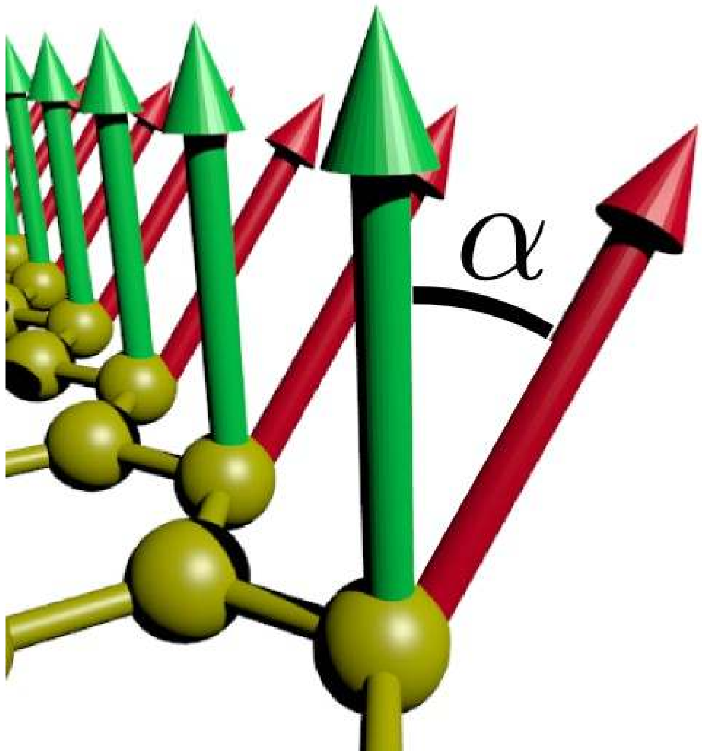
Magnetic edge anisotropy in graphene-like honeycomb crystals

J. L. Lado and J. Fernandez-Rossier



First Spinograph school, 27th March, Braga 2014

Motivation

- Zigzag edges host magnetic states

  (O. Yazyev yesterday)

- Spin-orbit coupling in honeycomb lattices creates gapless chiral edge states

  (Allan McDonald yesterday)

What is the interplay between spin-orbit physics and magnetism in graphene-like system?

We will focus in zigzag ribbons (1D translational invariance)

Spin-orbit in honeycombs

Why spin-orbit coupling in honeycomb systems is very appealing?

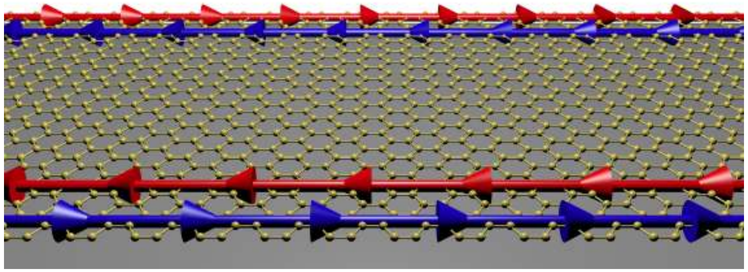
→ Simplest realization of the Quantum Spin Hall effect

Bulk gap (insulating)
Spin polarized counterpropagating edge channels (metallic)

Why graphene is not enough?

→ Effective coupling too low (0.1 ueV)

Don't worry, there are a bunch of materials :)



Material	t_{SO}	t
Graphene	0.1 μeV	2.7 eV
Silicene	0.16 meV	1.5 eV
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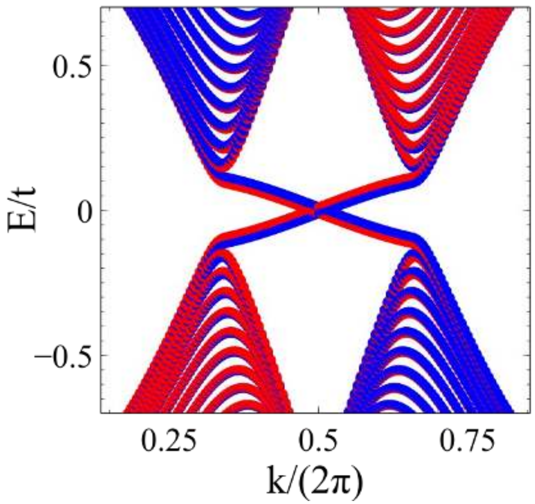
Double perovskyte	1 meV	0.1 eV

