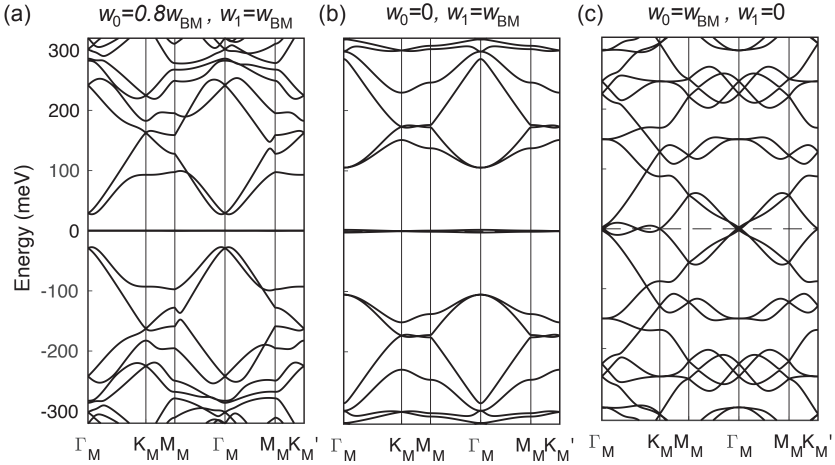
$w_{\mathrm{BM}} = 110\mathrm{meV}, w_0/w_1 = 0.8$

TBG band structure: effect of θ

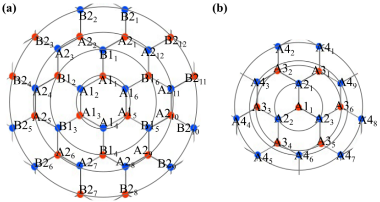


$$w_{\mathrm{BM}} = 110\mathrm{meV}, w_0/w_1 = 0.8$$

TBG band structure: effect of w_0, w_1



$w_{\mathrm{BM}} = 110\mathrm{meV}, \theta = 1.05^\circ$



Hexagon Model
Centered at Γ_M

Triangular Model
Centered at K_M

3- TBG: Symmetry

As usual, the first thing we should do once you have a new model is to find its symmetries and check its topological features if any (especially for a non-interacting system where topological characterization is a well-known territory)

Crystalline symmetries of graphene.

* C_{3z} → rotation along z by $\frac{2\pi}{3}$ (maps $A \to A$, $B \to B$)
* C_{2z} → rotation along z by π, it maps A to B and B to A, and K to K' in momentum space.

C_{2z} is no more a symmetry if you consider a single Dirac cone.

T time reversal symmetry: same story maps $k \to -k$ and thus swap the two valleys.

Symmetries of TBG

* C_{3z} is also a symmetry (representation $e^{\frac{2\pi i}{3}\sigma_z}$)

* C_{2z} and T cannot be considered as symmetries separately
But the combination $C_{2z}T$ leaves the BM model invariant.
Note that for the BM model, we assumed spinless fermions.
Thus even if T is antiunitary, we have $T^2 = 1$.
(as opposed to $T^2 = -1$ for spinful fermions)
With a proper gauge choice, the representation of $C_{2z}T$
can be written as $\sigma_x K$ where K is the complex conjugation.

* TBG has an additional symmetry: C_{2x}
it flips both the sublattices and layers.

$$C_{2x} = \sigma_x \tau_x .$$

But more "emergent" symmetries can be defined.

* conduct "particle-hole" transformation $P = i\tau_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

$$H(r) = i v_F \left(\tau_0 \vec{\partial}\cdot\vec{\sigma} + \frac{\theta}{2} \tau_z \vec{\partial} \wedge \vec{\sigma} \right) + \begin{pmatrix} 0 & T(r) \\ T^+(r) & 0 \end{pmatrix}$$

$$P H(\vec{r}) P^+ = i v_F \left(\tau_0 \underbrace{\vec{\partial}\cdot\vec{\sigma}}_{-\partial_{-\vec{r}}\cdot\vec{\sigma}} - \frac{\theta}{2} \tau_z \vec{\partial} \wedge \vec{\sigma} \right) - \begin{pmatrix} 0 & T^+(r) \\ T(r) & 0 \end{pmatrix}$$

$$= - H(-\vec{r}) + i v_F \theta \tau_z \vec{\partial} \wedge \vec{\sigma} \qquad \text{here } T^+(r) = T(-r))$$

