Topological electronic phases in graphene

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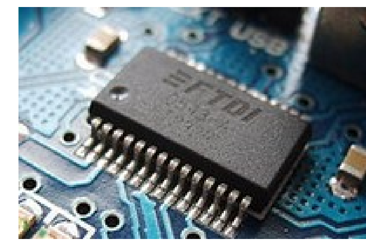
The role of quantum mechanics in science and technology

Quantum phenomena in today's technology

Medicine

Energy

Electronics

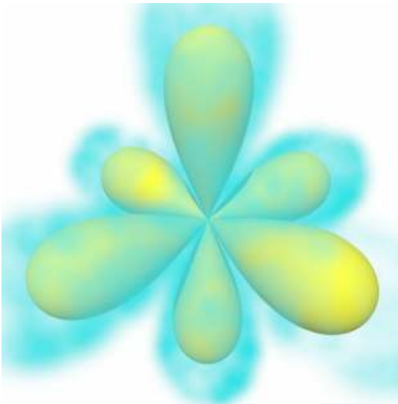
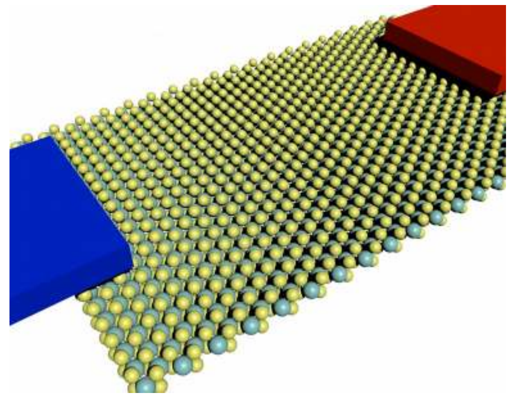
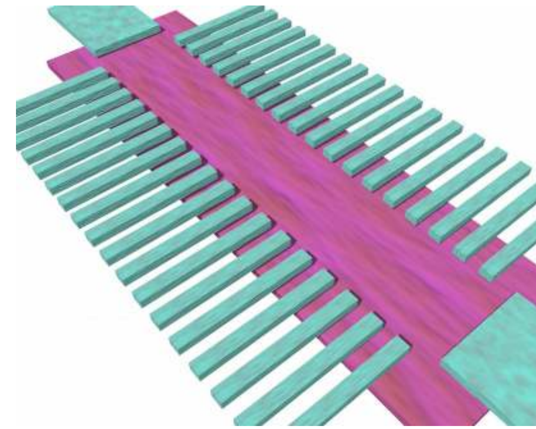


Atomic and quantum control in condensed matter opens new venues to exploit quantum physics

How can we create emergent behaviors?
→ Topological insulators, spin liquids, bad metals
How can we realize mathematical models?
→ Solitonic excitations, non abelian particles, highly entangled states
How can we exploit quantum phenomena?
→ Imaging techniques, quantum computing

Quantumness as a resource?

Losing quantumness

Size increase

But at some point

- Quantization is blurred away
- Coherence is lost
- Classical dynamics arises
- Planck's constant “disappears”

$$i\hbar\frac{\partial}{\partial t}\Psi = \mathcal{H}\Psi$$

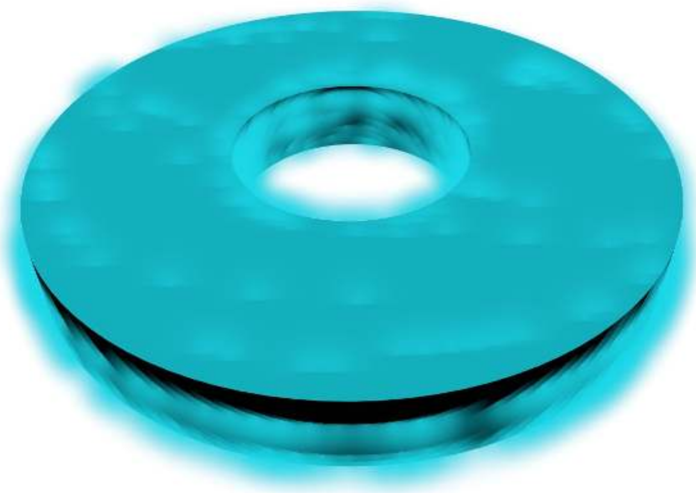
Quantum → Classical

Disorder
Imperfections
Fluctuations
Interactions
Decoherence
Temperature

Are quantum phenomena restricted to the nanoscale?

Quantumness in the macroscale

Superconductivity

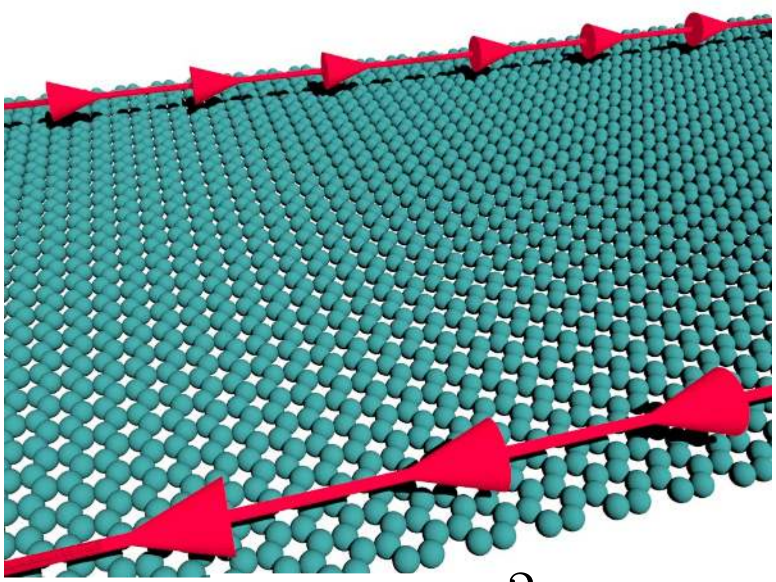


$$\Phi = \frac{h}{2e}$$

Many-body state

<u>Quantization</u> of flux

Quantum Hall effect



$$\sigma_{xy} = \nu \frac{e^2}{h}$$

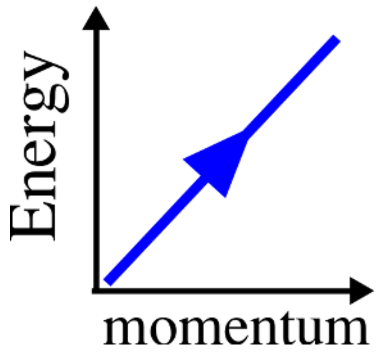
Single-particle state

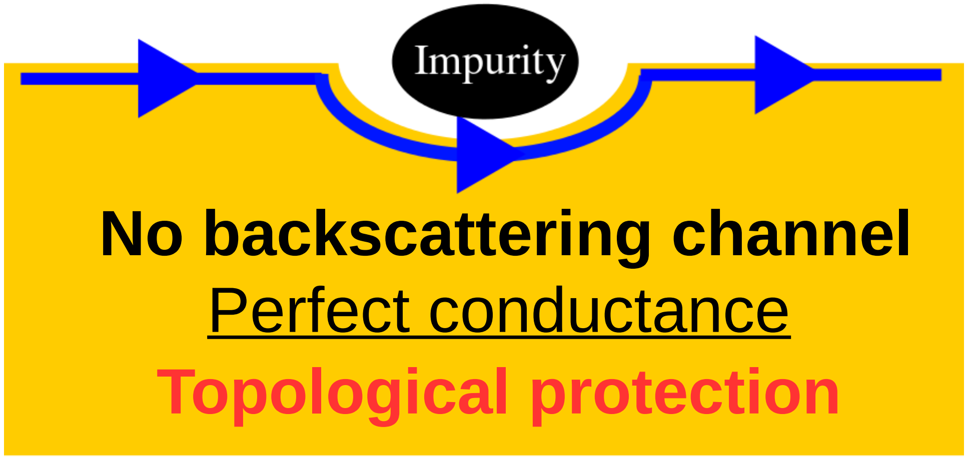
<u>Quantization</u> of conductance

Macroscopic quantum phenomena determine fundamental quantities with the highest precision

When defects no longer matter

Surface of Hall insulator



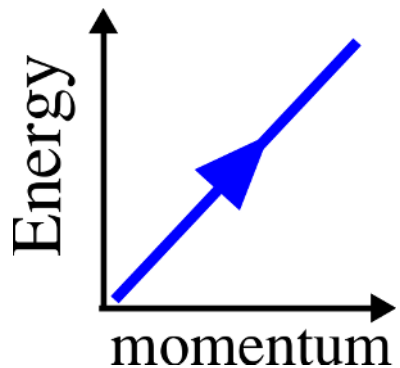


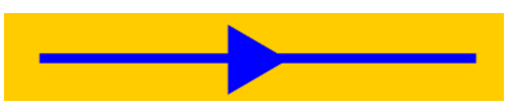
$$\sigma_{xy} = \frac{e^2}{h}\mathcal{C}$$	Hall conductance	**Physical observable**
$$\mathcal{C} = \frac{1}{2\pi}\int \Omega d^2 k$$	Chern number, **integer**	**Topological invariant**
$$\Omega = \partial_{k_x} A_y - \partial_{k_y} A_x$$	Berry curvature	**Geometrical properties of the Hamiltonian**
$$\vec{A} = i\langle\Psi\|\partial_{\vec{k}}\|\Psi\rangle$$	Berry connection	

Topology driven states

Hall insulator

2D system





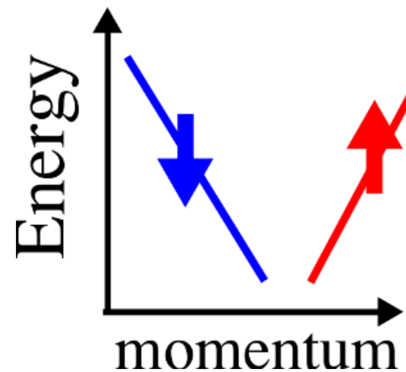
<u>1D Chiral metal</u>

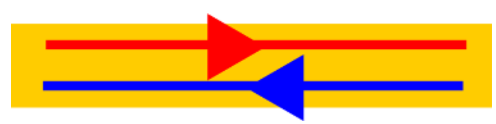
Absence of longitudinal resistance

Electronics

Spin Hall insulator

2D system





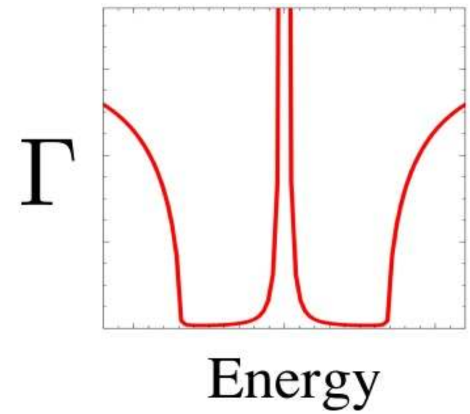
<u>1D Helical metal</u>

Pure spin flow without charge flow

Spintronics

Topological superconductors

1D system

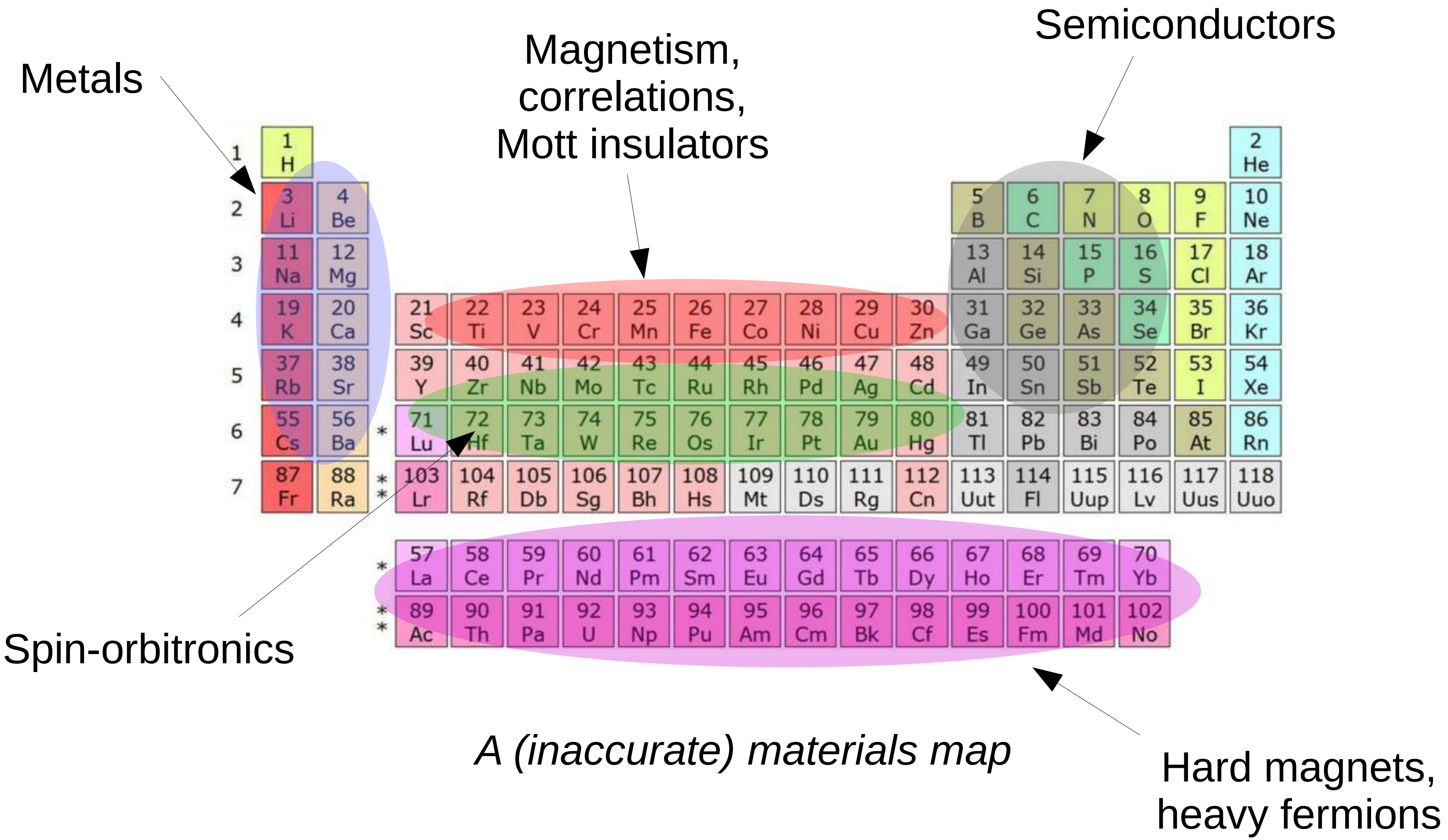


<u>0D Majorana bound states</u>

Anyonic braiding statistics

Quantum computing

A quest for topological materials

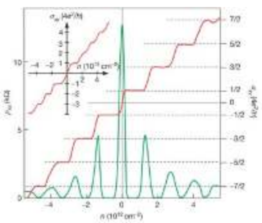


A (inaccurate) materials map

Where are the topological materials?