Spin-orbit in honeycombs

The tight binding model

Haldane model

→ Real hopping to first neighbors
→ Imaginary hopping to second neighbors
→ Breaks time-reversal symmetry
→ Chern number = 1
→ Topologycally protected edge channel



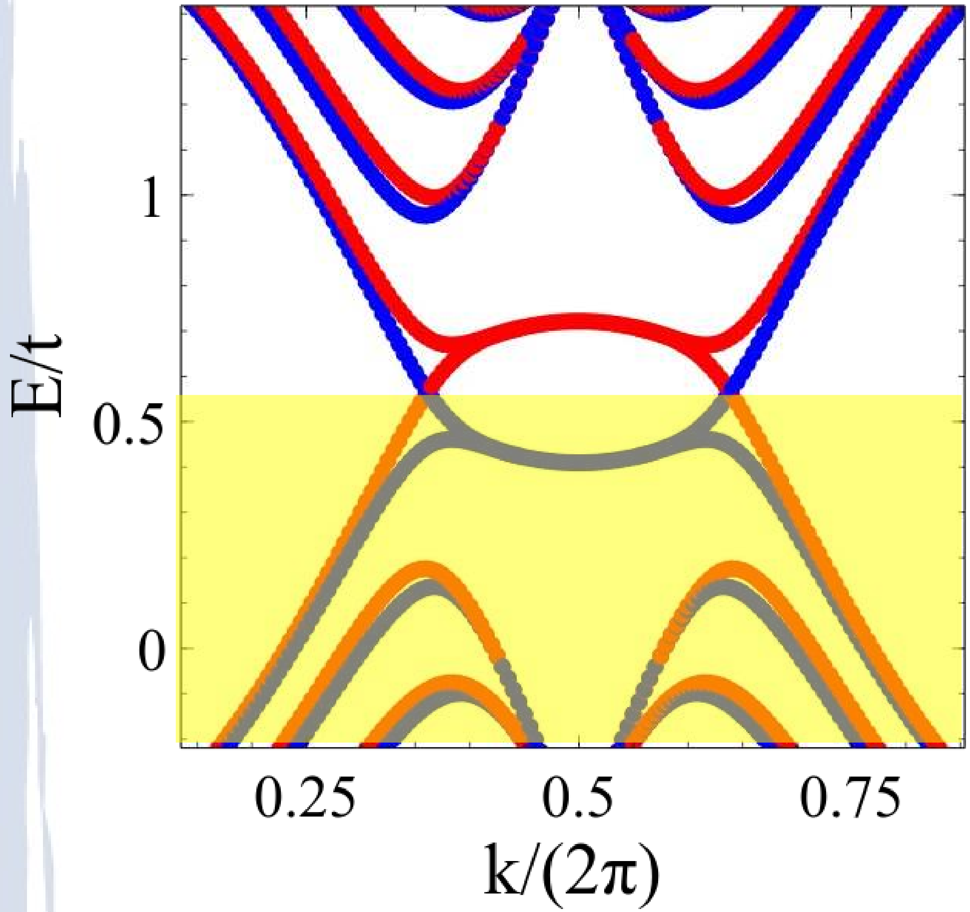
Kane-Mele model

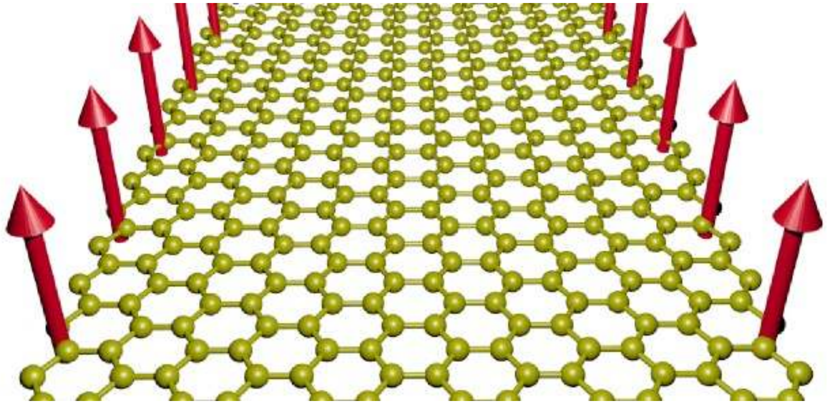
→ Two spin-depndent copies of the Haldane model
→ Preserves time reversal (TR)
→ Spin Chern number = 2
→ Edge channel protected against TR perturbations
→ Breaking of TR removes the protection

$$H = \sum_{\langle ij \rangle,\sigma} t c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{\langle\langle ij \rangle\rangle,\sigma} i t_{SO} \sigma \nu_{ij} c^{\dagger}_{i\sigma} c_{j\sigma}$$