If we neglect the term $\theta \tau_z \vec{\partial} \wedge \vec{\sigma}$ (we will discuss later this approximation), then we get.

$$P H(r) P^+ = - H(-r)$$

As such, P is an emergent symmetry of the model

Note that $P^2 = -1$

We can define $\mathcal{P} = P C_{2z} T$

This $\mathcal{P}$ is local in real space, anti-unitary and satisfies $\mathcal{P}^2 = -1$ (hint: sounds awfully close to time reversal symmetry for a spinful model).

* Chiral symmetry $C = \sigma_z$

Look back at $H(r)$. If $w_0 = 0$, the hamiltonian only contains σ_x and σ_y and thus anti-commutes with C

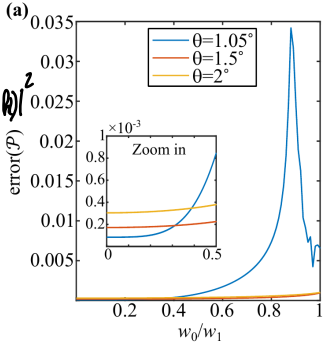
more generally: $C H(r) C^\dagger = -H(r) + 2 w_0 \tau_z \sigma_0 \sum_{j=1}^{3} e^{-i \vec{q}_j \vec{r}}$

$w_0 = 0$ is called the (first) chiral limit

Emergent symmetries

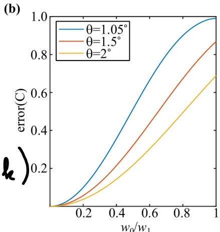
$$\text{error}(\mathcal{P}) = 1 - \frac{1}{\Omega_{mBZ}} \int dk \, |\langle u_1(k)|\mathcal{P}|u_{-1}(-k)\rangle|^2$$

index for the lower (-1) and upper band (+1)



$$\text{error}(C) = 1 - \frac{1}{\Omega_{mBZ}} \int dk \, |\langle u_1(k)|C|u_{-1}(k)\rangle|^2$$

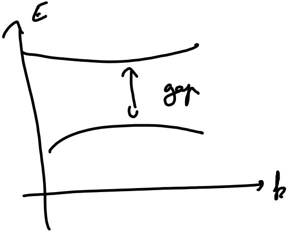
(both symmetries anticommute and thus relate E to $-E$ but $\mathcal{P}$ changes k to $-k$)



4- TBG: Topology

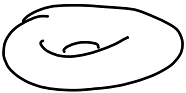
A Short introduction to Chern Insulators and topology.

What is a Chern insulator?



1. it is an insulator.

2. $\vec{k}$

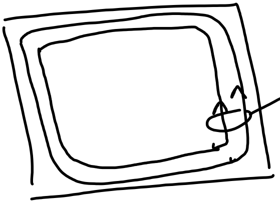


BZ

$|\psi(k)\rangle$

Bloch sphere.

Chern number: How many times you cover the Bloch sphere by spanning the BZ.

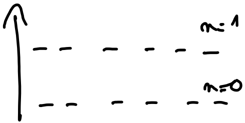


Chern number C

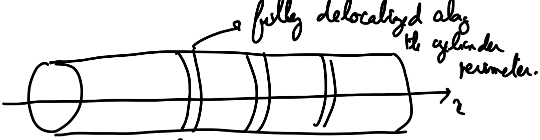
C chiral edge states.

robust edge mode due to the impossibility of backscattering.