Materials with topological states

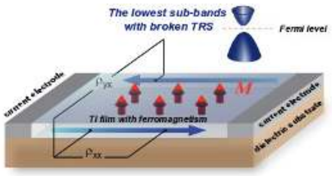
Quantum Hall effect



graphene

Nature 438, 197-200 (2005)

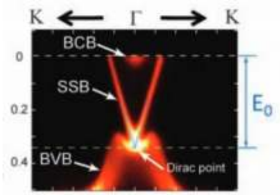
Quantum Anomalous Hall effect



Cr-doped $(Bi,Sb)_2Te_3$

Science 340.6129 (2013): 167-170

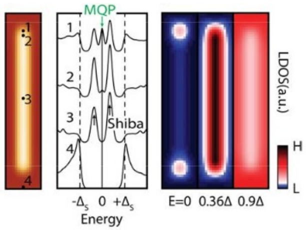
Quantum Spin Hall effect



Bi_2Se_3

Science 325.5937 (2009): 178-181

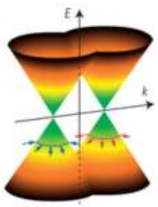
Topological superconductor



Fe@Pb

Science 346.6209 (2014): 602-607

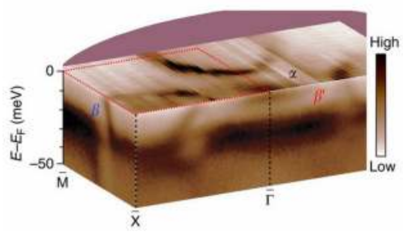
Weyl semimetal



TaAs

Nature Physics 11, 724–727 (2015)

Topological Kondo insulator



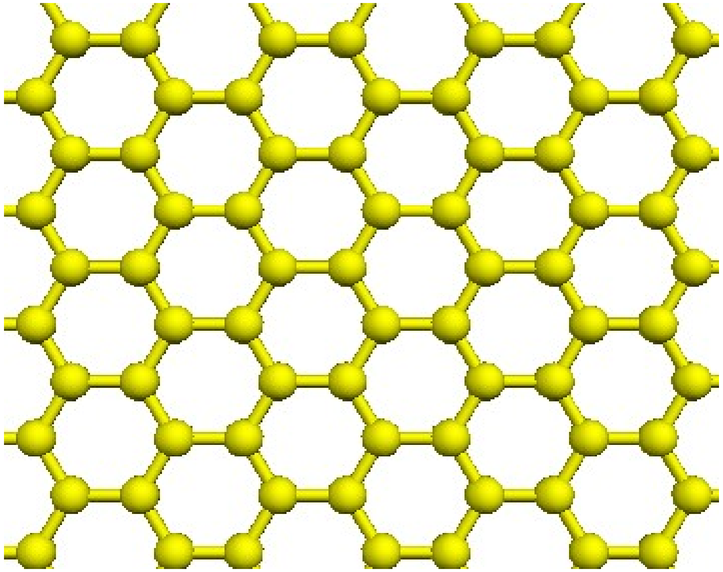
SmB_6

Nature Communications 5, 4566 (2014)

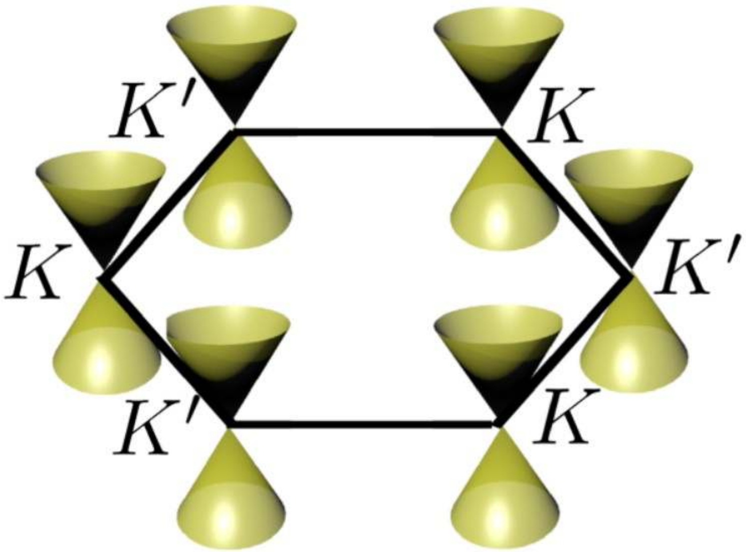
Topological states are not restricted to certain elements

The electronic structure of graphene

Honeycomb lattice



Electronic spectrum



Dirac dispersion at the Fermi energy

Masless electrons

Berry phase: source of “topologicality”

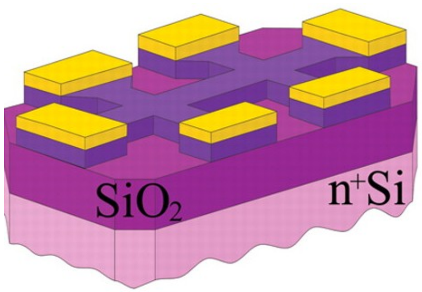
$$\mathcal{H} = v_F[\sigma_x p_x + \sigma_y p_y]$$

$$\oint \vec{A} \cdot d\vec{k} = \pm\pi$$

Tunability of graphene

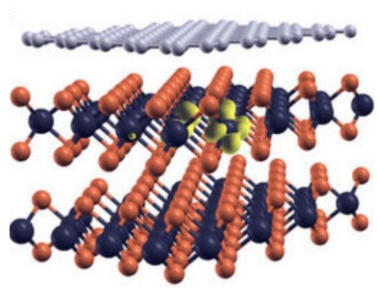
Field effect doping

Science 306.5696
666-669 (2004)



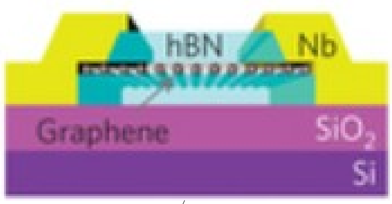
Spin-orbit proximity

Nature communications 5,
4875 (2014)



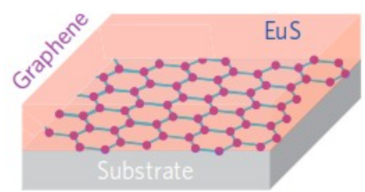
Superconducting transport

Nature Physics 12.4
318-322, (2016)



Exchange proximity

Nature Materials 15,
711–716 (2016)



$$\mathcal{H} = \mathcal{H}_0 + \mu c_i^\dagger c_i + \mathcal{H}_{SOC} + \Delta[c^\dagger_{i,s} c^\dagger_{i,s'} + c_{i,s'} c_{i,s}] + J\vec{m}\cdot\vec{\sigma}_{s,s'} c^\dagger_{i,s} c_{i,s'}$$

Can we exploit graphene's tunability to engineer topological states?

Core ideas of this thesis

How to exploit the interplay of Dirac points, helical states, magnetism and superconductivity?

How to create topological states without having to rely on spin orbit coupling?

References

Magnetic Edge Anisotropy in Graphene-like Honeycomb Crystals

J. L. Lado, J. Fernández-Rossier

Physical Review Letters 113 (2), 027203 (2014)

Quantum Anomalous Hall effect in graphene coupled to skyrmions

J. L. Lado, J. Fernández-Rossier

Physical Review B 92 (11), 115433 (2015)

Noncollinear magnetic phases and edge states in graphene quantum Hall bars

J. L. Lado, J. Fernández-Rossier

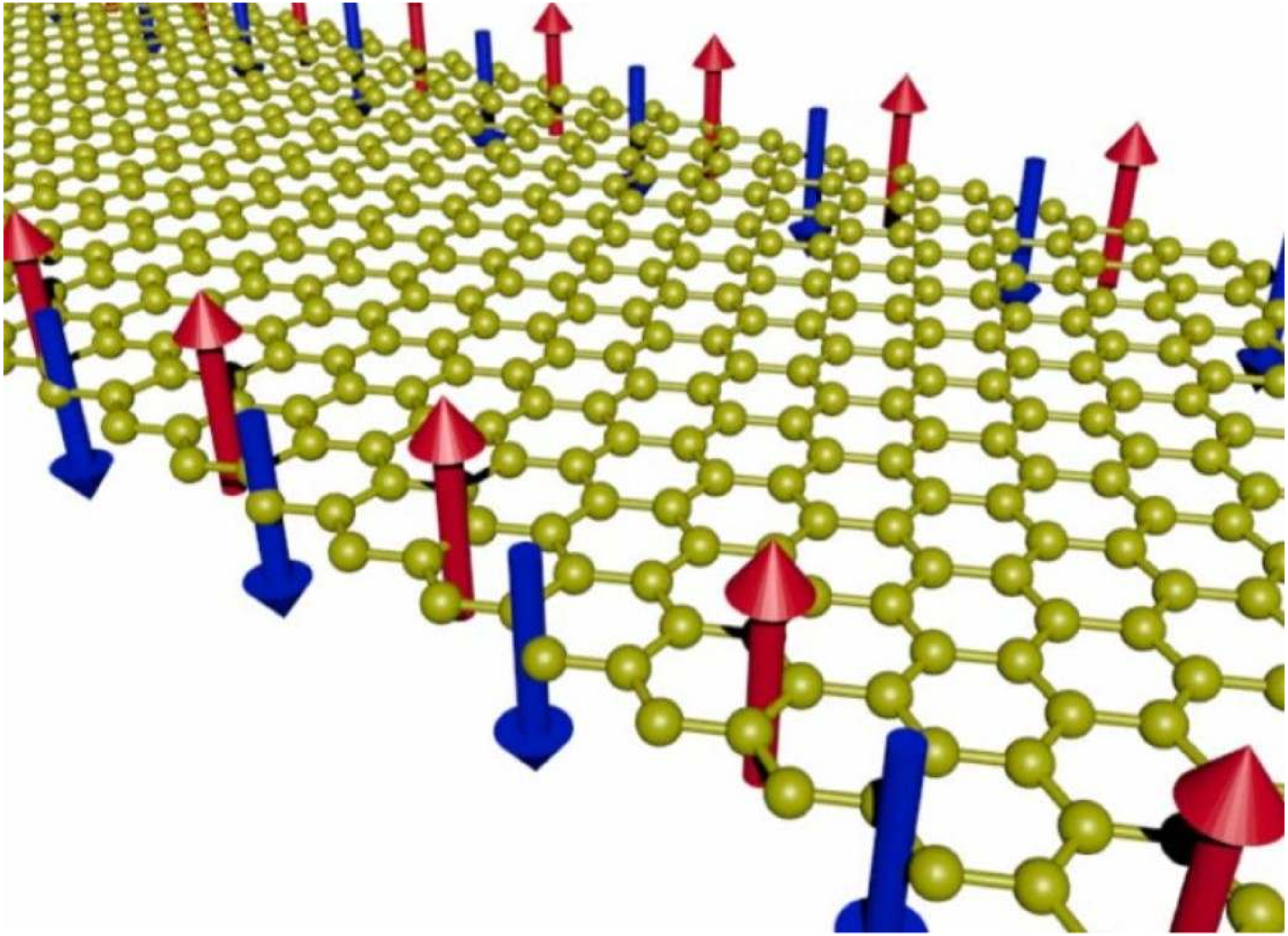
Physical Review B 90 (16), 165429 (2014)

Majorana zero modes in graphene

P. San-Jose, J. L. Lado, R. Aguado, F. Guinea, J. Fernández-Rossier

Physical Review X 5 (4), 041042 (2015)

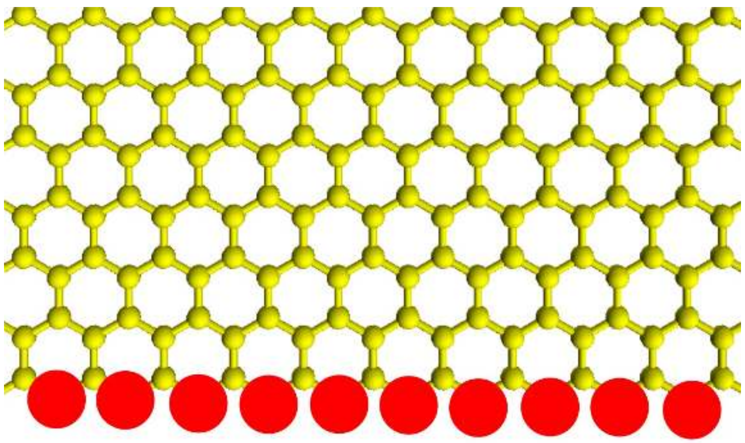
Intrinsic quantum spin Hall effect and magnetism in graphene



Two different edge states

Geometrical origin

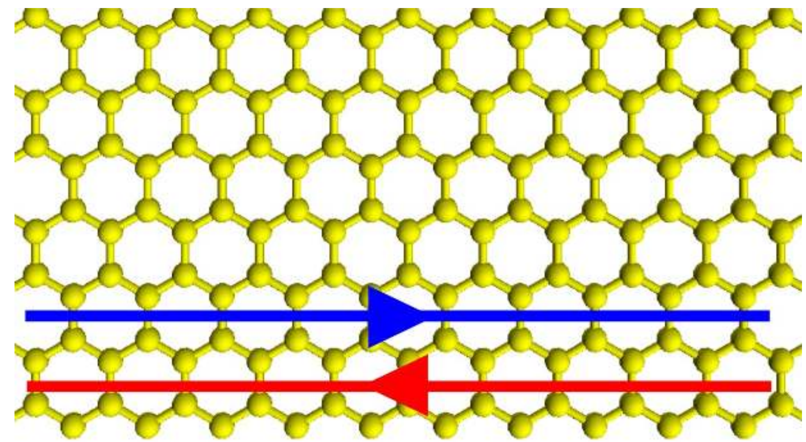
<u>Zigzag edge states:</u>
<u>Stoner instability</u>



Lieb theorem

Topological origin

<u>Helical states</u>



Z_2 topological invariant

$$\mathcal{H} = \sum_{\langle i,j\rangle} t c_j^\dagger c_i + \lambda_{SO} \sum_{\langle\langle i,j\rangle\rangle} \nu_{i,j} s_z c_j^\dagger c_i + U \sum_i c_{i,s}^\dagger c_{i,s} c_{i,s'}^\dagger c_{i,s'}$$

Kinetic energy

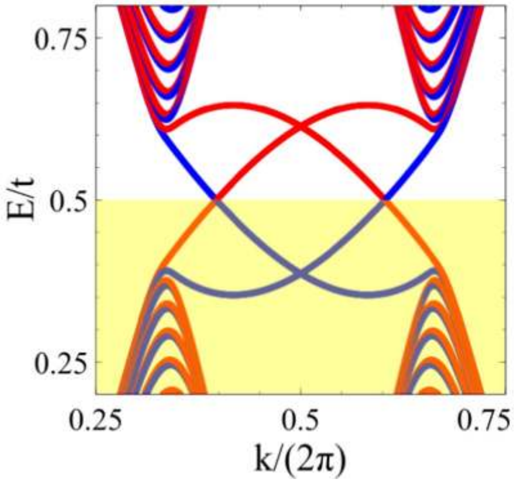
Spin-orbit coupling

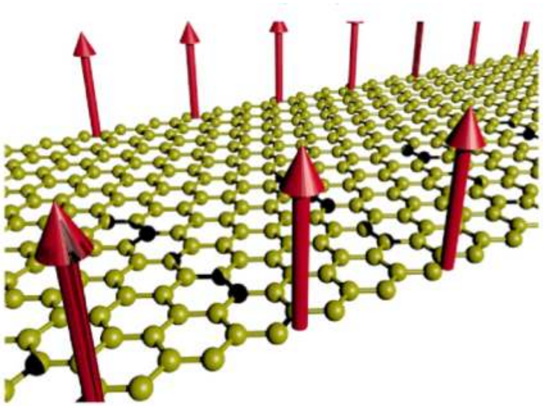
Electronic interaction (Hubbard)

How does the intrinsic localized magnetism interact with a helical metal?