Magnetism in zig-zag ribbons

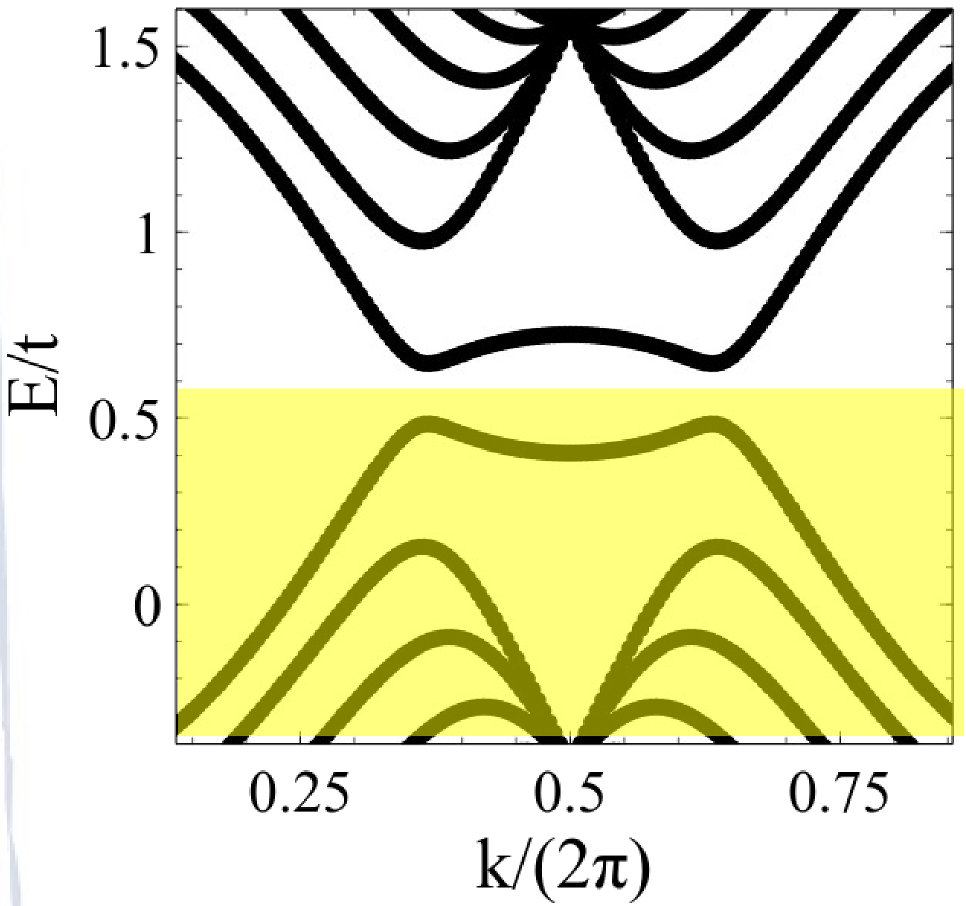
Ferro (metallic)

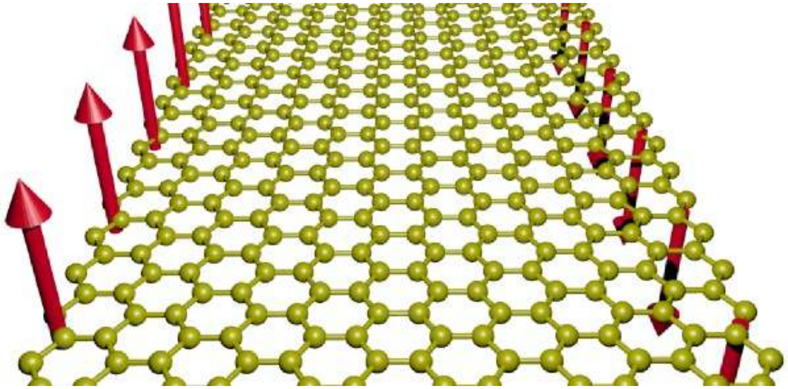




Magnetism in zig-zag ribbons

Antiferro (insulating)



