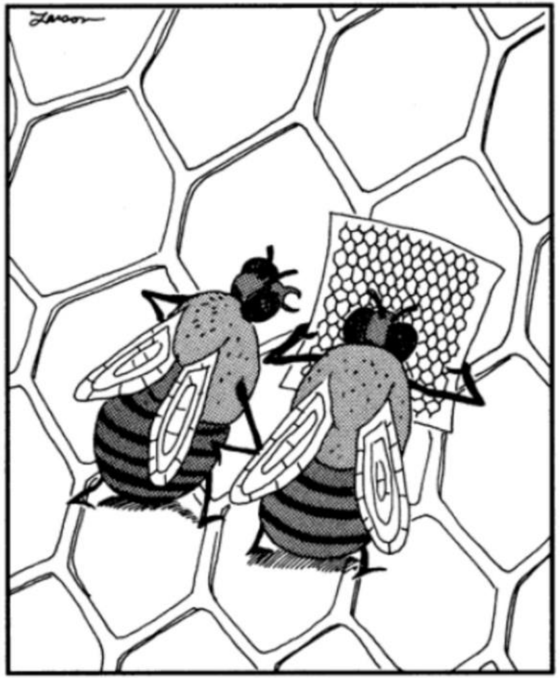
Quantum Spin Hall Effect in Graphene



"Face it, Fred—you're lost!"

Taylor S., Kai S., Benjamin S., Kathryn W., Penghao Z.

C. L. Kane and E. J. Mele, Phys. Rev. Lett. **95**, 226801 -- (2005)

Quick Overview

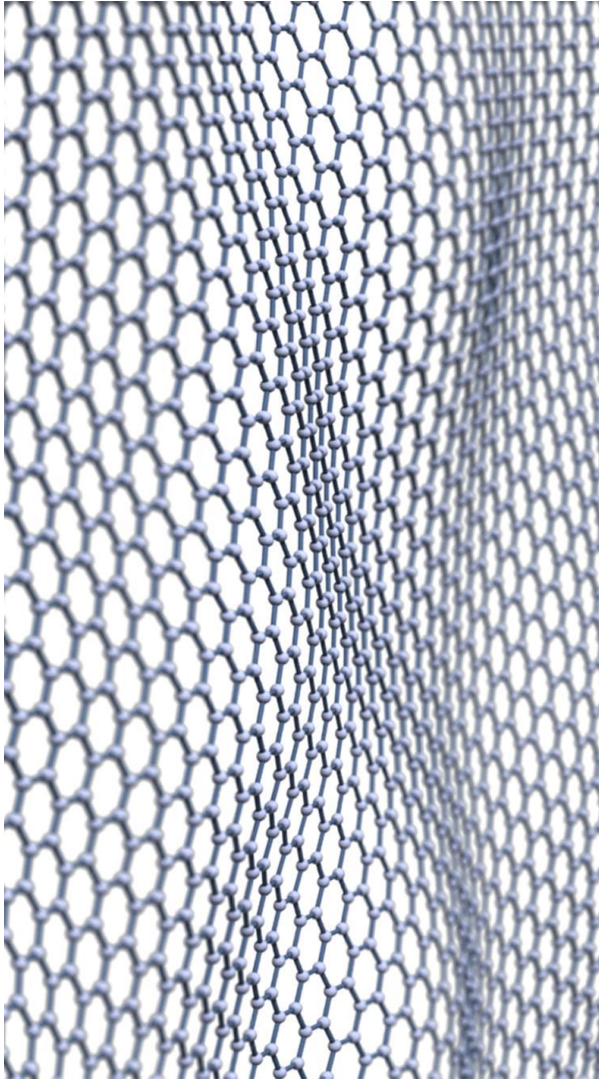
First the Motivation.

Go over the original simplified version of Graphene’s Hamiltonian symmetries.

Explanation of how Kane and Mele completed the Hamiltonian symmetry by adding spin to the hamiltonian.

Introduce the Spin Hall Effect (the implications) along with the experimental considerations.

And finally another summary along with our critiques of the paper.