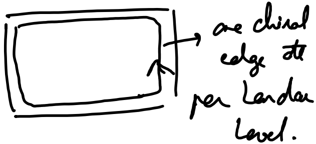
<u>example</u>: Landau levels (requires an external magnetic field)



Landau levels, perfectly flat band, Chern number $C=1$ per band.



on a cylinder

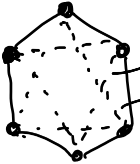


<u>quantization of the Hall conductance</u>

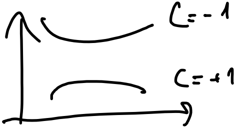
$C \neq 0 \Rightarrow$ obstruction to have (exponentially) localized Wannier orbitals (, i.e. no lattice realization of a single band
$\rightarrow$ no Hubbard model and no atomic limit)

A lattice realization? (Haldane 88) but two bands

graphene + NNN



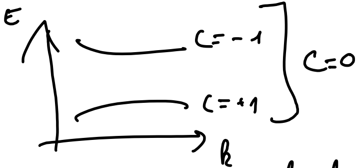
gap at the Dirac points



overall, the time reversal symmetry is not broken $\Rightarrow$ total Chern number is 0, But $C = \pm 1$ per band.

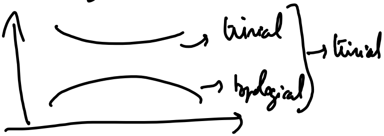
(graphene would like so much to be a topological phase) reverse the argument I have a topological band, how do I trivialize it?

face with fire: you need another topological band (with the proper Chern number)



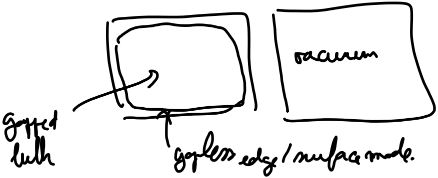
strong topology

That was the situation until 2017. With the development of crystalline topological insulators (Bernevig / Vishwanath / Fang) was discovered fragile topology.

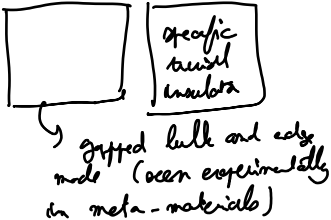


"fragile" is a misnomer. First, it does not say how large is the gap.

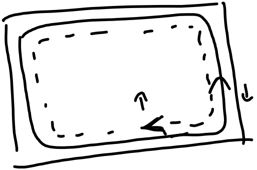
Second, it cannot be trivialized by "any" trivial band.



versus



Can we have a situation like this?



Not protected unless you have time reversal symmetry (think about adding spin and playing with $T^2 = -1$ and its antiunitary behavior, protect the crossing in the band structure)

protected but only mod 2.

Z_2 topological insulator (Kane and Mele 2005, once again based on graphene + a sci-fi spin orbit coupling) example of a time reversal protected TI.

Last but not least: How does magnetic field affect a Chern insulator.

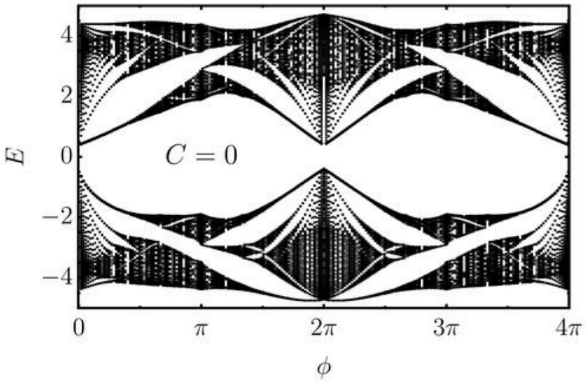
Magnetic length $l_B = \sqrt{\frac{\hbar}{eB}} \simeq \frac{26\,nm}{B^{1/2}[T]}$

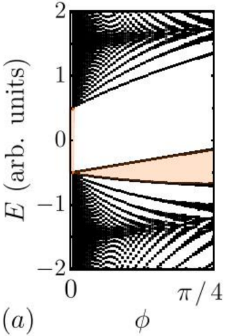
when $l_B \simeq$ to the atomic scale / lattice spacing you get the Hofstadter butterfly

For pure graphene $a = 0.142\,nm \rightarrow B \sim 10^4 T$.

moiré $l \simeq 13\,nm \rightarrow B \sim$ a few teslas

Hofstadter and topology





What about a Chern insulator?