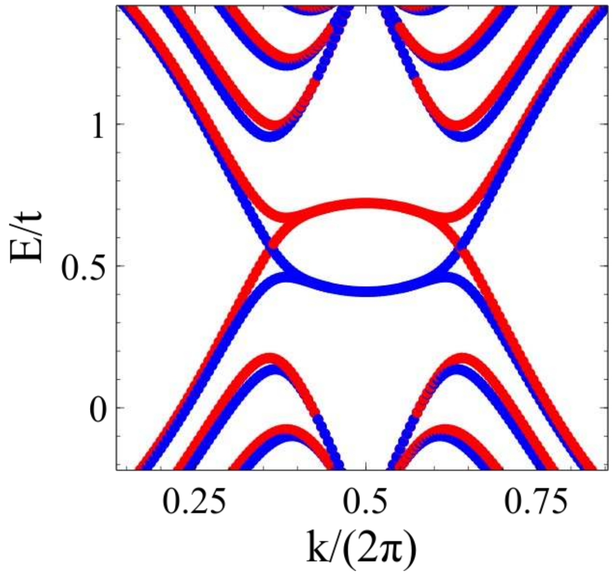


Metallic zig-zag ribbons

Two ways of getting a metallic zigzag ribbon

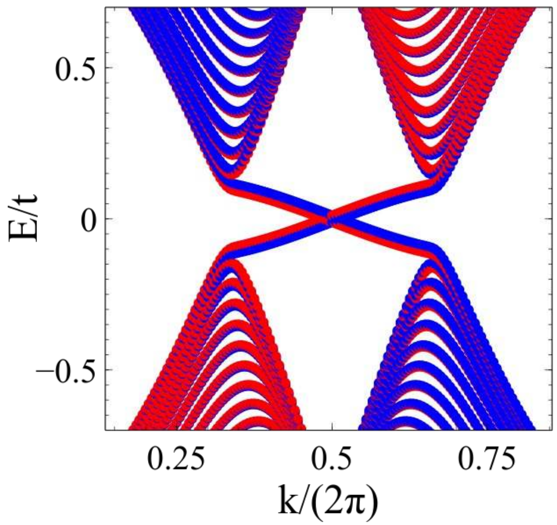
Ferromagnetic edge configuration

(Interaction at mean field level)



Quantum Spin effect edge channels

(Non interacting, triggered by spin-orbit)



What if both are present?

Magnetism and SOC in zig-zag ribbons

Calculated using a Hubbard model (local Coulomb interaction)
solved in a mean field **collineal** approximation

$$H = \sum_{\langle ij \rangle, \sigma} t c^\dagger_{i\sigma} c_{j\sigma} + \sum_{\langle\langle ij \rangle\rangle, \sigma} i t_{SO} \sigma \nu_{ij} c^\dagger_{i\sigma} c_{j\sigma} + H_{\text{int}}$$

$$H_{int} = U \sum n_{i\uparrow} n_{i\downarrow}$$

$$H_{int} = U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

Fixed direction calculations

The goal

→ Study the magnetic anisotropy of the system fixing the magnetization direction

How?