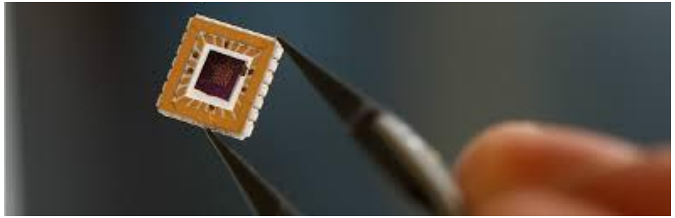


Why Is/Was Graphene Interesting and Useful?

- Graphene is a 2-D material (first to be isolated).
- Geim and Novoselov isolated single-layer using the “scotch-tape” method (2004).
  - 2010 Nobel Prize “for groundbreaking experiments regarding the two-dimensional material graphene.”
  - This paper: submitted 2004, published 2005.
- It's the strongest material in the world. It's completely flexible, and it's more conductive than copper.

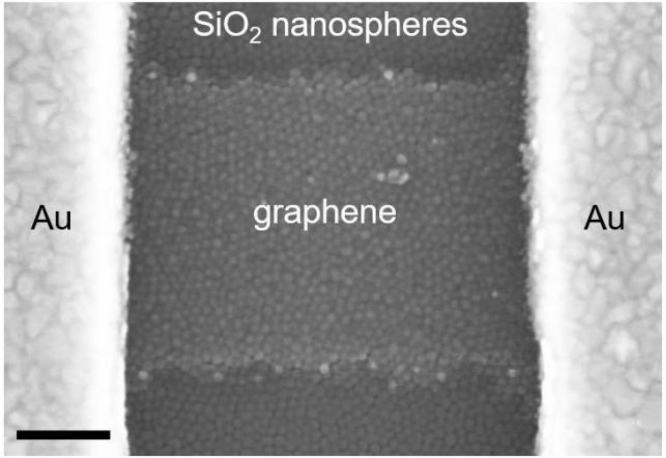
Graphene Today

Potential graphene applications include lightweight, thin, flexible, yet durable circuits.



Medical : Graphene could pave the way for bionic devices in living tissues.

UIUC: Our own colleagues are using graphene to research new physics.



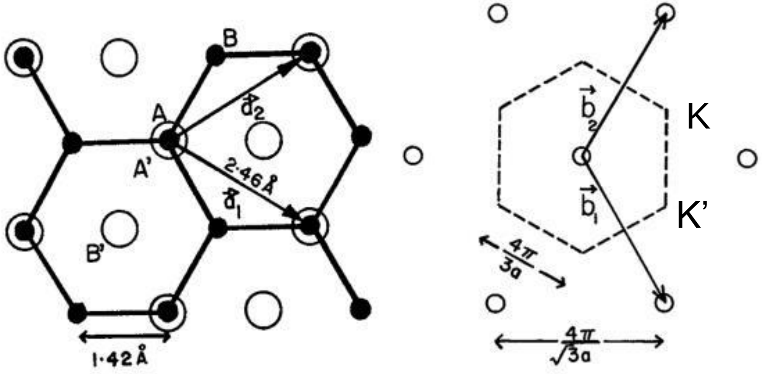
Electron transport in strain superlattices of graphene

Y Zhang, Y Kim, MJ Gilbert, N Mason

Everyday : High-power graphene supercapacitors could make batteries obsolete.

Graphene’s Structure and Symmetries

- We want to model graphene. We will demand some symmetries.
- Inversion
  - Invert about the center of a plaquette, for example.
- Time reversal
  - Imagine pausing and then tracing motion backwards
  - Example: B field.
    - B field is due to charge in motion.
    - Time reversal sends $\vec{B} \to -\vec{B}$



Hamiltonian of Graphene Without Spin

- Hamiltonian in real space (at low energy):

$$\mathcal{H}_0 = -i\hbar v_F \psi^\dagger(\sigma_x\tau_z\partial_x + \sigma_y\partial_y)\psi.$$