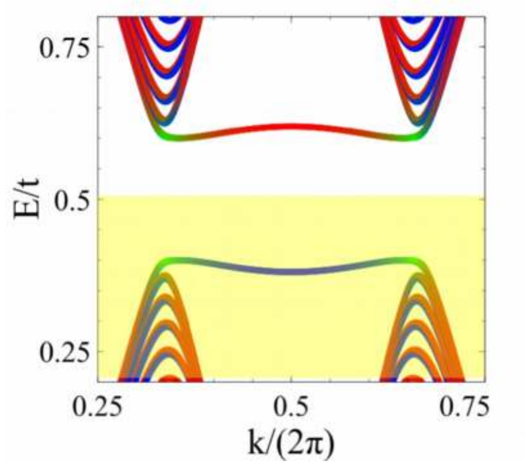
Magnetic dependent transport

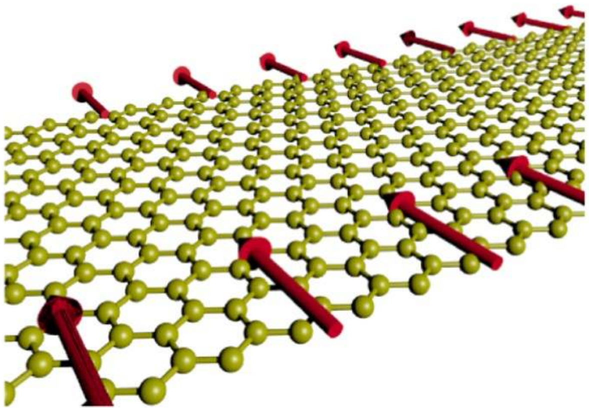
Off-plane magnetism, helical metal, gapless





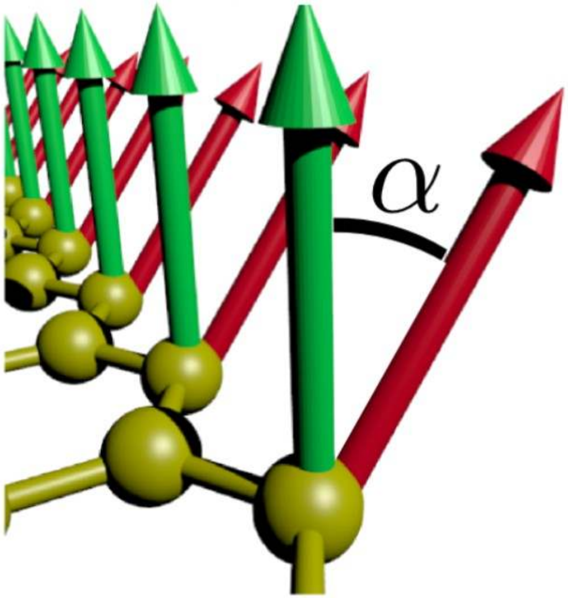
In-plane magnetism, gapped



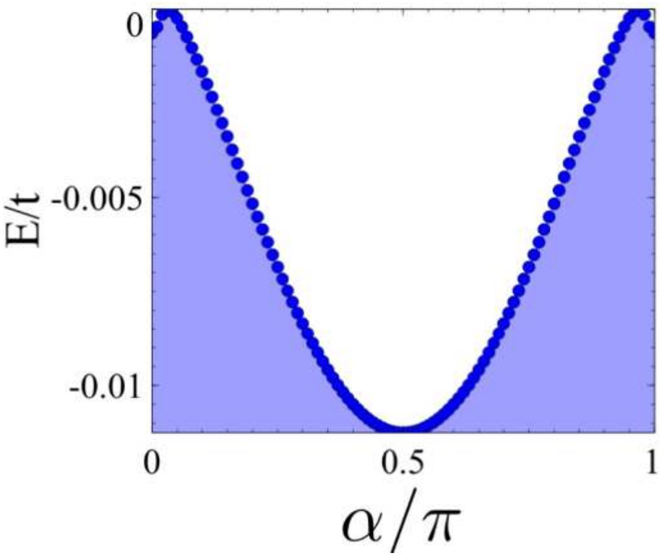


Gap and energy versus angle

Angle-dependent ground state



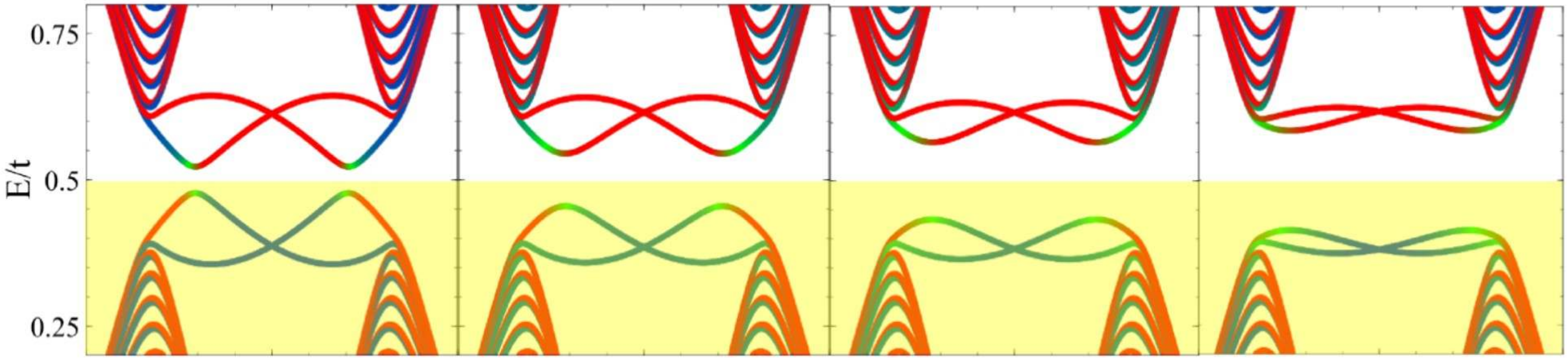
Lowest energy is the in-plane solution



Almost off-plane

Increasing angle

Almost in-plane



Anisotropy in graphene-like

How important is the magnetic anisotropy in different materials?

Material	t_{SO}	t
Graphene	0.1-5.0 μeV	2.7 eV
Silicene	0.16 meV	1.5 eV
Germanene	2.5 meV	1.4 eV
Stanene	8-30 meV	1.3 eV
MOF	1 meV	0.3 eV
Perovskite bilayer	1 meV	0.1 eV

$$\Delta E \approx c_1 \frac{t_{SO}^2}{t}$$

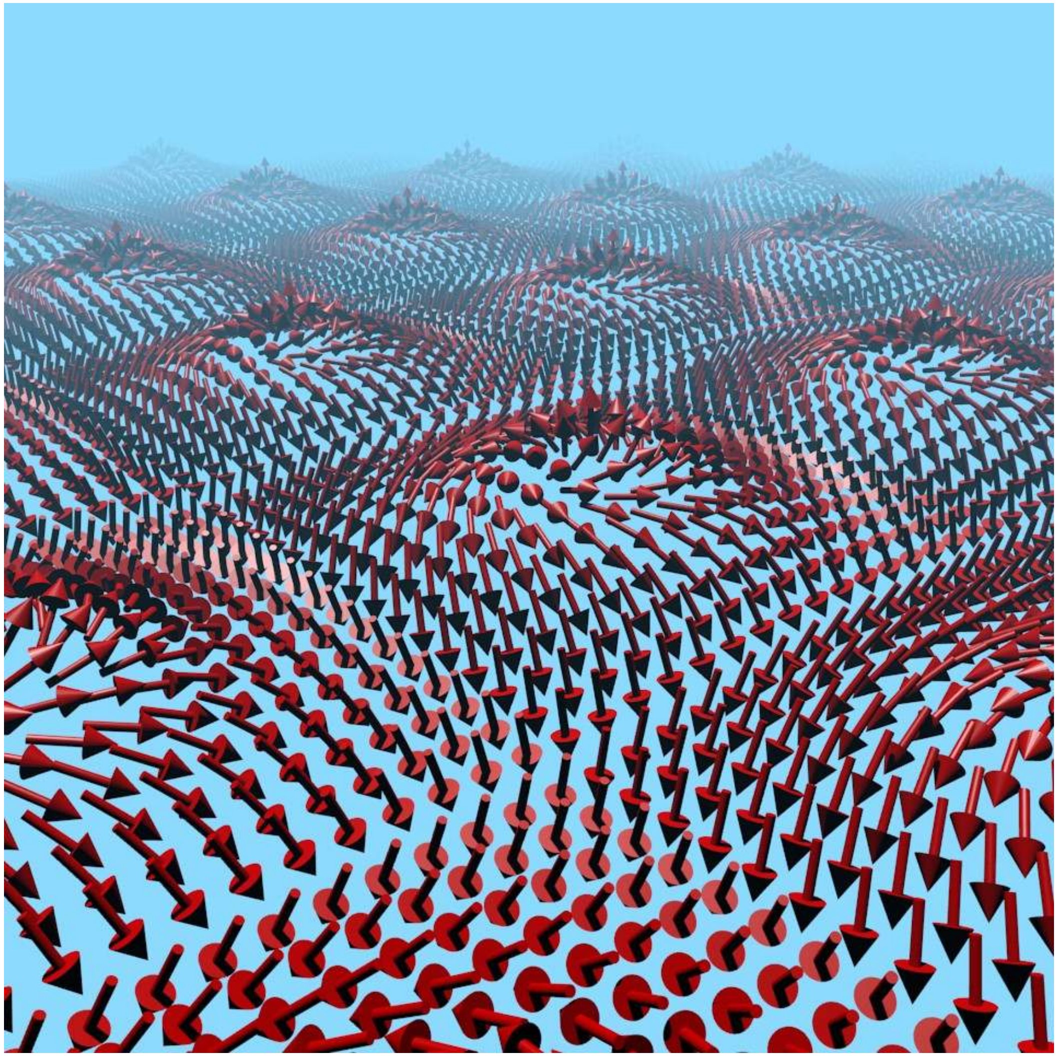
Anisotropy **negligible in graphene** but sizable in stanene (4 meV)

The (doomed?) fate of topological states in graphene

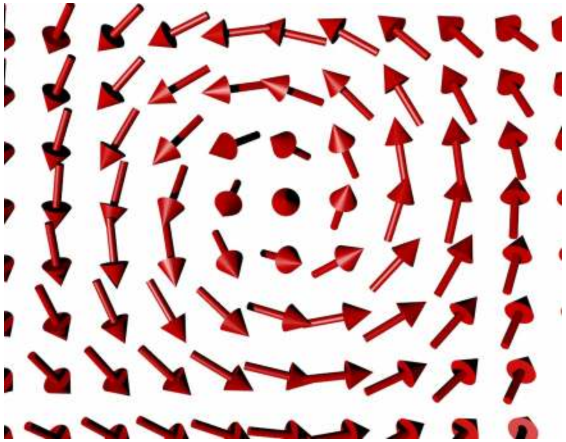
Does the lack of spin-orbit coupling (SOC) turn graphene into a bad material for topological states?

Can there be Quantum anomalous Hall without SOC?
Can there be Quantum spin Hall without SOC?
Can there be Majorana states without SOC?

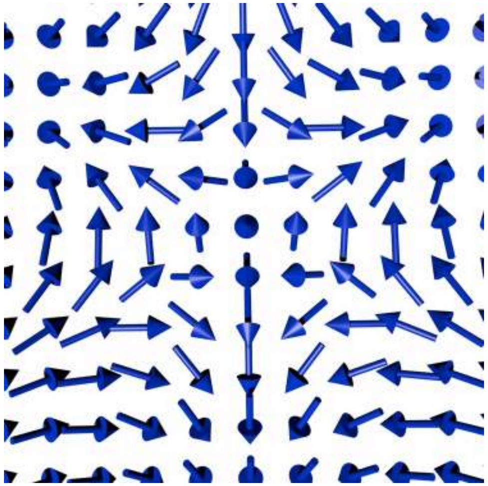
Chiral magnetism: skyrmions



$C_{Sky} = +1$

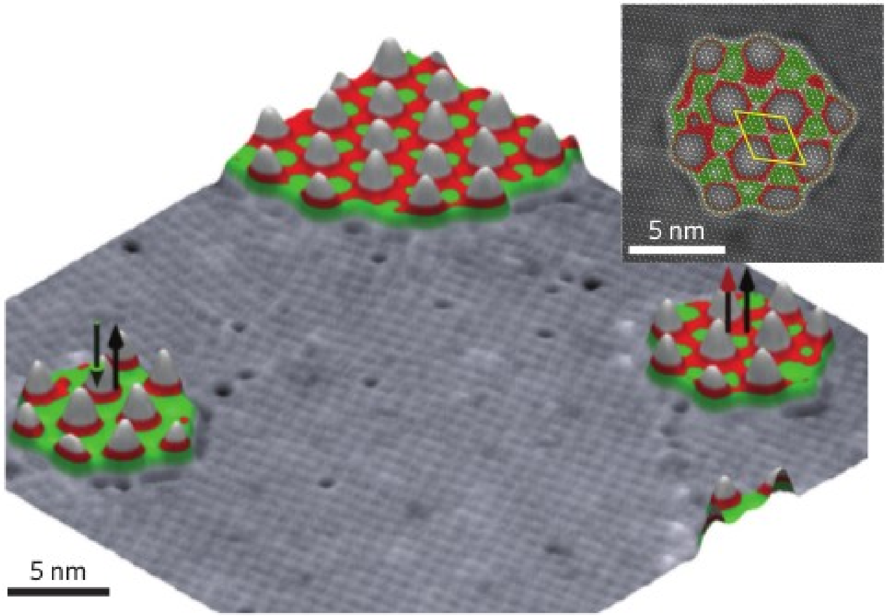


$C_{Sky} = -1$



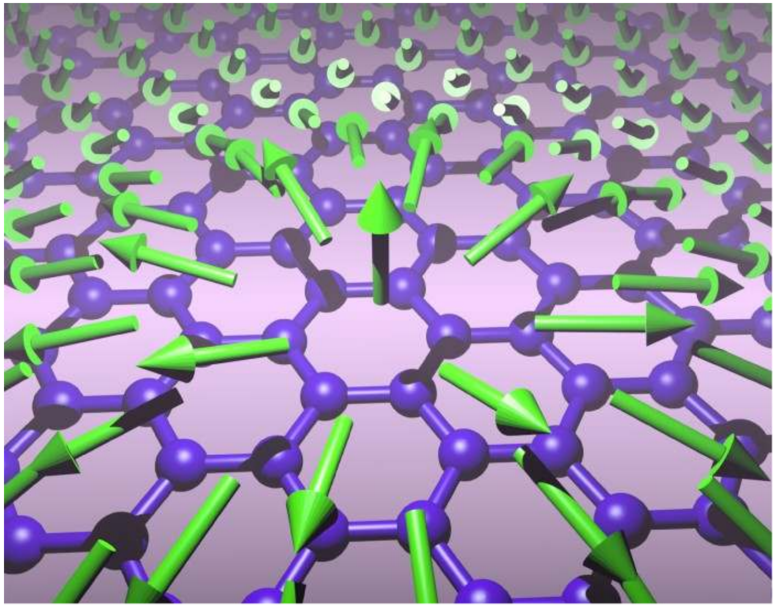
Graphene on skyrmions

Graphene on skyrmions
in Fe@Ir(111)



Nature Nanotechnology 9,
1018–1023 (2014)

What is the effect of an insulating skyrmion lattice in graphene?



Electronic structure: graphene@skyrmions

$$\mathcal{H} = t c_j^\dagger c_i + J \vec{m}_i \cdot \vec{\sigma}_{s,s'} c_{i,s'}^\dagger c_{i,s}$$

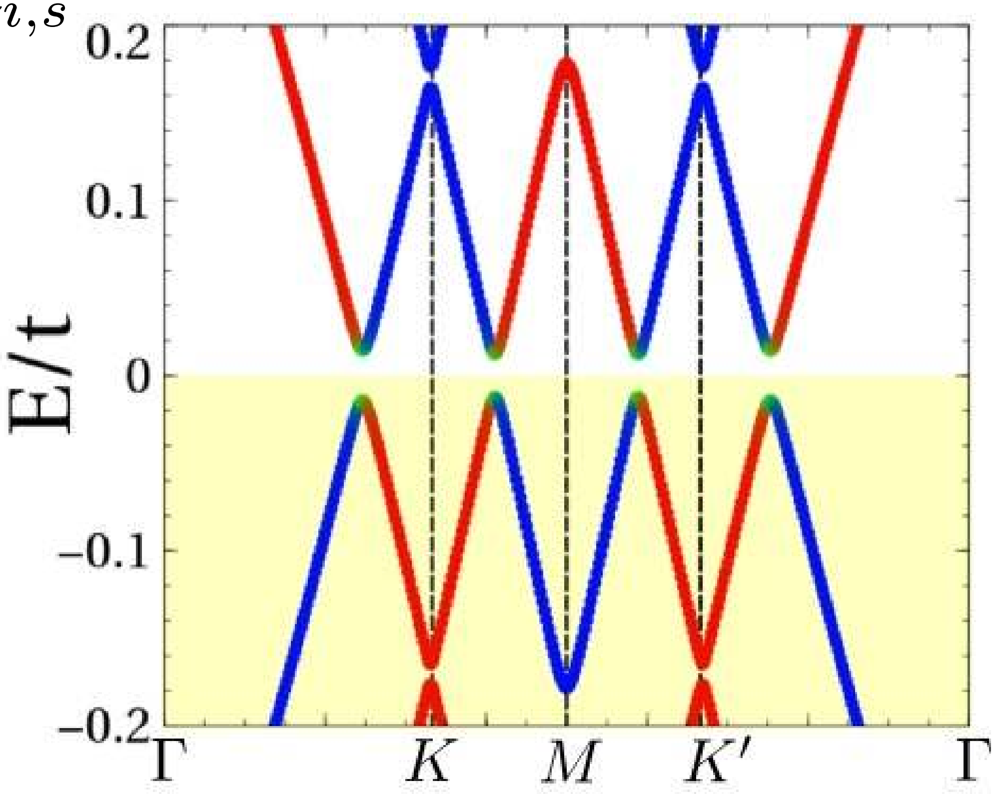
Kinetic energy

Exchange interaction with the skyrmion

$$C_{Sky} = \frac{1}{4\pi} \int \hat{m} \cdot (\partial_x \hat{m} \times \partial_y \hat{m}) dA$$

How is the topological invariant of the skyrmions transmited to graphene electrons?