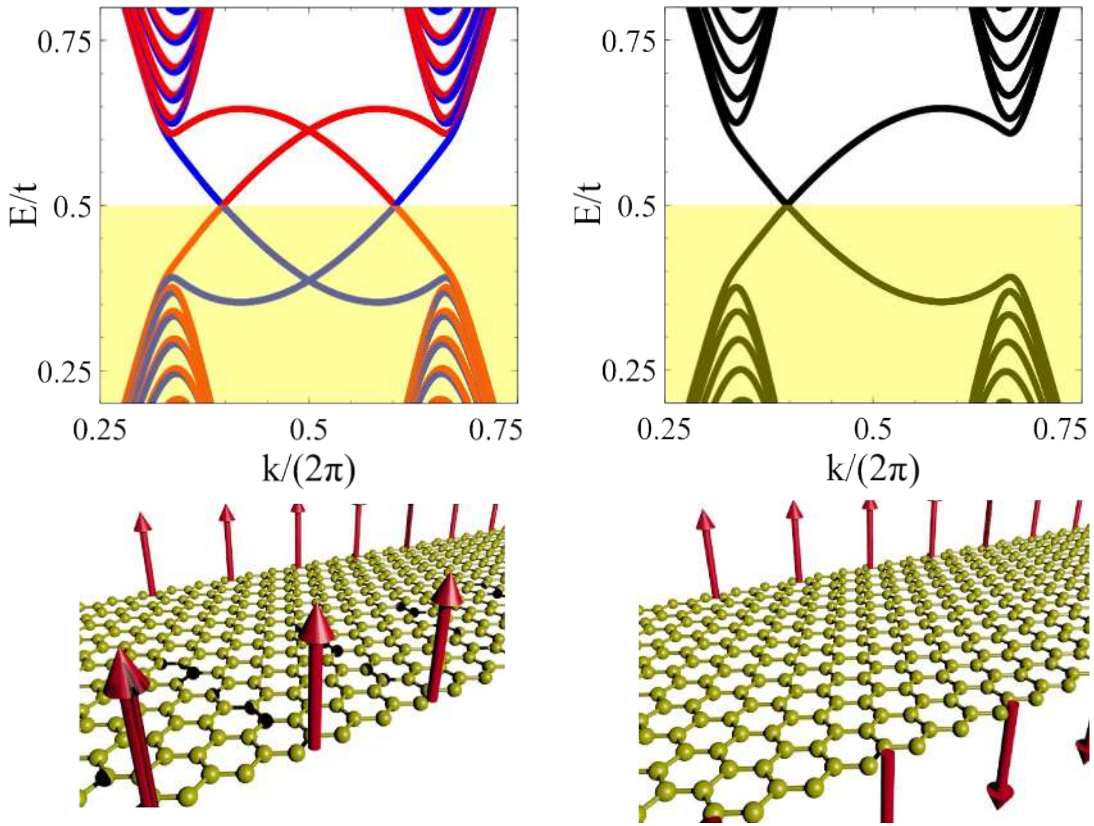
→ Express the densities in the desired quantization axis
→ Retain only the direct term of the contractions (Wick theorem)
Broken rotation symmetry!!!
→ True ground state checked with full non collineal calculation

$$H_{int} = U n_{i\uparrow(\alpha)} n_{i\downarrow(\alpha)}$$

$$H_{MF} = U[\langle n_{i\uparrow(\alpha)}\rangle n_{i\downarrow(\alpha)} + n_{i\uparrow(\alpha)}\langle n_{i\downarrow(\alpha)}\rangle - \langle n_{i\uparrow(\alpha)}\rangle\langle n_{i\downarrow(\alpha)}\rangle]$$

Off-plane solution (U and SOC)