$\sigma_z = \pm 1$ states on the A(B) sublattice

$\tau_z = \pm 1$ states at the K(K') points

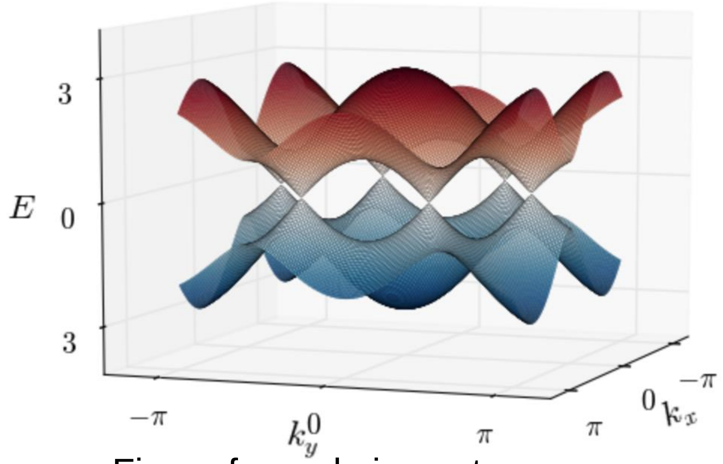
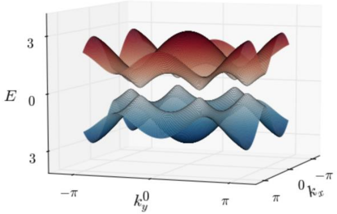


Figure from nbviewer topocm wk4_haldane

- Hamiltonian in k space (Fourier transform $\mathcal{H}_0$):

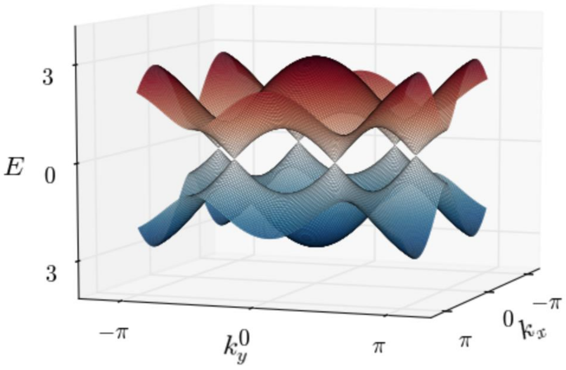
$$-i\hbar\partial_x \to k_x,\ -i\hbar\partial_y \to k_y$$

- Note: There is no σ_z in the Hamiltonian!
  - This is because it will open a gap and breaks time reversal+parity!



What Do Time Reversal and Parity Do to the Hamiltonian

	Time reversal (T)	Parity (P)
$(I_2,\ \vec{\tau})$	$\vec{\tau} \to -\vec{\tau} \qquad I_2 \to -I_2$	$\vec{\tau} \to -\vec{\tau} \qquad I_2 \to -I_2$
$(I_2,\ \vec{\sigma})$	$\vec{\sigma} \to \vec{\sigma} \qquad I_2 \to I_2$	$\sigma_x \to \sigma_x, \sigma_y \to -\sigma_y, \sigma_z \to -\sigma_z$ $I_2 \to I_2$

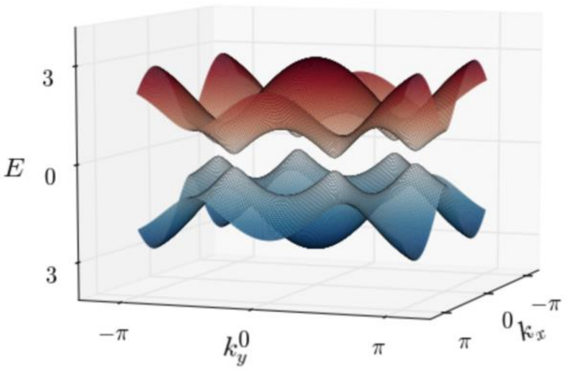


Add terms $\sigma_z \otimes I_2$

Breaks P

Add terms $\sigma_z \otimes \tau_z$

Breaks T



But Electrons Have Spin...

- Without spin we learn:
    - Demanding time reversal + parity symmetries 100% guarantees that there is no gap.
- **Question:** If we take spin into account and demand that our system be invariant under time reversal+parity, do the results change when compared to the spinless case?
- $S \to -S$ under time reversal, where S is the spin.
- A spin orbit term like $S \cdot L \to (-S) \cdot (-L)$ is left invariant under time reversal (and also under parity), where L is the orbital angular momentum.