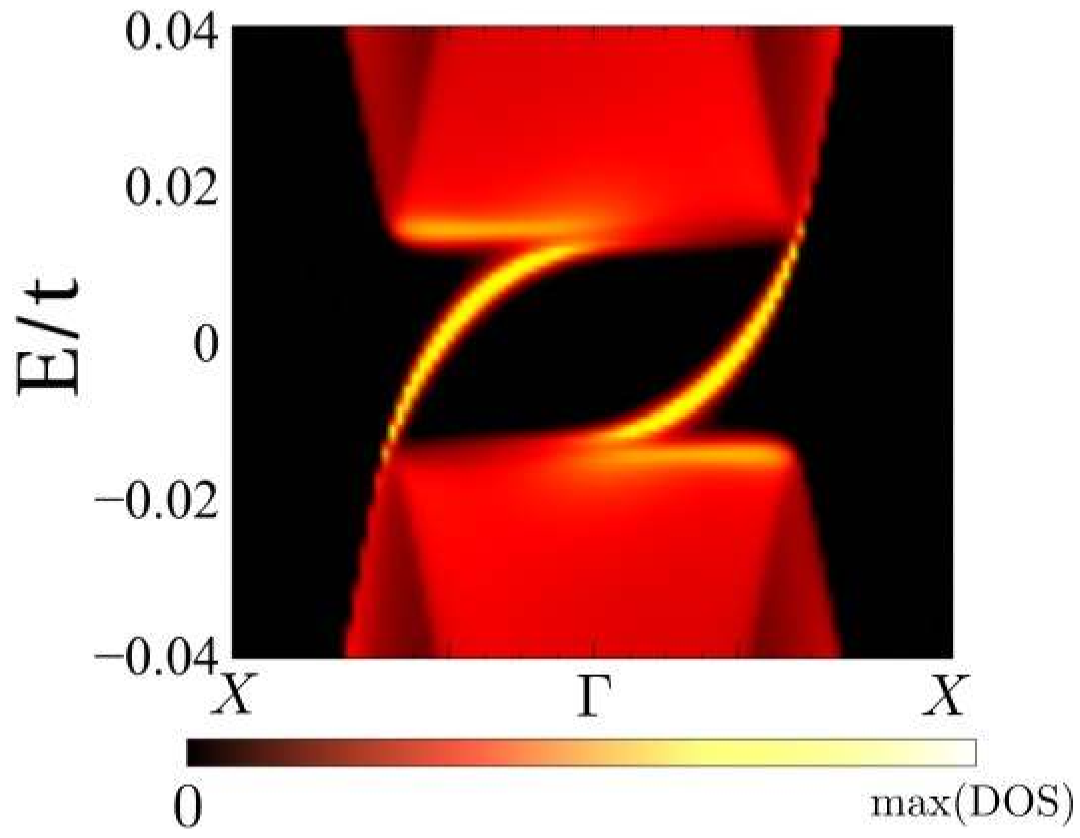
Graphene band structure



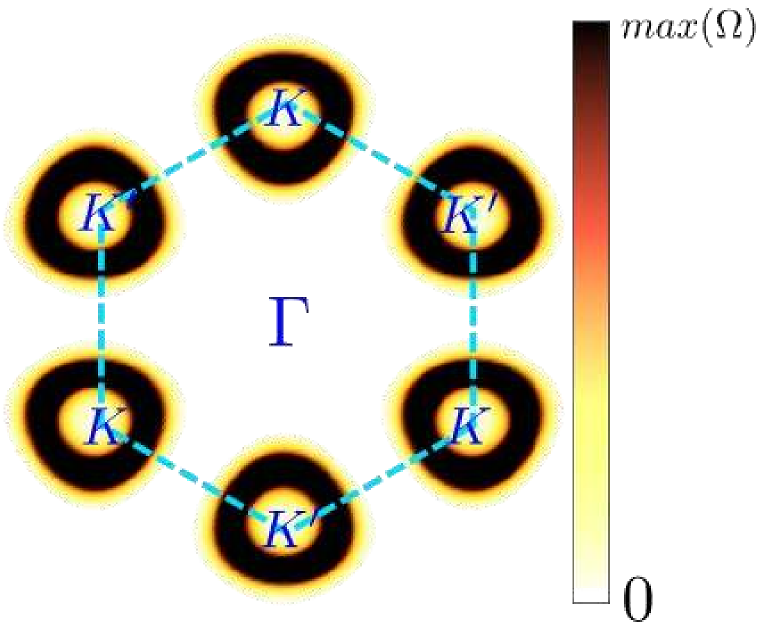
Gapped electronic spectrum

Bulk and edge correspondence

Surface spectral function



Berry curvature



Chern number

$$\mathcal{C} = 2$$

But why does graphene become a Chern insulator?

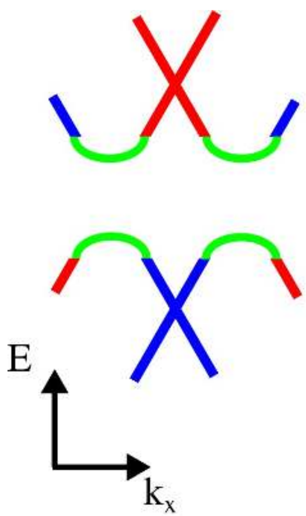
Chern number is zero for a coplanar spin texture $\vec{m} = m_x\sigma_x + m_z\sigma_z$

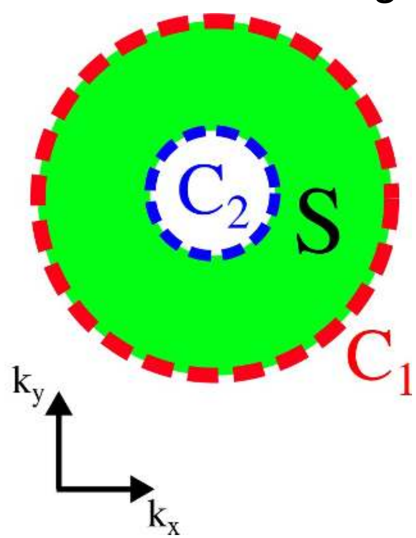
$$\mathcal{H} = \mathcal{H}^* \Longrightarrow \Omega(\vec{k}) = -\Omega(-\vec{k}) \rightarrow \mathcal{C} = 0$$

Conjugation symmetry

Non coplanar magnetism with net exchange

Stokes theorem in the anticrossing





$$\mathcal{C} = \frac{1}{\pi}\left[\oint_{C_1} \vec{A}\cdot d\vec{k} + \oint_{C_2} \vec{A}\cdot d\vec{k}\right]$$

$$\oint \vec{A}\cdot d\vec{k} = \pm\pi$$ Dirac point

$$\mathcal{C} = 0, \pm 2$$

Topological imprinting

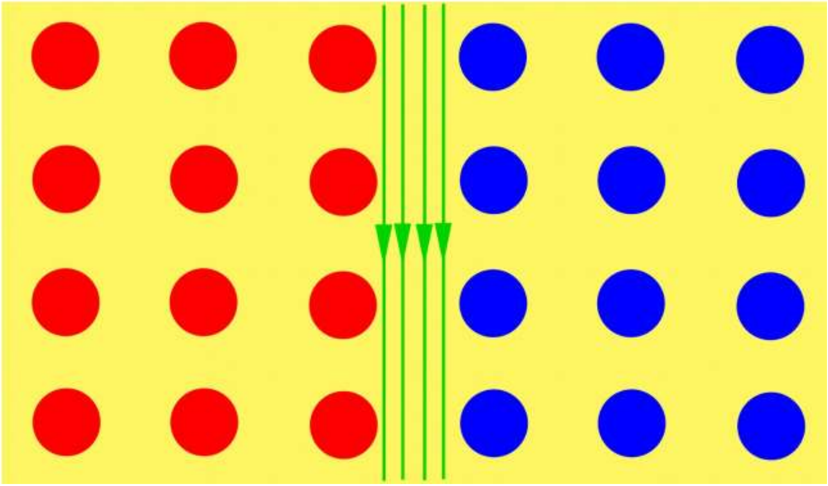
The topology of the skyrmion texture is imprinted in graphene electrons