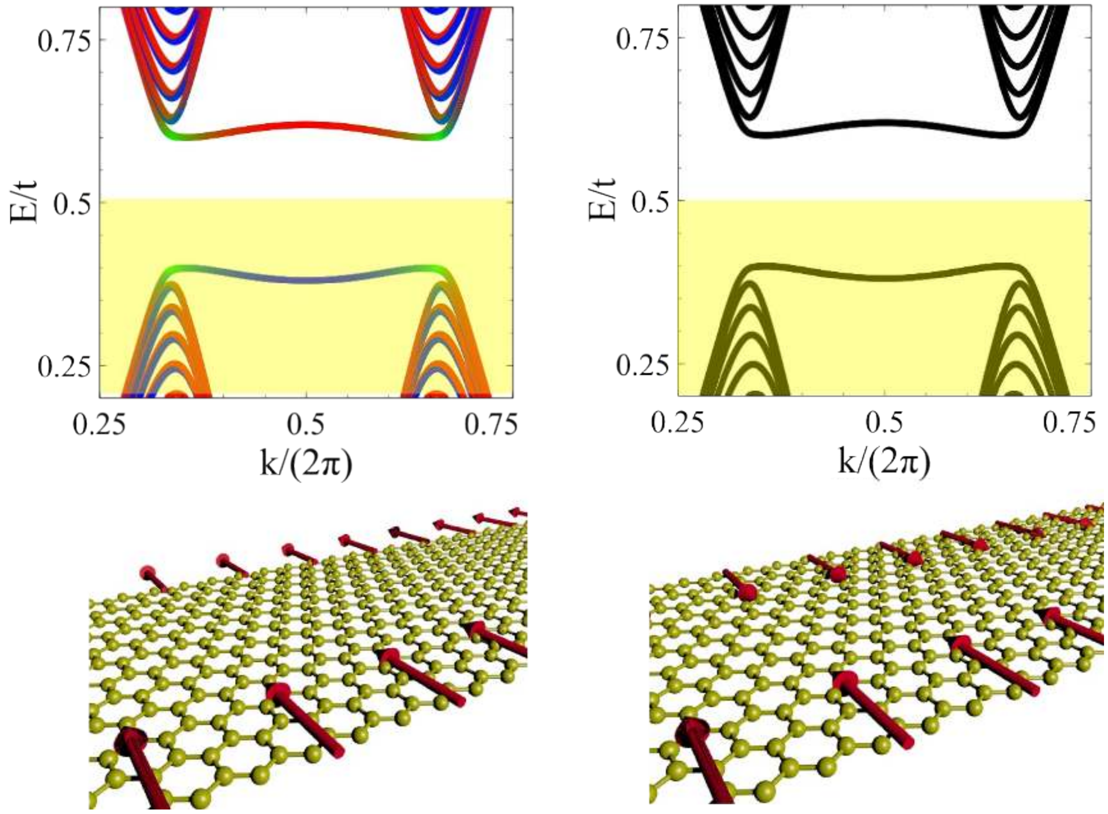
Gapless edge channels



Quantum spin Hall effect even in the presence of time reversal breaking!!!!

In-plane solution (U and SOC)