Graphene with Spin May Have a Spin-Orbit Term in the Hamiltonian

- Working in the low energy case, Kane and Mele add a spin-orbit coupling term to the Hamiltonian:

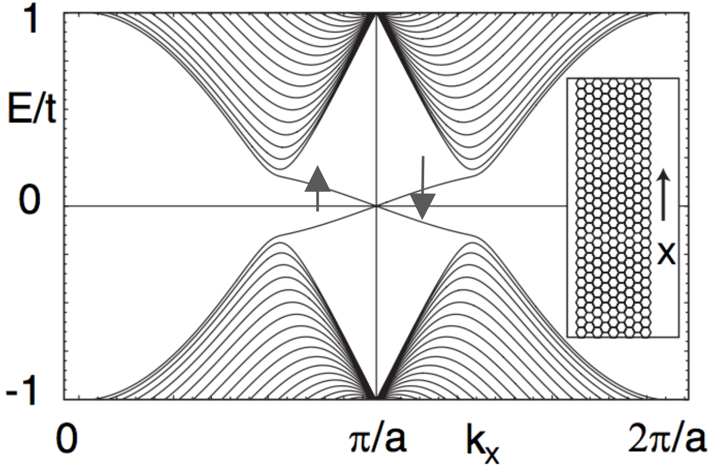
$$\mathcal{H}_{\mathrm{SO}} = \Delta_{so}\psi^\dagger \sigma_z \tau_z s_z \psi.$$

- Based on the table before, we see that this is invariant under time reversal and parity.

Adding Spin-Orbit Opens a Gap and Gives Non-trivial Edge States

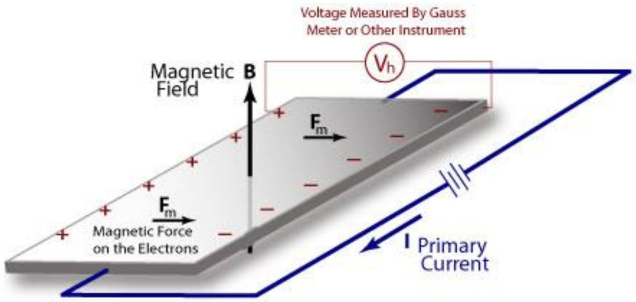
- Do the calculation for zigzag edges.
  - Edges states expected by Laughlin's argument.
  - The edge states, instead of being flat, have a slope.
  - Recall $\hbar\vec{v} = \nabla_{\vec{k}} E\left(\vec{k}\right)$. Thus, these edge states have non-zero velocity.

Calculation of E(k) with spin-orbit

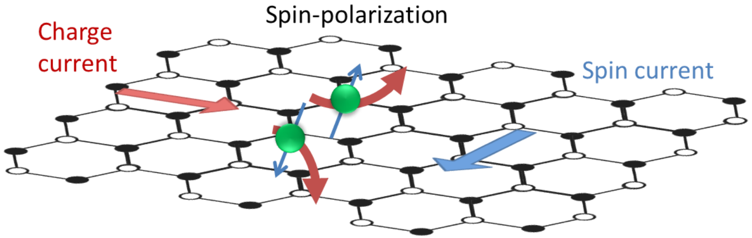


The Spin Hall Effect is the Accumulation of Spin on Boundaries

- The Hall effect has electrons accumulated on the boundaries.
- Spin hall effect is the accumulation of spin on the boundaries.
- A “quantum spin hall effect” is seen in graphene with the spin-orbit term included.