$$\mathcal{C} = 2C_{Sky}$$

Chern number of graphene electrons

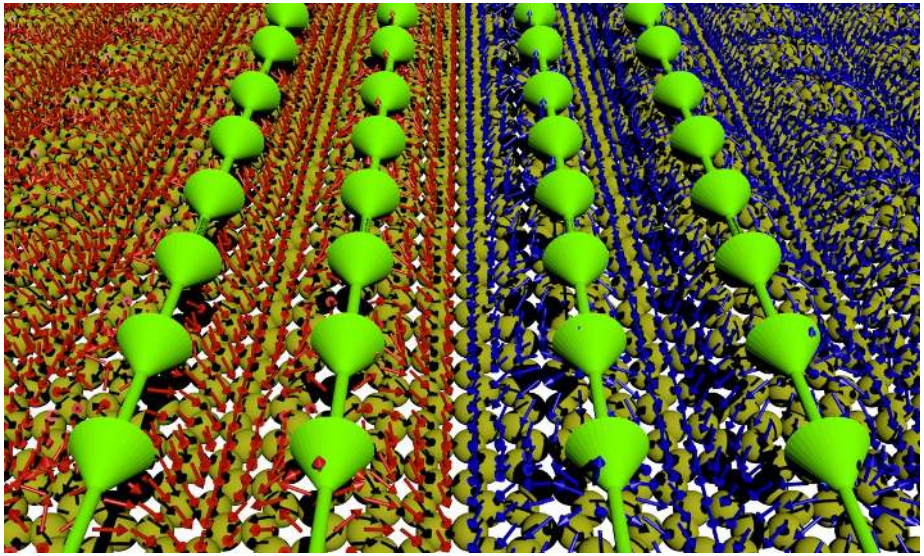
Winding number of the Skyrmion

$C_{Sky} = +1$ $C_{Sky} = -1$

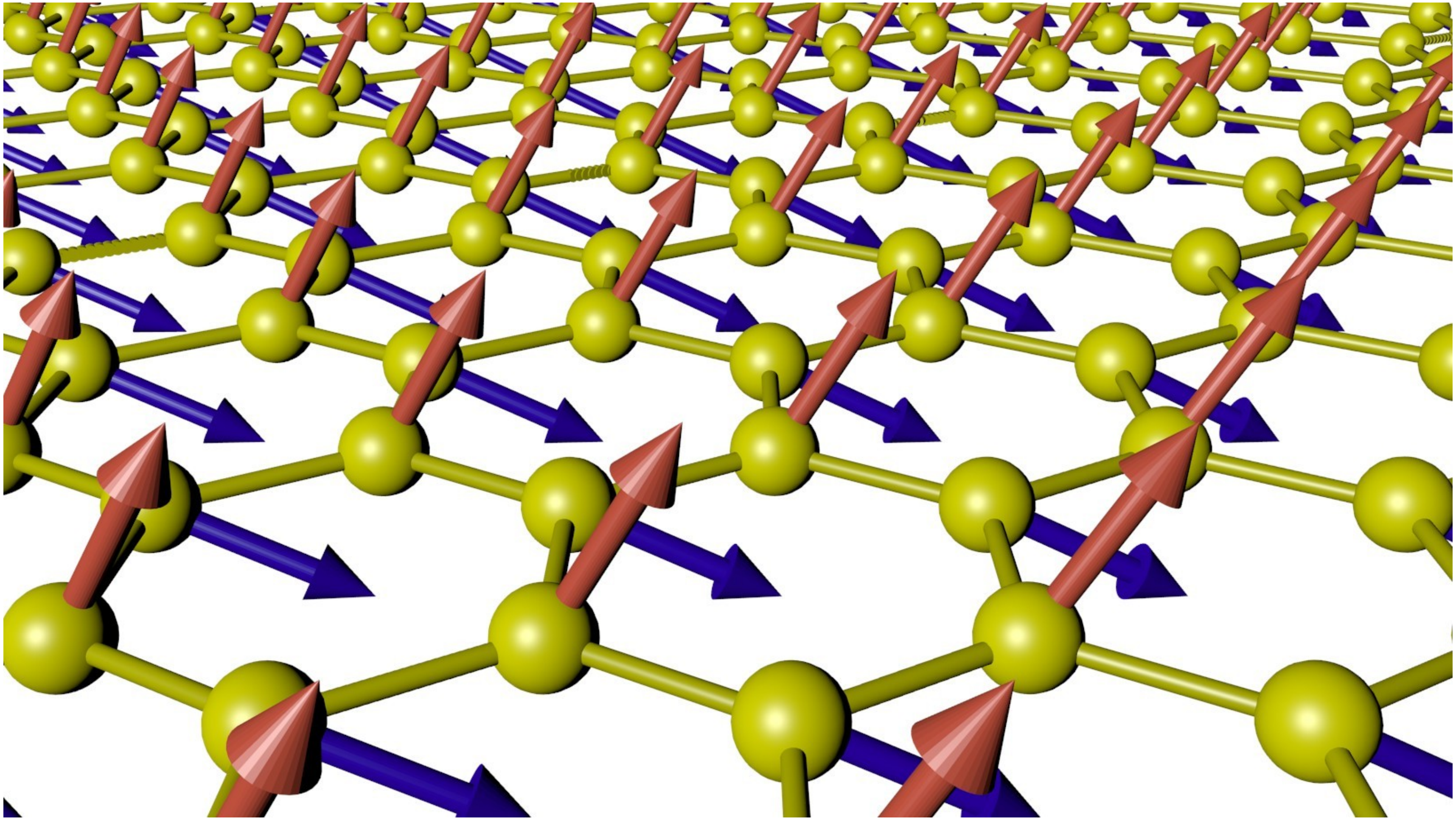


$\mathcal{C} = +2$ $\mathcal{C} = -2$

Four interface states

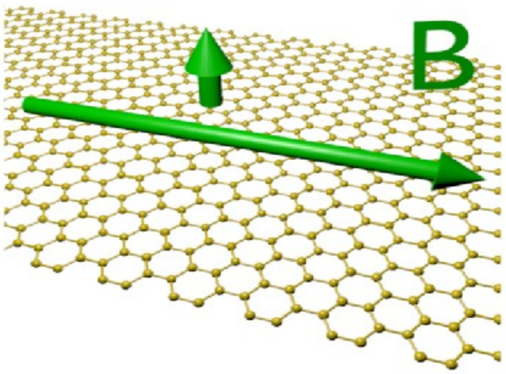


Ferromagnetism, antiferromagnetism and canted magnetism in graphene

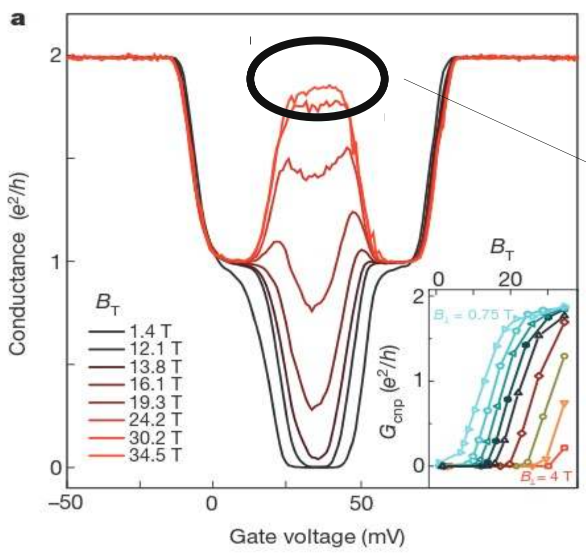


Quantum Hall graphene

Graphene in tilted magnetic field

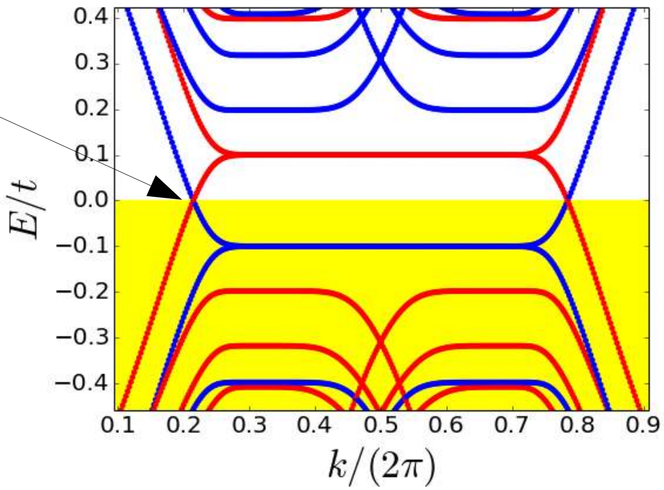


Tranisition with in-plane field



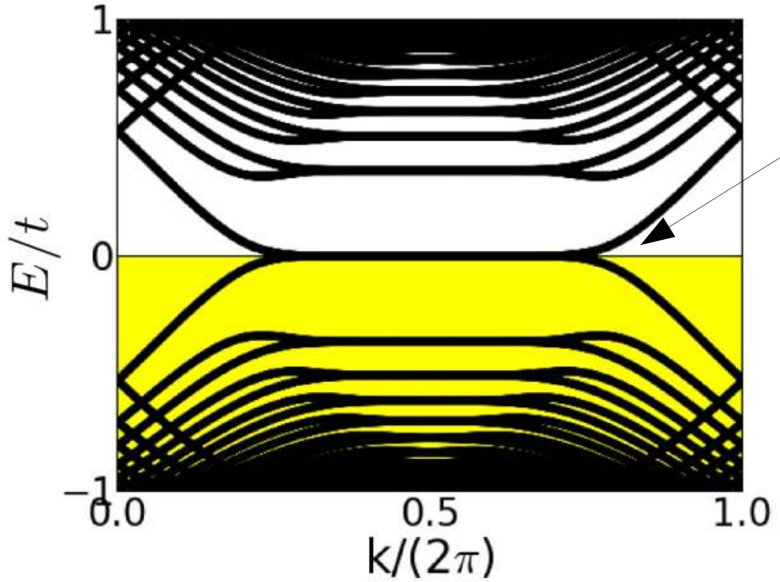
Nature 505, 528–532 (2014)

Ferromagnetic Hall state



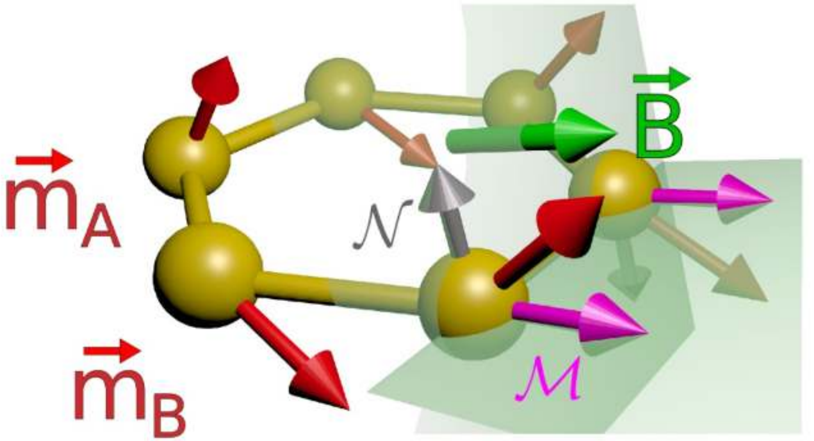
What is the origin of the phase transition with magnetic field?

Quantum Hall graphene



Large density of states
Electronic instability

Order parameters $\mathcal{N}, \mathcal{M}$



Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j \rangle} t(B_z) c_j^\dagger c_i + \sum_i \vec{B} \cdot \vec{\sigma}_{s,s'} c_{i,s'}^\dagger c_{i,s} + U c_{i,s}^\dagger c_{i,s} c_{i,s'}^\dagger c_{i,s'}$$

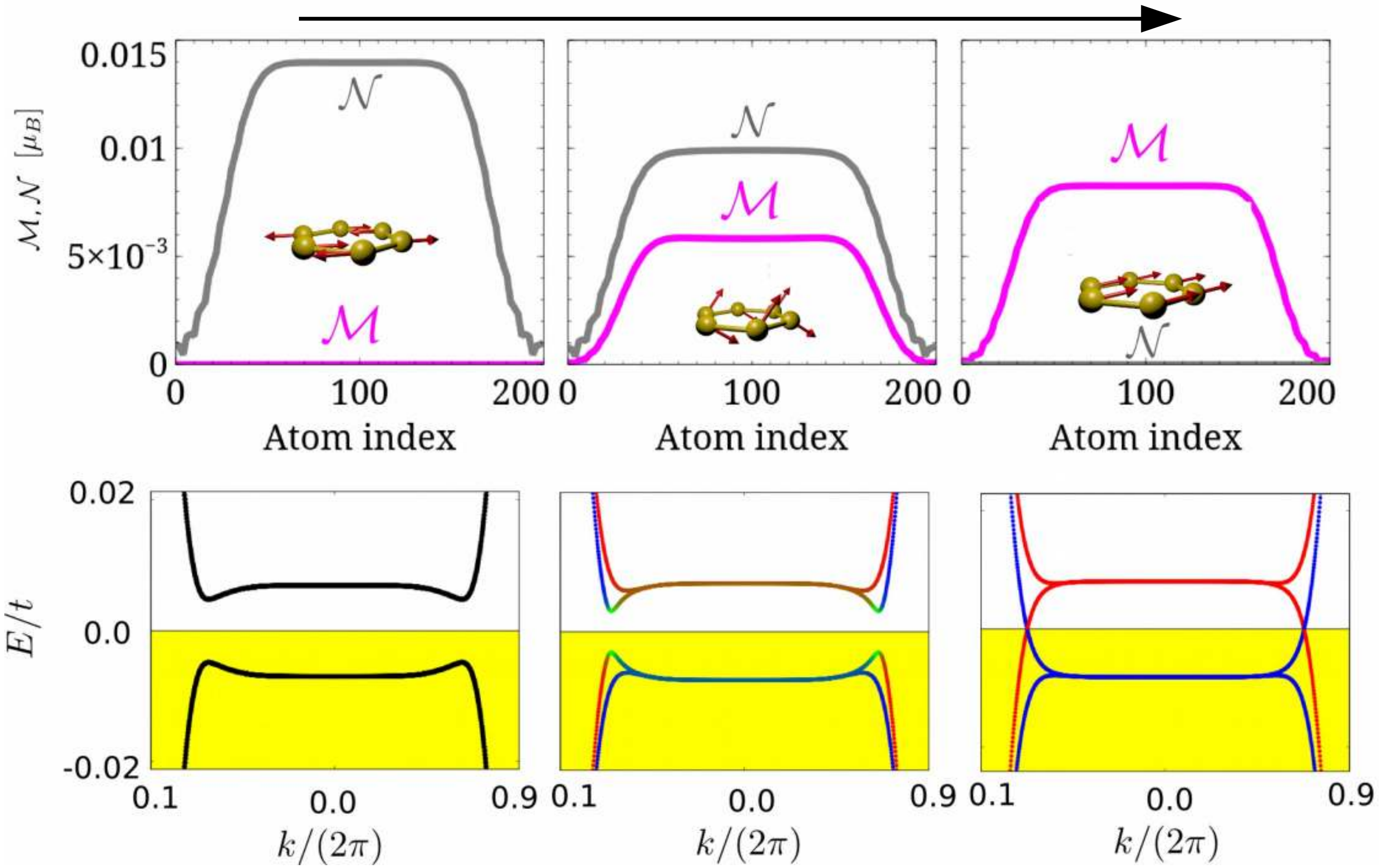
Kinetic energy + gauge field,
off-plane magnetic field

Zeeman term,
in-plane magnetic field

Hubbard interaction,
solved with mean field

Quantum Hall transition in graphene

Increasing in-plane magnetic field



Antiferromagnet

Canted antiferromagnet

Ferromagnet

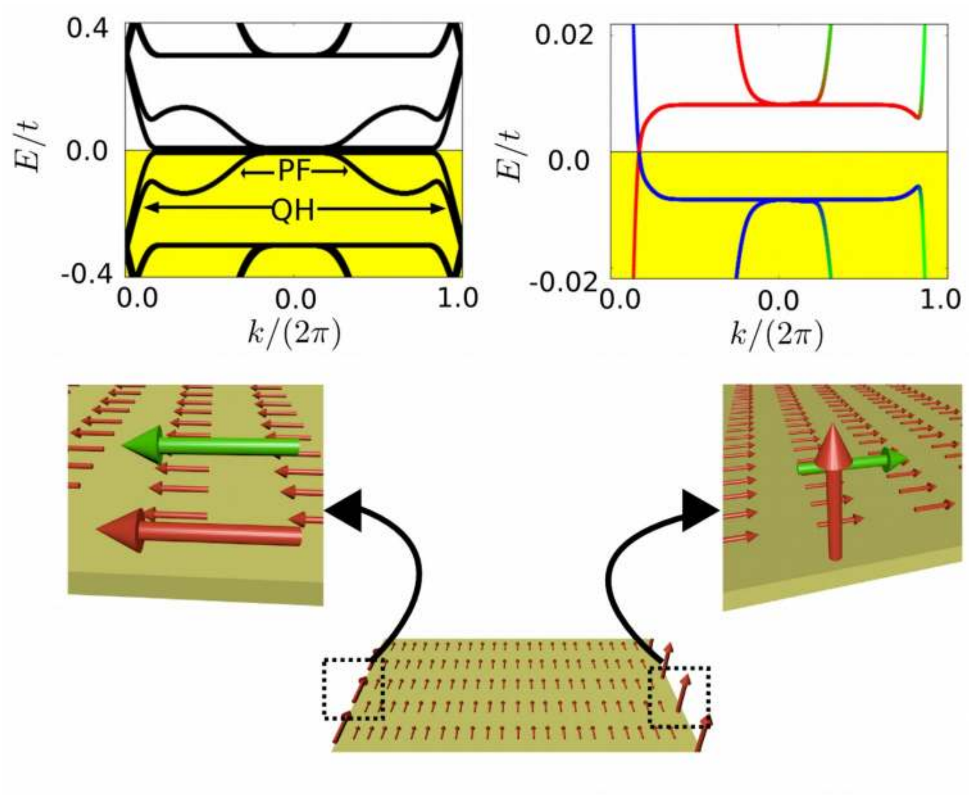
Insulator

Insulator

Helical metal

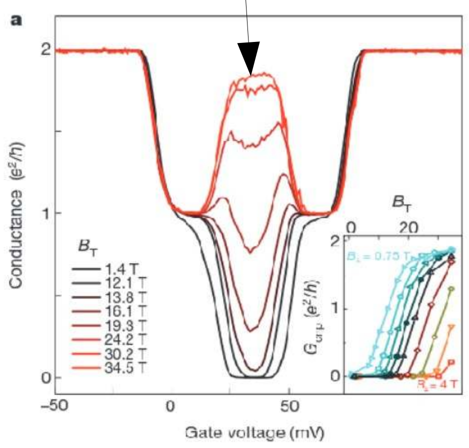
Interaction between localized moments and helical states

Spin fluctuations in localized moments gap-out helical states



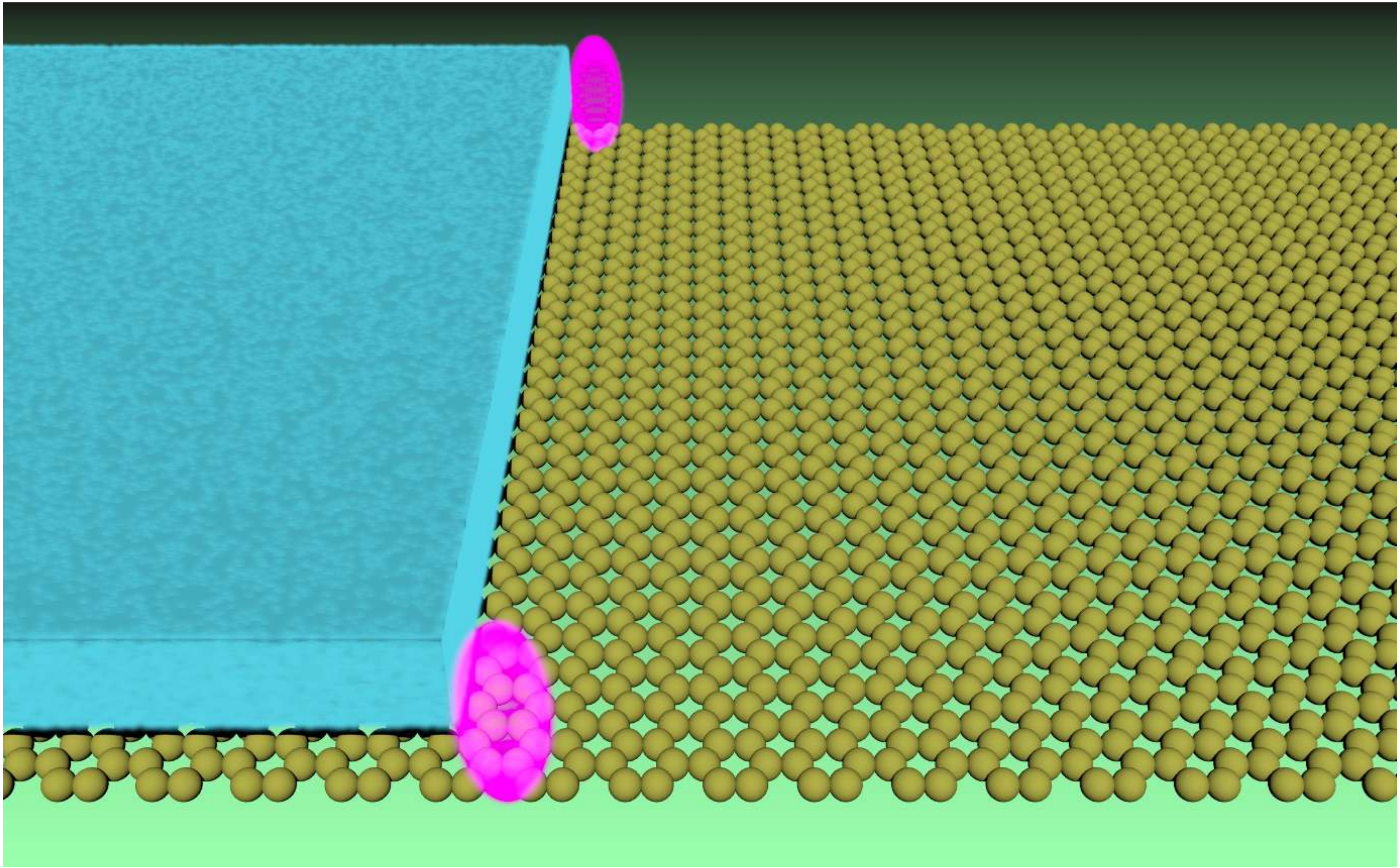
Possible origin of not perfect quantization