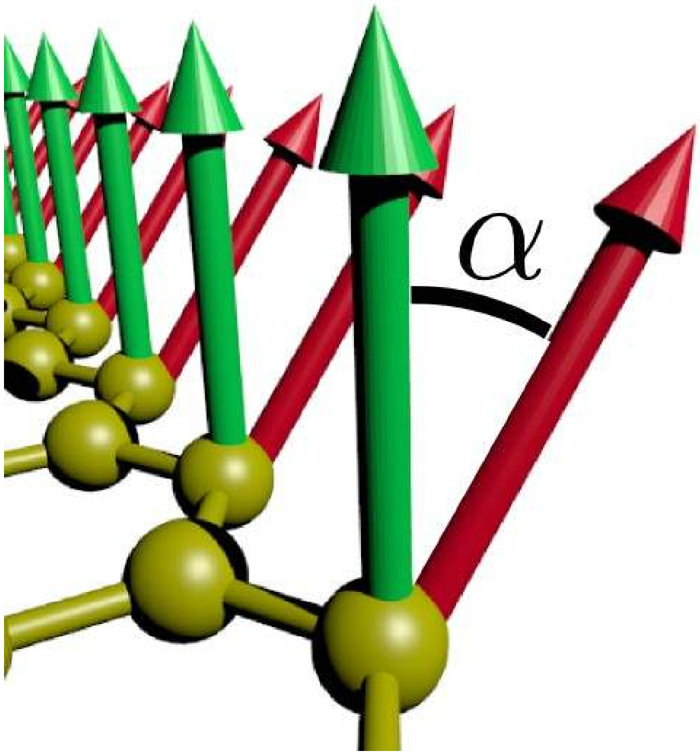
Gapped edge channels

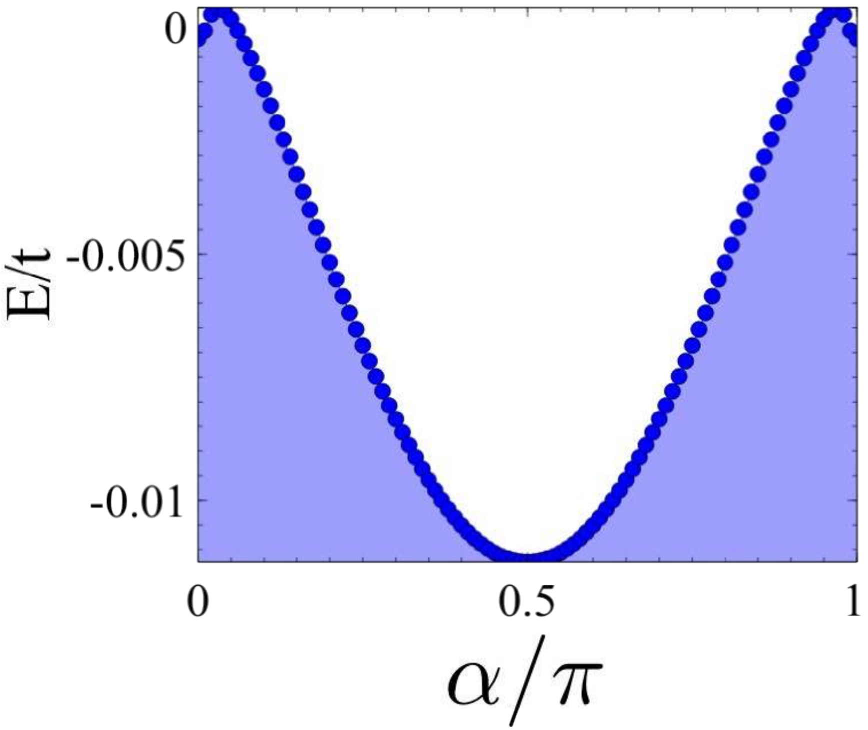


Uppon breaking of TR, the existence of gapless states is no longer guaranteed

Dependence with the angle

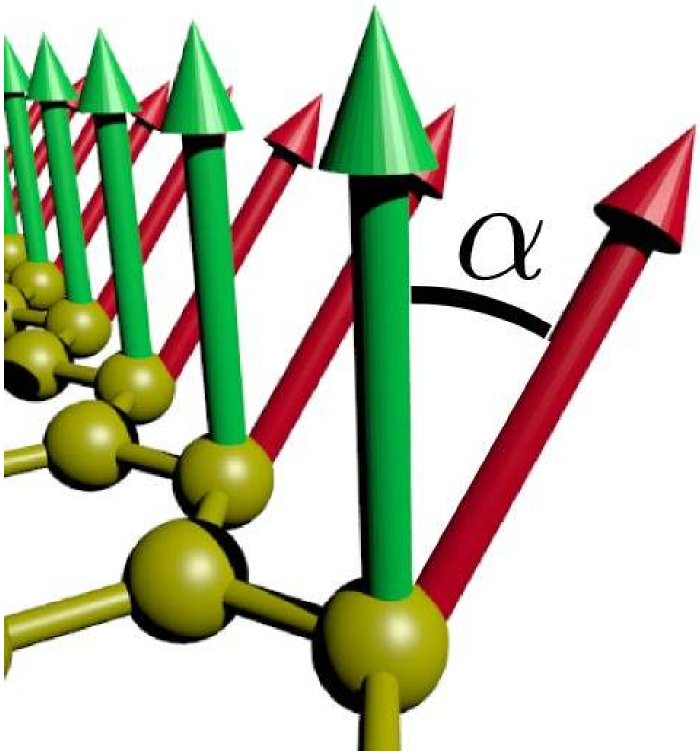