https://sites.google.com/site/joshshalleffectcache/



https://en.wikipedia.org/wiki/Spin_Hall_effect

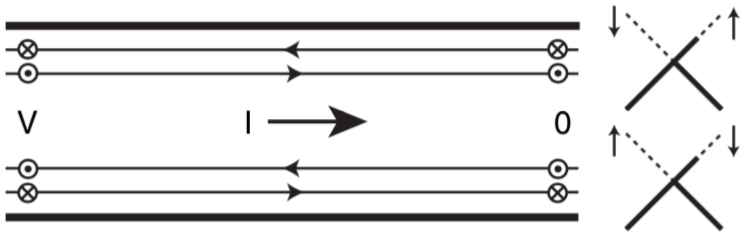
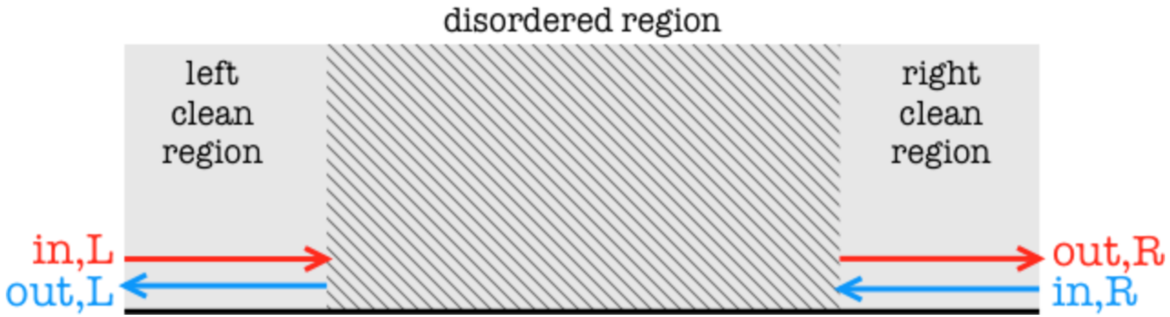


Figure 2a) from Kane & Mele’s Paper

Does Disorder on the Edges Change the Results?



$$|\Psi, \mathrm{L}\rangle = \sum_{n=1}^{N} \alpha_{n,\mathrm{L}} \ |n, \mathrm{L}\rangle + \beta_{n,\mathrm{L}} \mathcal{T} \, |n, \mathrm{L}\rangle$$

$$|\Psi, \mathrm{R}\rangle = \sum_{n=1}^{N} \alpha_{n,\mathrm{R}} \ |n, \mathrm{R}\rangle + \beta_{n,\mathrm{R}} \mathcal{T} \, |n, \mathrm{R}\rangle$$

$$\begin{pmatrix} \beta_{\mathrm{L}} \\ \beta_{\mathrm{R}} \end{pmatrix} = S \begin{pmatrix} \alpha_{\mathrm{L}} \\ \alpha_{\mathrm{R}} \end{pmatrix}$$

$$S = \begin{pmatrix} r & t \\ t' & r' \end{pmatrix}$$

Figures from Figure from nbviewer topocm wk5_qshe

If the Disorder is Time Reversal Invariant...

- The upshot is that the S matrix satisfies the following: $S = \mathcal{T}^2 S^T$
- The time reversal operator squared can be +1 or -1.
- If it is -1, then there is always a mode such that t=1 (in other words r=0) so it is perfectly transmitted!
    - This means the results are fairly robust and therefore it makes sense to go and do an experiment to test the predictions.
        - The results don't need approximations like ``approximate the cow as spherical...''

Conclusions

- Adding spin in graphene Hamiltonian
    - Time Reversal and Inversion symmetries still satisfied
    - Non-trivial insulating behavior
        - Gap in bulk
        - Propagating edge states exist where the bulk is gapped

- Citations: 2,936 (Web of Science)

- Historical significance of this paper
    - Contributed to start of “Band Revolution”
    - Increased interest in topology in band theory

- Scientific Validity ✓
- Importance ✓
- Broad Interest ✓
- Accessibility ✗

Trivial and Nontrivial Critiques...

- Notation is overly terse for a general audience
- Paper is not accessible to a general audience
- Several trivial typos found in the paper

Typo 1

$$\mathcal{H} = \sum_{\langle ij\rangle\alpha} t c^\dagger_{i\alpha} c_{j\alpha} + \sum_{\langle\langle ij\rangle\rangle\alpha\beta} i t_2 \nu_{ij} s^z_{\alpha\beta} c^\dagger_{i\alpha} c_{j\beta}. \qquad (6)$$

The first term is the usual nearest neighbor hopping term. The second term connects second neighbors with a spin dependent amplitude. $\nu_{ij} = -\nu_{ji} = \pm 1$, depending on the orientation of the two nearest neighbor bonds $\mathbf{d}_1$ and $\mathbf{d}_2$ the electron traverses in going from site j to i. $\nu_{ij} = +1\,(-1)$ if the electron makes a left (right) turn to get to the second bond. The spin dependent term can be written in a coordinate independent representation as $i(\mathbf{d}_1 \times \mathbf{d}_2) \cdot \mathbf{s}$. At low energy (6) reduces to (2) and (3) with $\Delta_{so} = 3\sqrt{3}t_2$.