Nature 505, 528–532 (2014)



Coupling of a helical metal with localized moments

Topological superconductivity in graphene



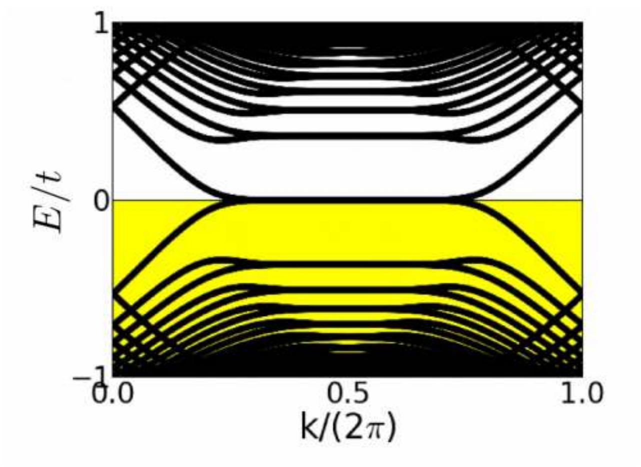
Topological superconductivity in graphene: the recipe

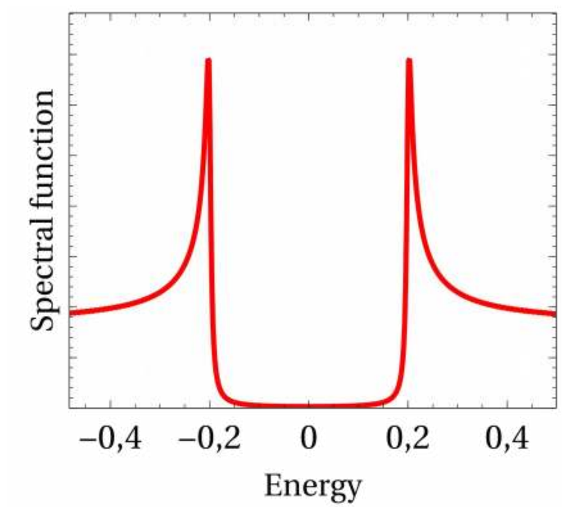
Kinetic energy and magnetic gauge field

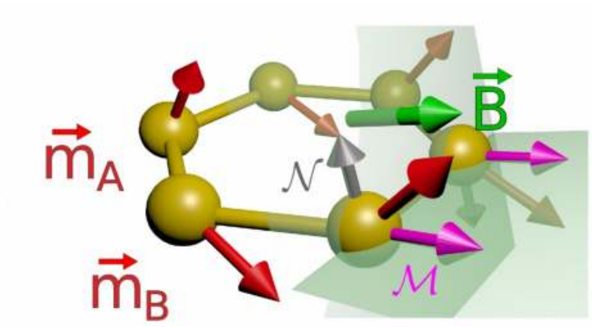
Superconducting pairing

Interaction driven and Zeeman

$$\mathcal{H} = t_{ij}(B_z)c_j^\dagger c_i + \Delta[c_{i,s}^\dagger c_{i,s'}^\dagger + c_{i,s'}c_{i,s}] + J\vec{m}_i \cdot \vec{\sigma}_{s,s'}c_{i,s}^\dagger c_{i,s'}$$





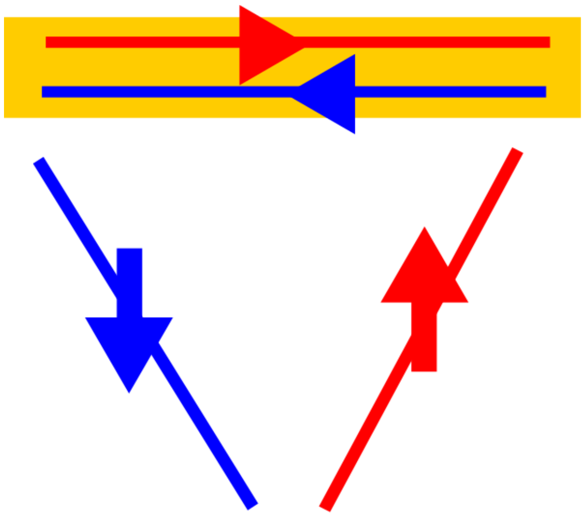


Are these three ingredients enough to create topological superconductivity?

How to create Majorana bound states in graphene

<u>Goal</u>: Engineer a Kitaev chain $H = \sum_n t c^\dagger_{n+1} c_n + \Delta c_n c_{n+1} + c.c.$

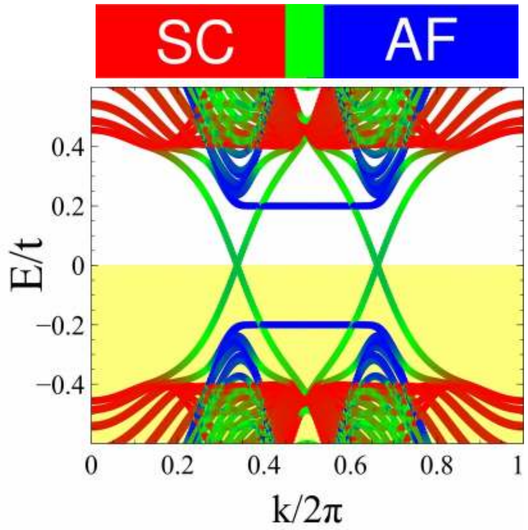
Helical states +
s-wave superconductivity



Relies on the Landau level
structure of graphene

<u>Ferromagnetic</u>
<u>Quantum Hall state</u>

Solitonic superconducting states +
breaking of conjugation and rotation symmetry

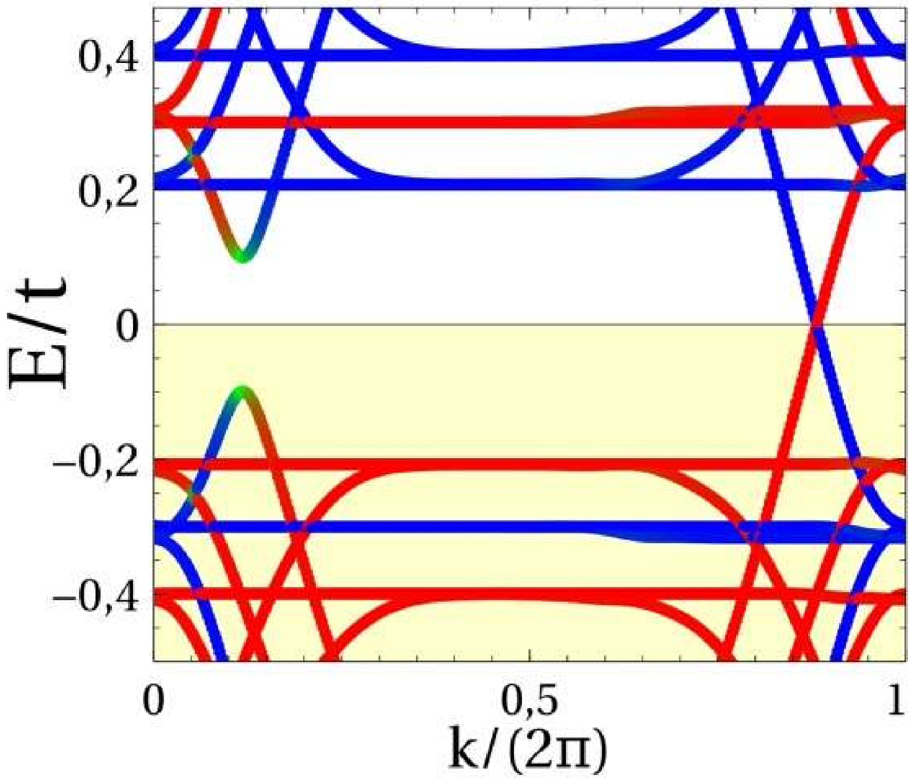


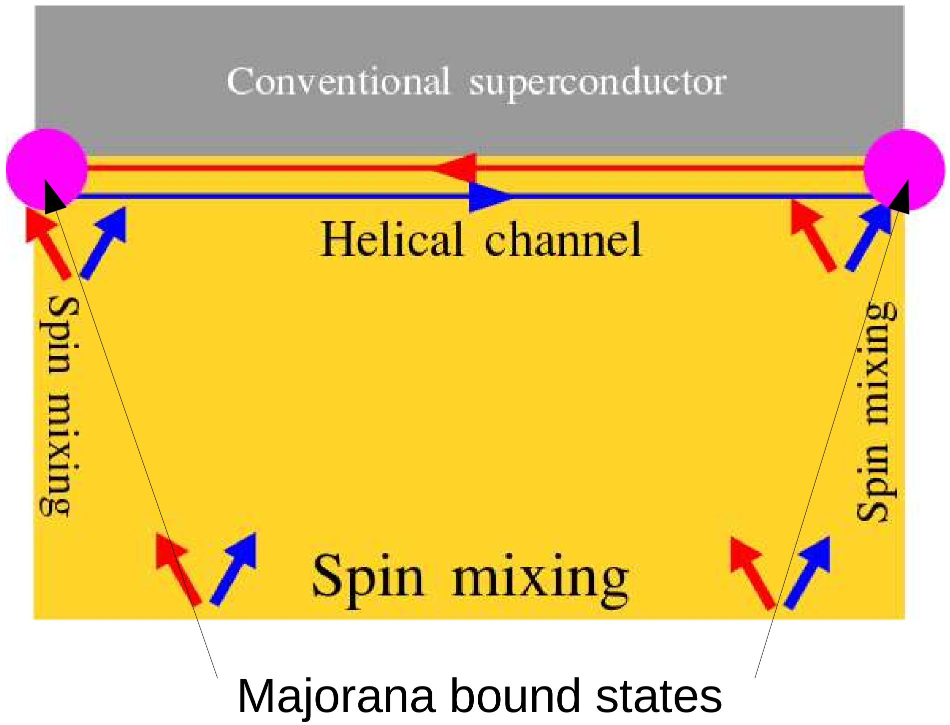
Relies on valley states
originated by valley Chern numbers

<u>Antierromagnetic</u>
<u>Quantum Hall state</u>

None of them require spin orbit coupling

Majoranas in ferromagnet Hall graphene



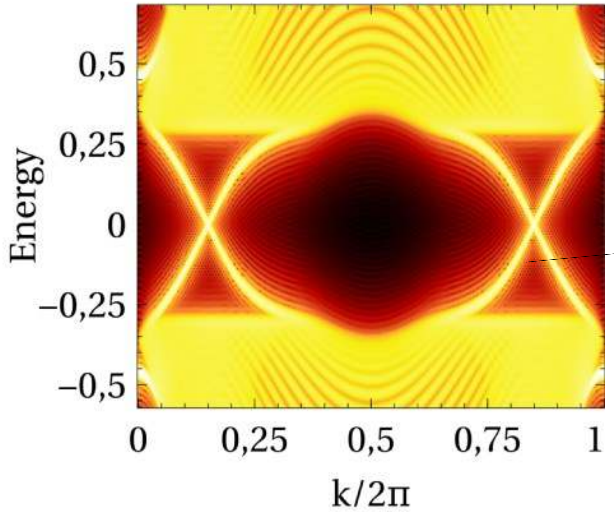


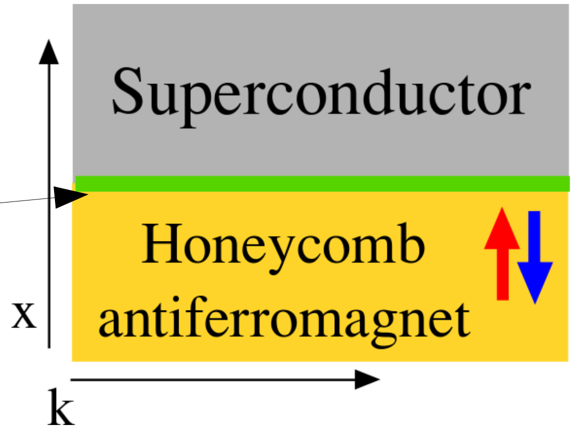
Analogous to interface between Z_2 insulator and superconductor

Interface between superconductor and honeycomb antiferromagnet

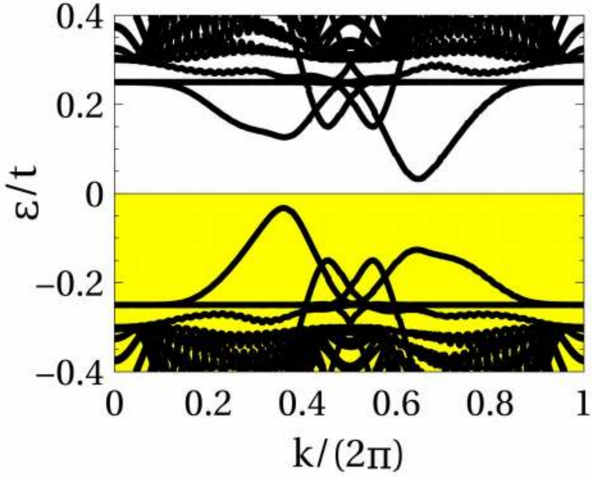
Solitonic solution in the interface superconductor-antiferromagnet

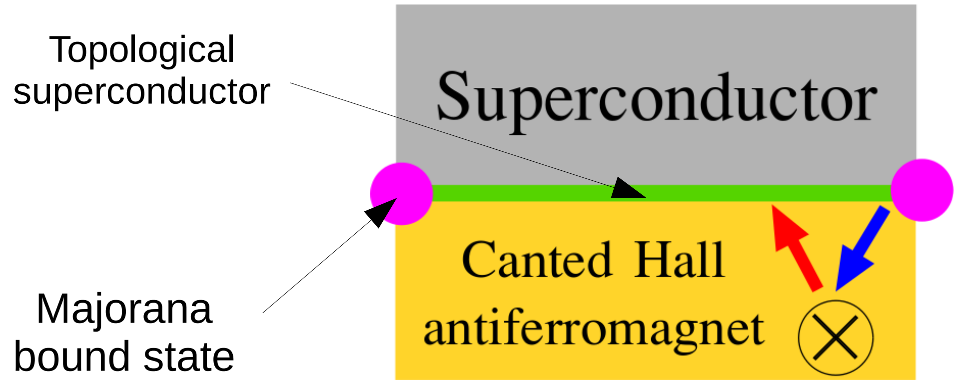
$$H = \gamma_1 m(x) + \gamma_2 p + \gamma_3 \Delta_{SC}(x) \qquad \phi(x) = N e^{-\int_0^x [m(x') - \Delta_{SC}(x')] dx'} \phi_0$$





Topological superconductor in the canted Hall antiferromagnet

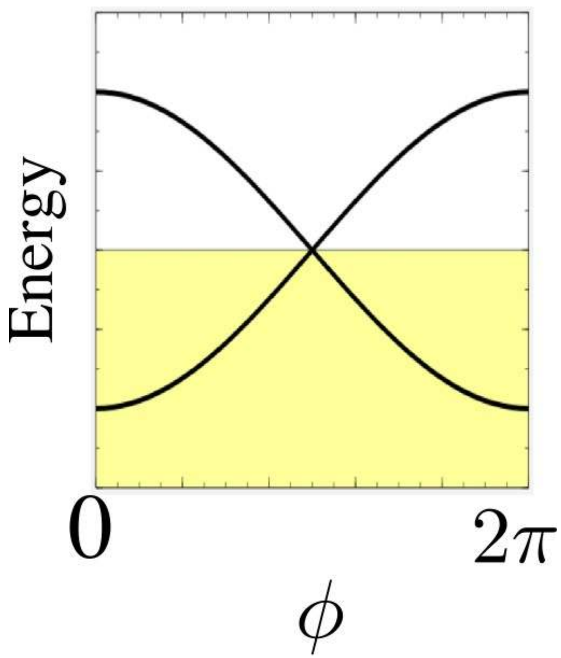




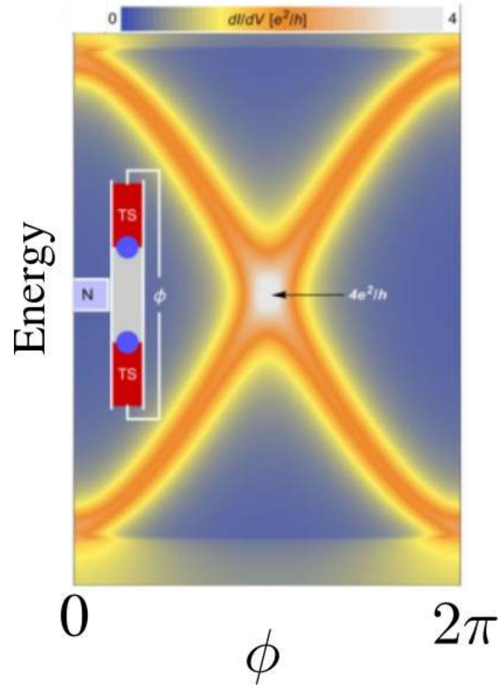
Experimental signatures of Majorana states, Josephson effect