→ close the gap as soon as you add any infinitesimal amount of magnetic flux.

Streda formula: the filling factor of the band at non-zero flux depends on the Chern number.

$$\sigma_{xy} = \frac{\partial n}{\partial B} \quad / \quad \text{Chern insulator } \sigma_{xy} = C\frac{e^2}{h}.$$

$$\underbrace{\delta n}_{\text{variation of the density}} \;\hat{=}\; \underbrace{C}_{\text{Chern number}} \;\; \delta B \longrightarrow \text{magnetic field.}$$

$\left(\delta \nu = C \frac{\Phi}{\Phi_0}\right)$ — Φ_0: quantum of flux $\frac{h}{e}$

tracking of $\delta\nu$ or δn changes to keep an insulator while tuning B gives access to C.

Back to TBG

Is there any topology in the active bands of TBG?

* $C_{2z}T$ leads to fragile topology
* $\mathcal{P}$ leads to strong topology similar to the $\mathbb{Z}_2$ TI ($\mathcal{P}^2 = -1$ non unitary symmetry)

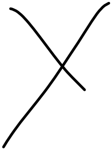
As a consequence, you cannot capture the physics of the two active bands using a two band model for $C_{2z}T$ or any additional number of bands for $\mathcal{P}$ ($\mathcal{P}$ imposes to have additional bands per pair, cancelling each other)

The chiral symmetry is also helpful.

Thanks to $C_{2z}T$, you can always describe at a given k points for the two active bands, using 2 wavefunctions with opposite Chern number $e_Y = \pm 1$ (but they might not be eigenstates of H).

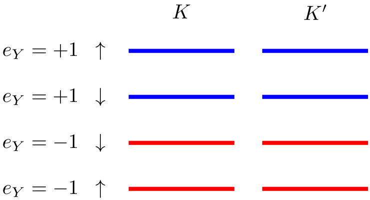
If you include the chiral symmetry, then the Chern basis becomes also the eigenstates of chiral sym. You can then think about the two active bands as 2 bands with opposite Chern number.

<u>To recap</u>: think about TBG as two active bands with non trivial topology, times 2 for the degree valley of freedom, times 2 if you include back the spin: a total of 8 bands.

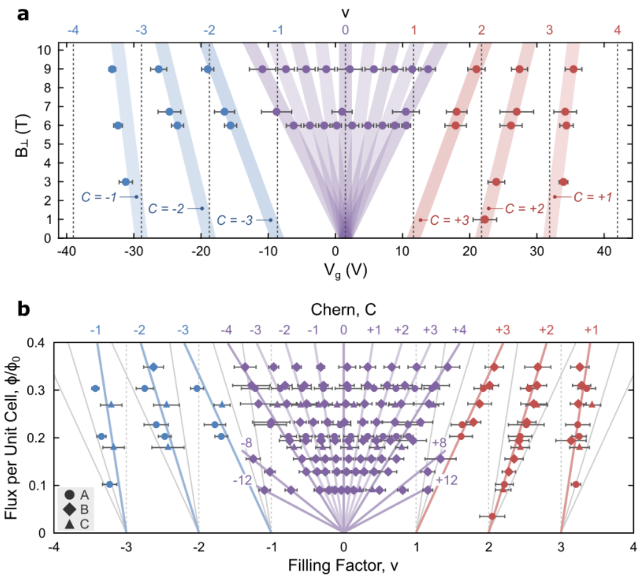


If you forget for one moment the kinetic energy, you have 8 massively degenerate bands. Why shall we get any insulator at e.g. $\nu = -3$ or $\nu = -1$? Interaction.

- Filling factor $\nu = -4, \ldots, 4$.
- Charge neutrality at $\nu = 0$.
- Chiral limit, each band has its own Chern,spin,valley quantum numbers.



Quantized magnetic-field response in TBG



Nuckolls et al., Nature (2020)