The edge states can be seen by solving (7) in a strip

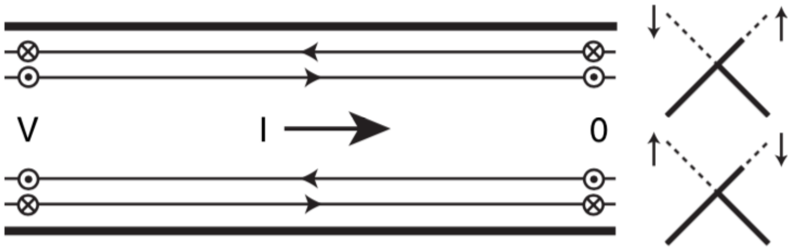
Typo 2

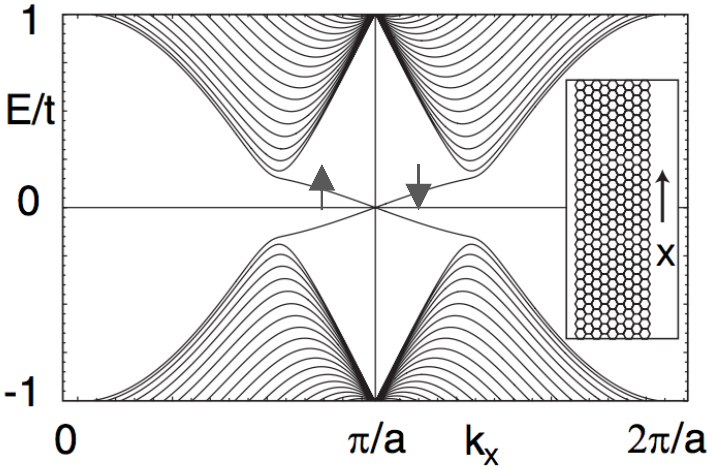
The magnitude of Δ_{so} may be estimated by treating the microsopic SO interaction

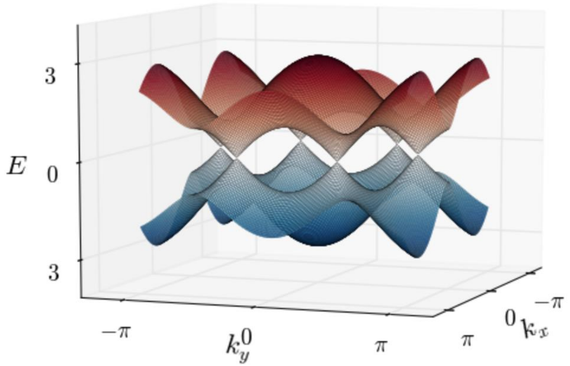
$$V_{\mathrm{SO}} = \frac{\hbar}{4m^2c^2}\mathbf{s} \cdot (\nabla V \times \mathbf{p}) \qquad (7)$$

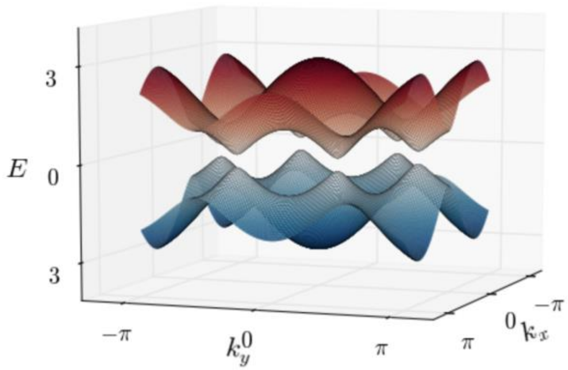
in first order degenerate perturbation theory. We thus evaluate the expectation value of (8) in the basis of states

Questions?


V
I
0


1
E/t
0
-1
0
π/a
k_x
2π/a
x


3
E
0
3
$-\pi$
k_y 0
π
$-\pi$
0 k_x
π


3
E
0
3
$-\pi$
k_y 0
π
$-\pi$
0 k_x
π