4π Josephson effect

Eigenvalue spectrum

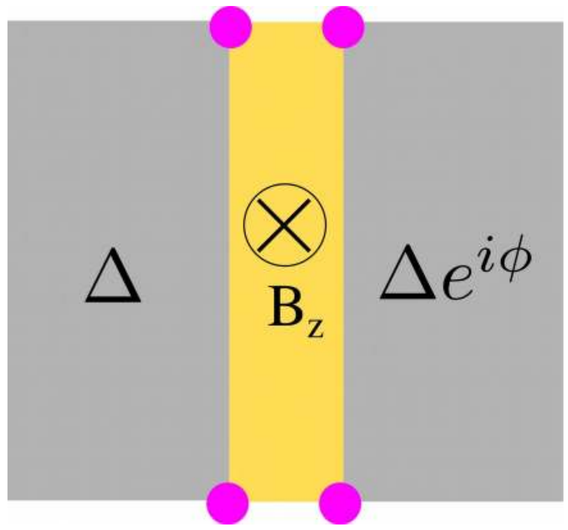


Transport signal

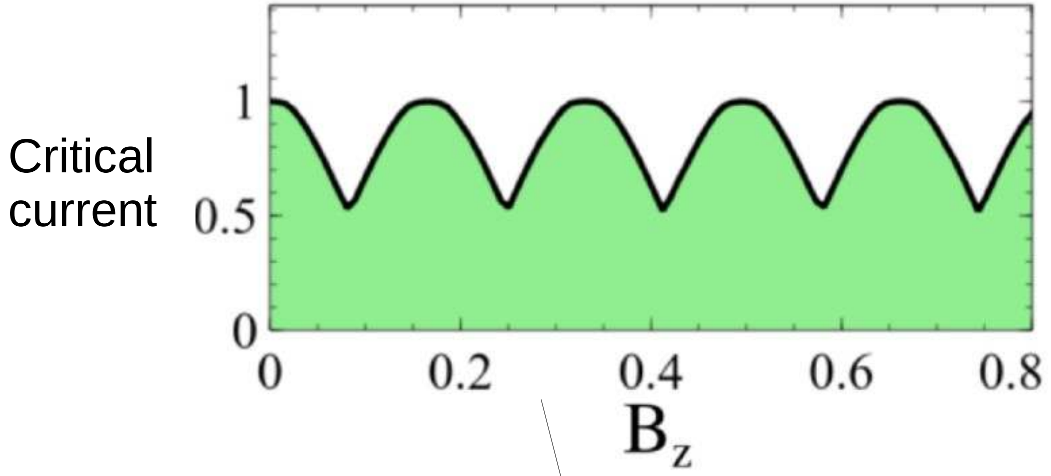


Experimental signatures of Majorana states, Fraunhofer

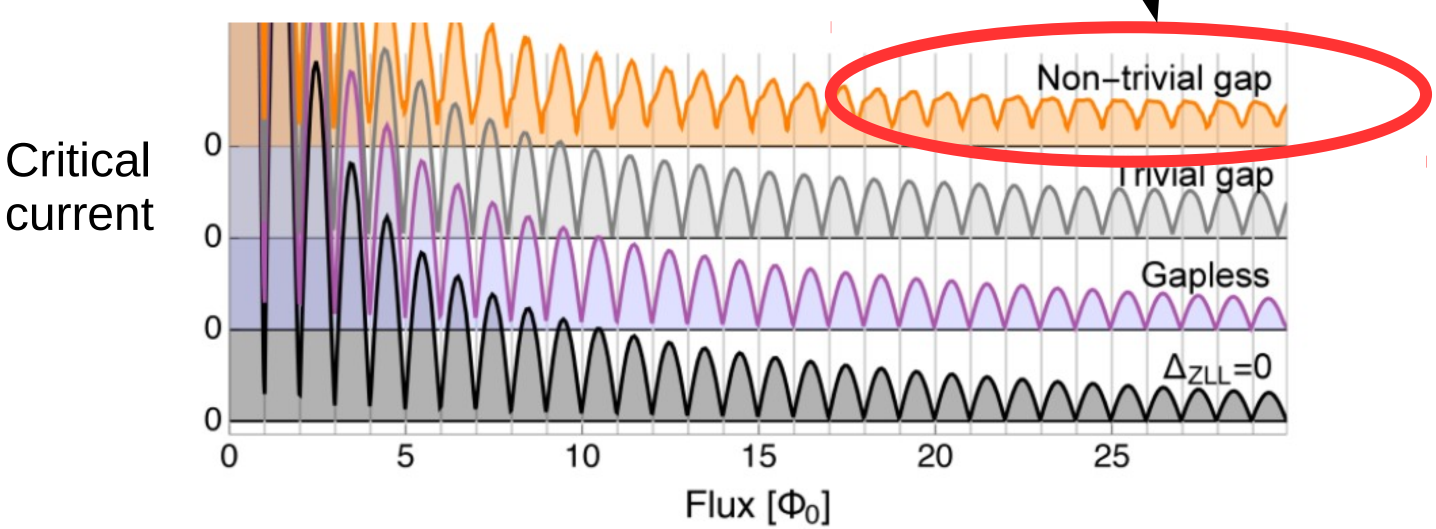
Fraunhofer geometry



Toy model with four Majoranas



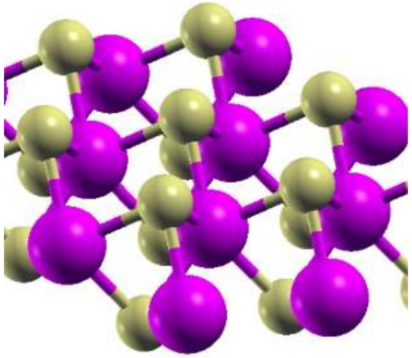
Graphene Majoranas setup

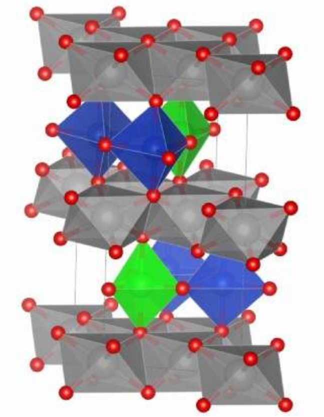


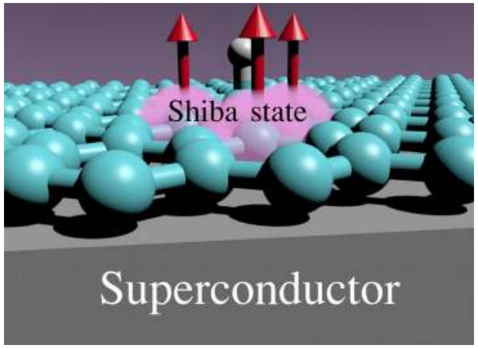
Summary

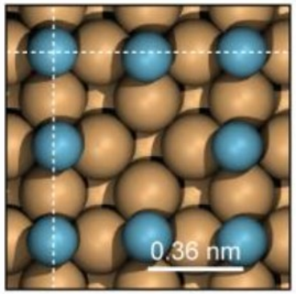
- **Quantum anomalous Hall effect in graphene**
  - **Skyrmions** imprint topology in graphene, Chern number is controled by skyrmion chirality
- **Quantum spin Hall effect in graphene**
  - Magnetic and topological states can be **tuned by in-plane magnetic field** in the quantum Hall regime
- **Topological superconductivity in graphene**
  - **Majorana bound states** appear at the interface of a superconductor and ferromagnetic or canted quantum Hall graphene

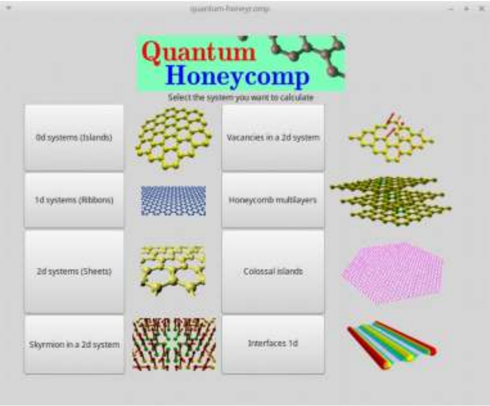
Epilogue: Short items









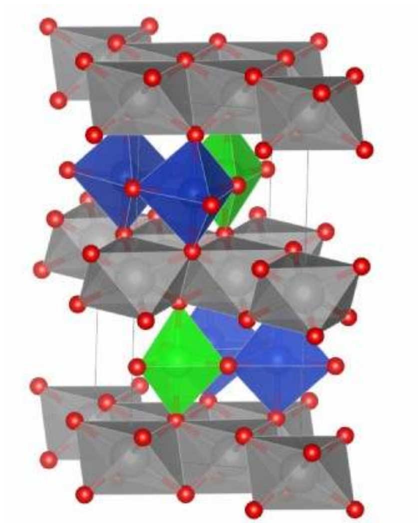


Quantum spin Hall in oxides

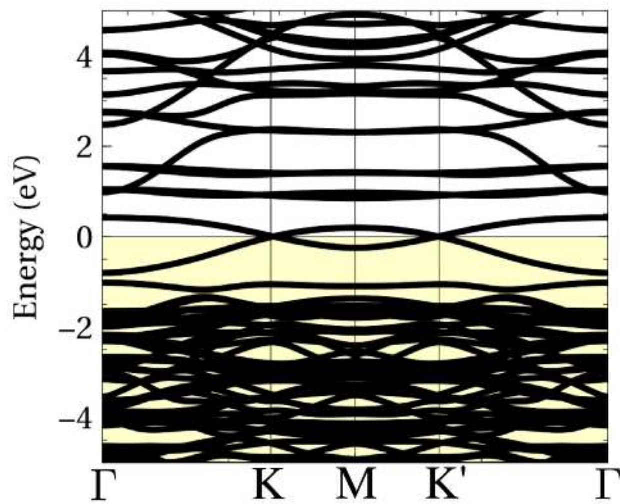
Dirac insulator in oxides

$$\mathrm{InZn}_{1/3}\mathrm{Ag}_{1/3}\mathrm{V}_{1/3}\mathrm{O}_3$$

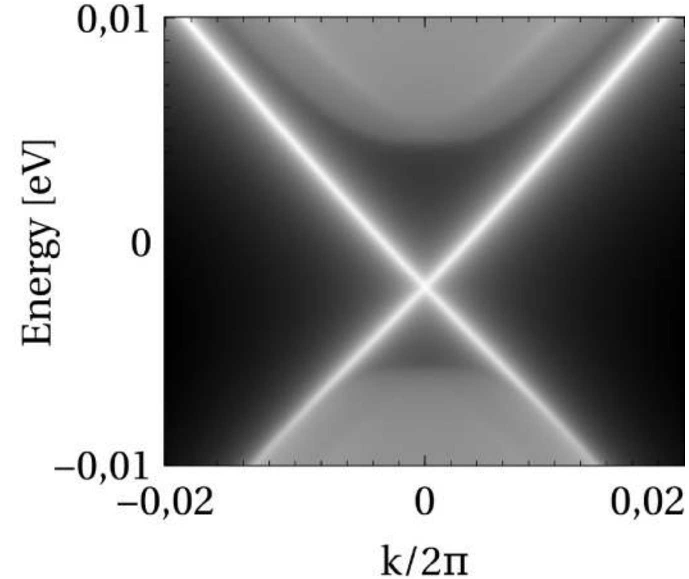
Crystal structure



Band structure



Surface spectral function



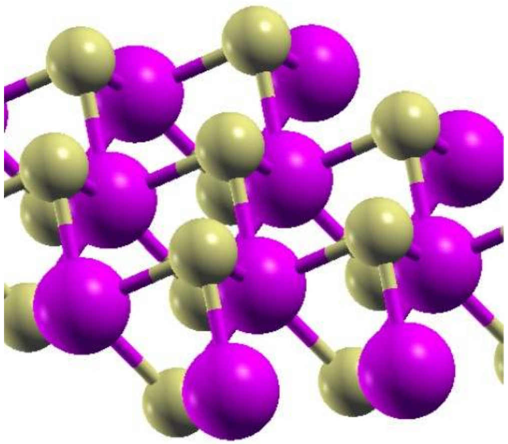
Dirac electrons in an oxide
Realization of the Kane-Mele model in the d_{z^2} manifold

J. L. Lado, V. Pardo, arXiv:1604.05554, (submitted) 2016

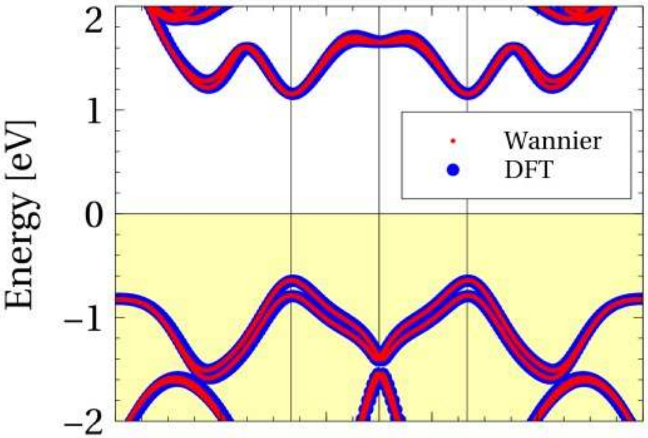
Landau levels in 2D materials

Quantum Hall effect starting from density functional theory

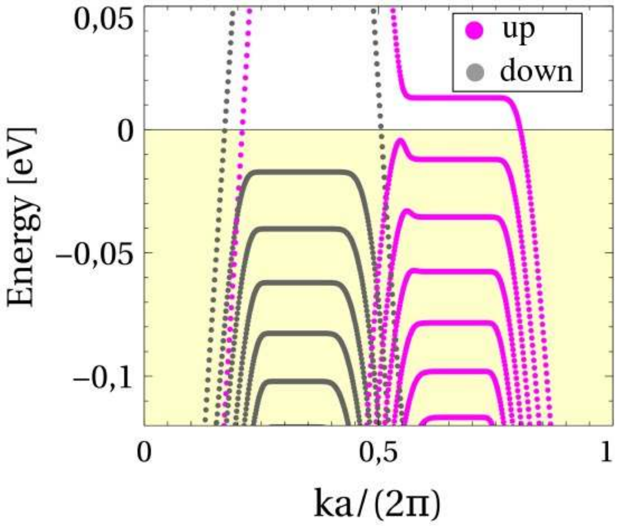
MoS_2 structure



Bulk band structure



Landau levels



Real space Hamiltonian

$$H_{2D} = \sum_{n,m} \sum_{i,j} t_{ij}^{\vec{n}-\vec{m}} c^{\dagger}_{\vec{m},j} c_{\vec{n},i}$$

Peierls coupling to gauge field

$$\hat{t}_{ij}^{N-M} \rightarrow \hat{t}_{ij}^{N-M} e^{i\phi_{ij}^{N,M}}$$

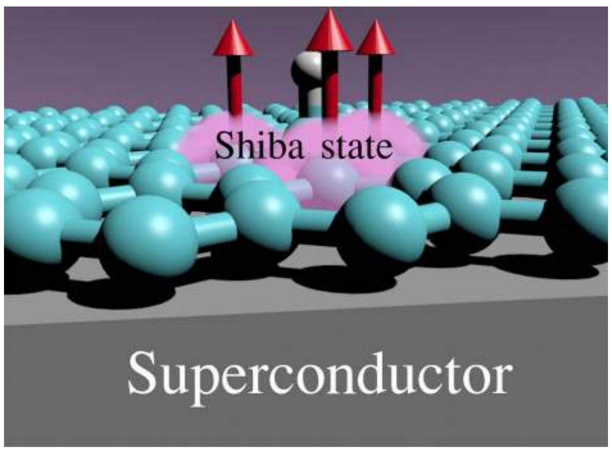
Wannier transformation

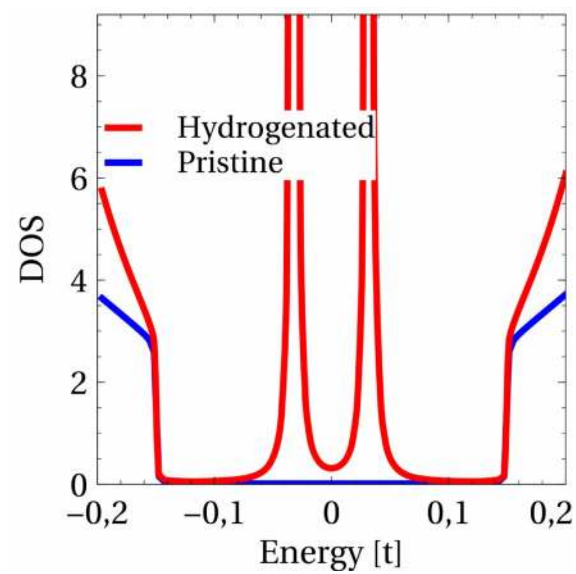
$$|\vec{n},\mu\rangle = \frac{1}{(2\pi)^2} \int e^{i\vec{n}\cdot\vec{k}} U(\vec{k})_{\mu,\nu} |\vec{k},\nu\rangle d^2k$$

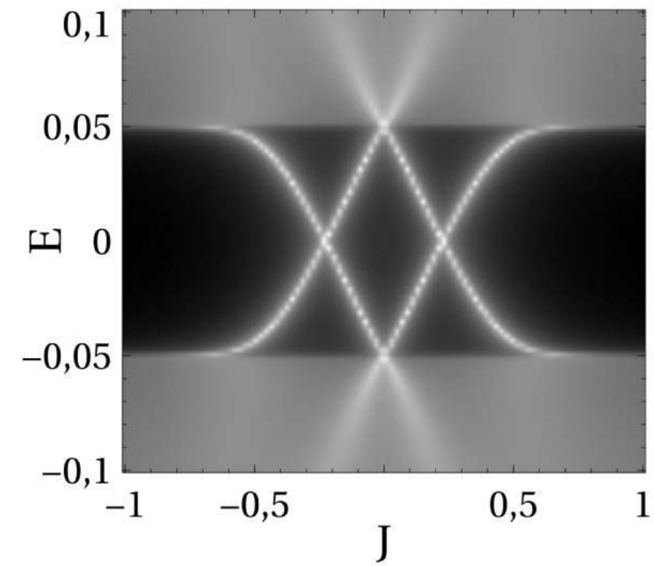
J. L. Lado, J. Fernandez-Rossier, arXiv:1606.03038, submitted (2016)

Yu-Shiba-Rusinov states in graphene

Single hydrogenation creates Shiba states in graphene







Conventional Shiba theory breaks down

YSR energy

Superconducting pairing

$$E_S = \Delta \frac{1 - (\pi \frac{S}{2} J \rho)^2}{1 + (\pi \frac{S}{2} J \rho)^2}$$

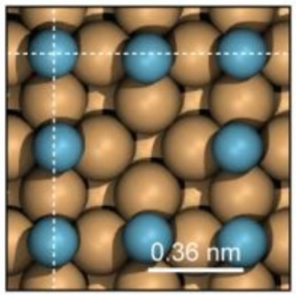
Exchange coupling

DOS (zero in graphene)

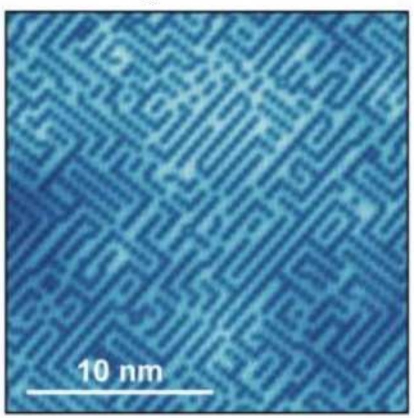
J. L. Lado, J. Fernández-Rossier, 2D Materials 3 (2), 025001 (2016)

An atomic scale rewritable memory

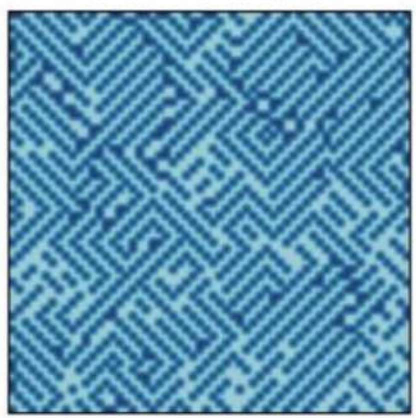
Vacancies in Cl on Cu (001)



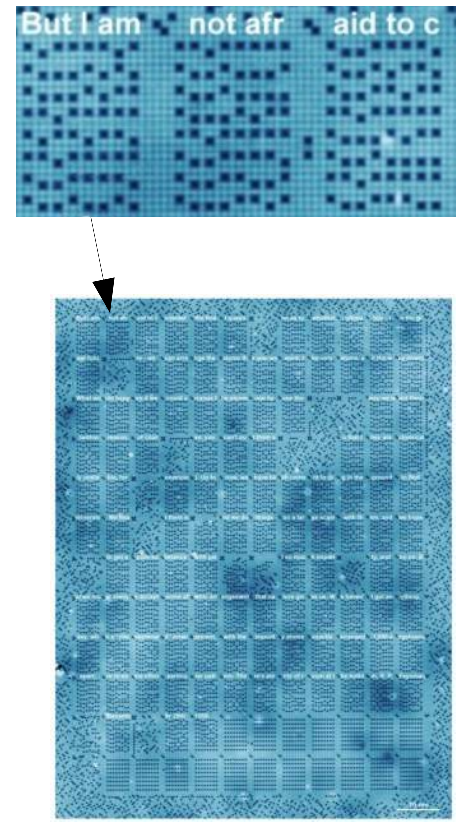
Experiment



Density functional theory
and Montecarlo

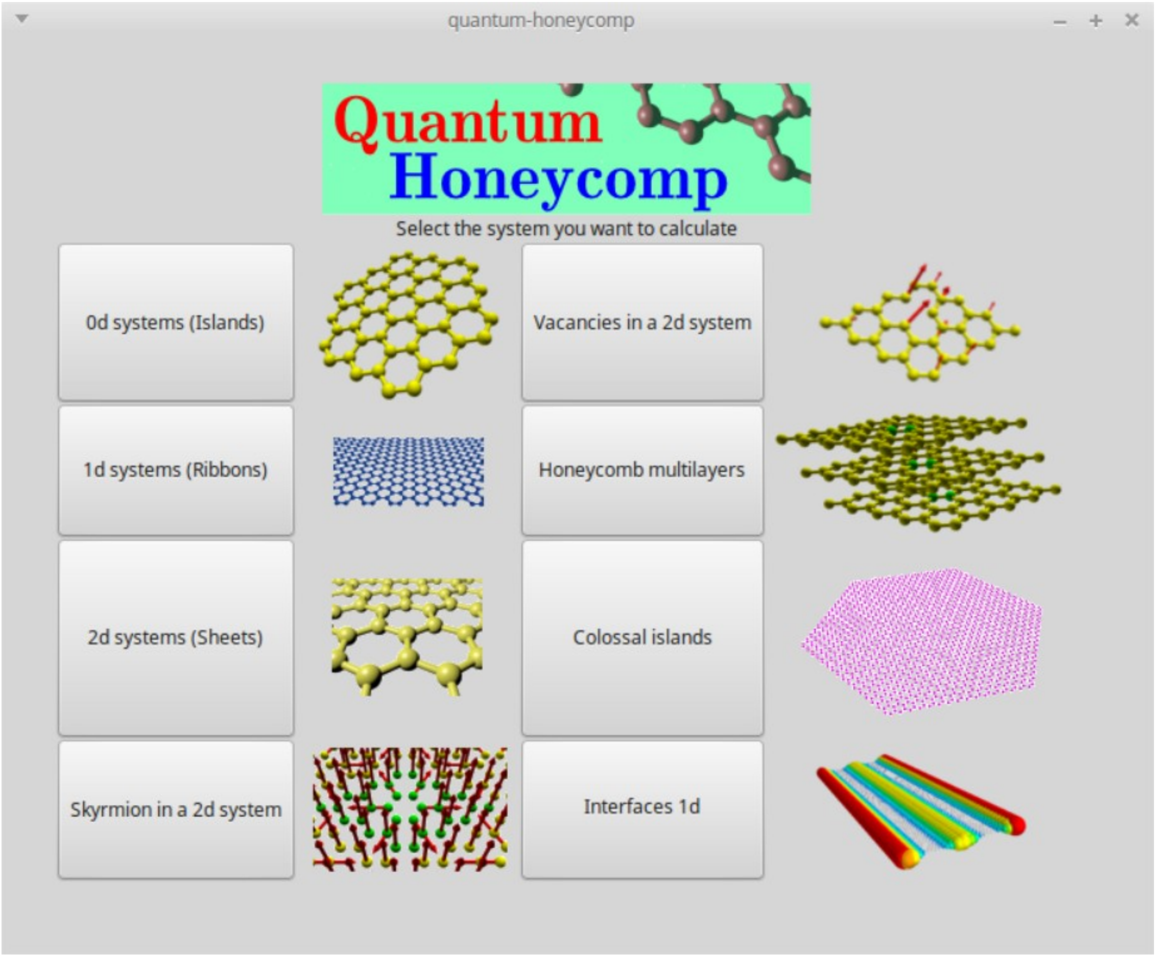


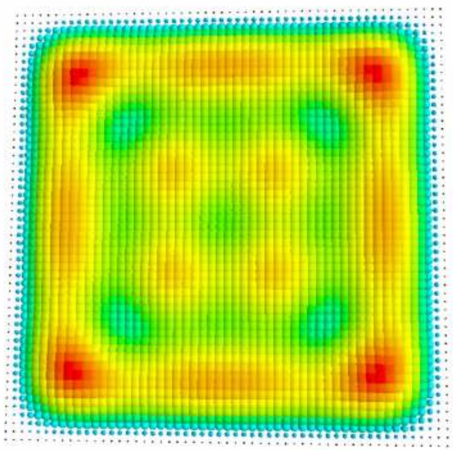
Recording using vacancy manipulation
(AF Otte group, Delft, Netherlands)

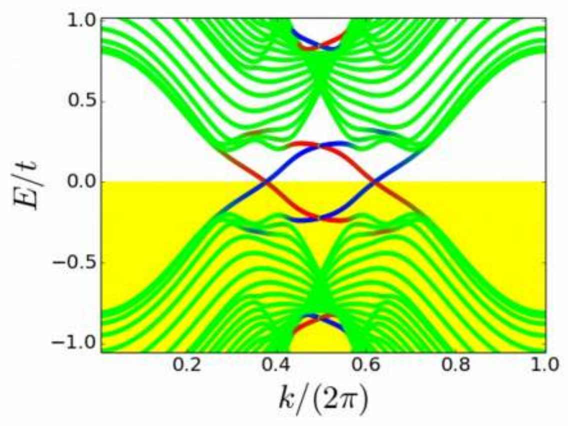


FE Kalff, MP Rebergen, E Fahrenfort, J Girovsky,
R Toskovic, JL Lado, J Fernández-Rossier, AF Otte
Nature Nanotechnology (2016)

Quantum Honeycomp



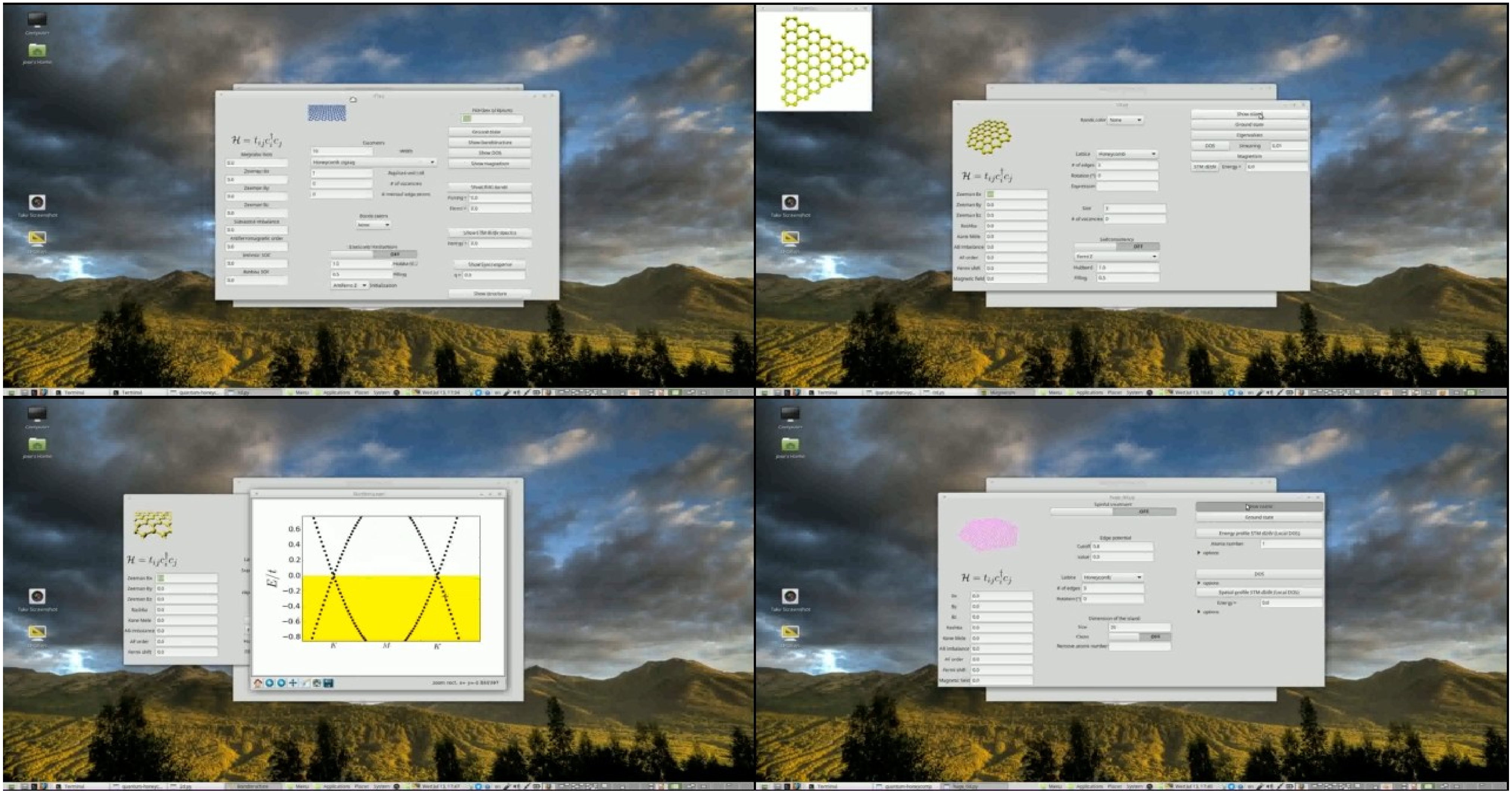




Open source and user friendly interactive program

https://sourceforge.net/projects/quantum-honeycomp/

Quantum Honeycomp



Acknowledgements

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Spinograph

Spintronics in Graphene

Thank you!