Energy anisotropy

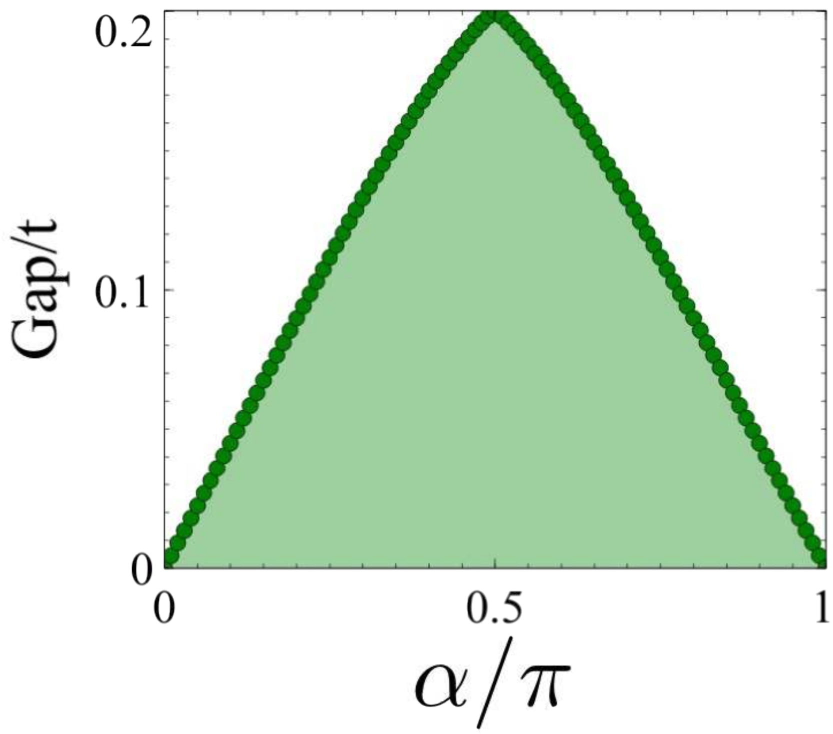




Dependence with the angle

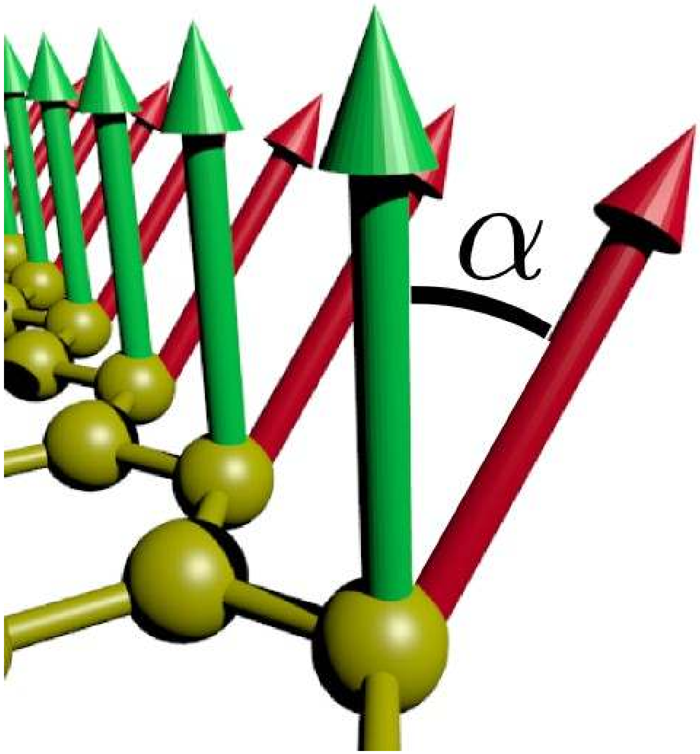
Gap anisotropy

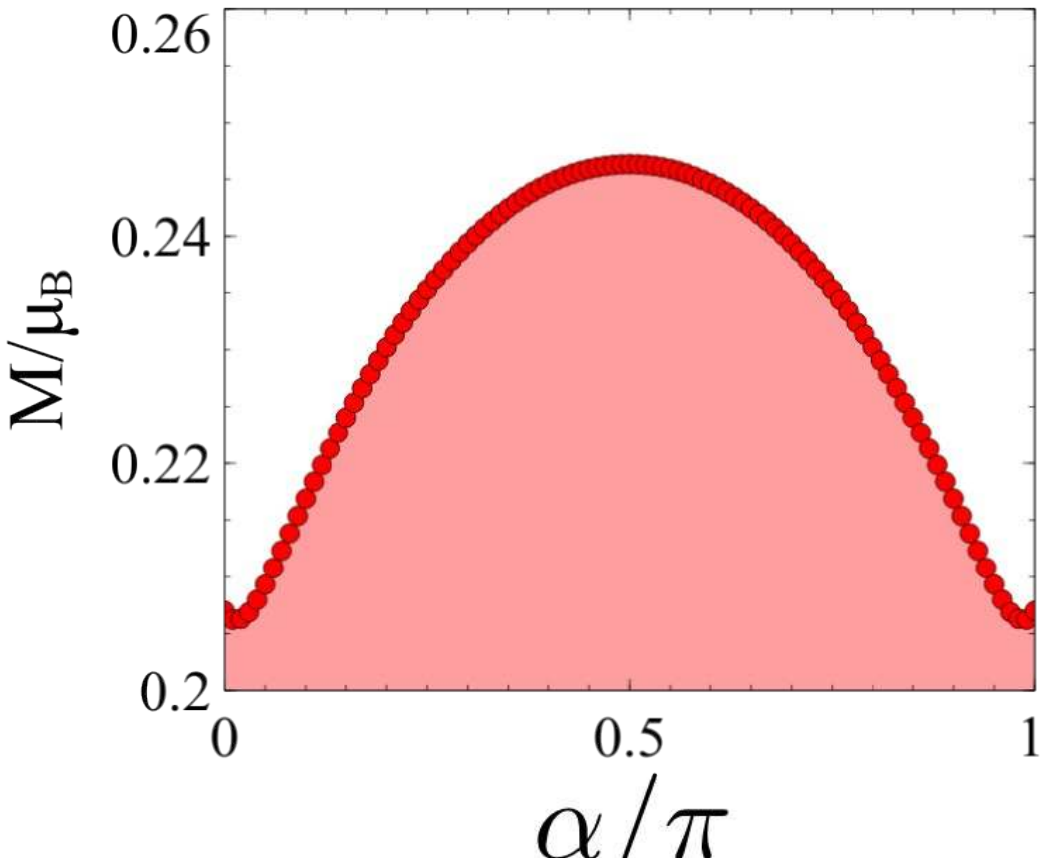




Dependence with the angle

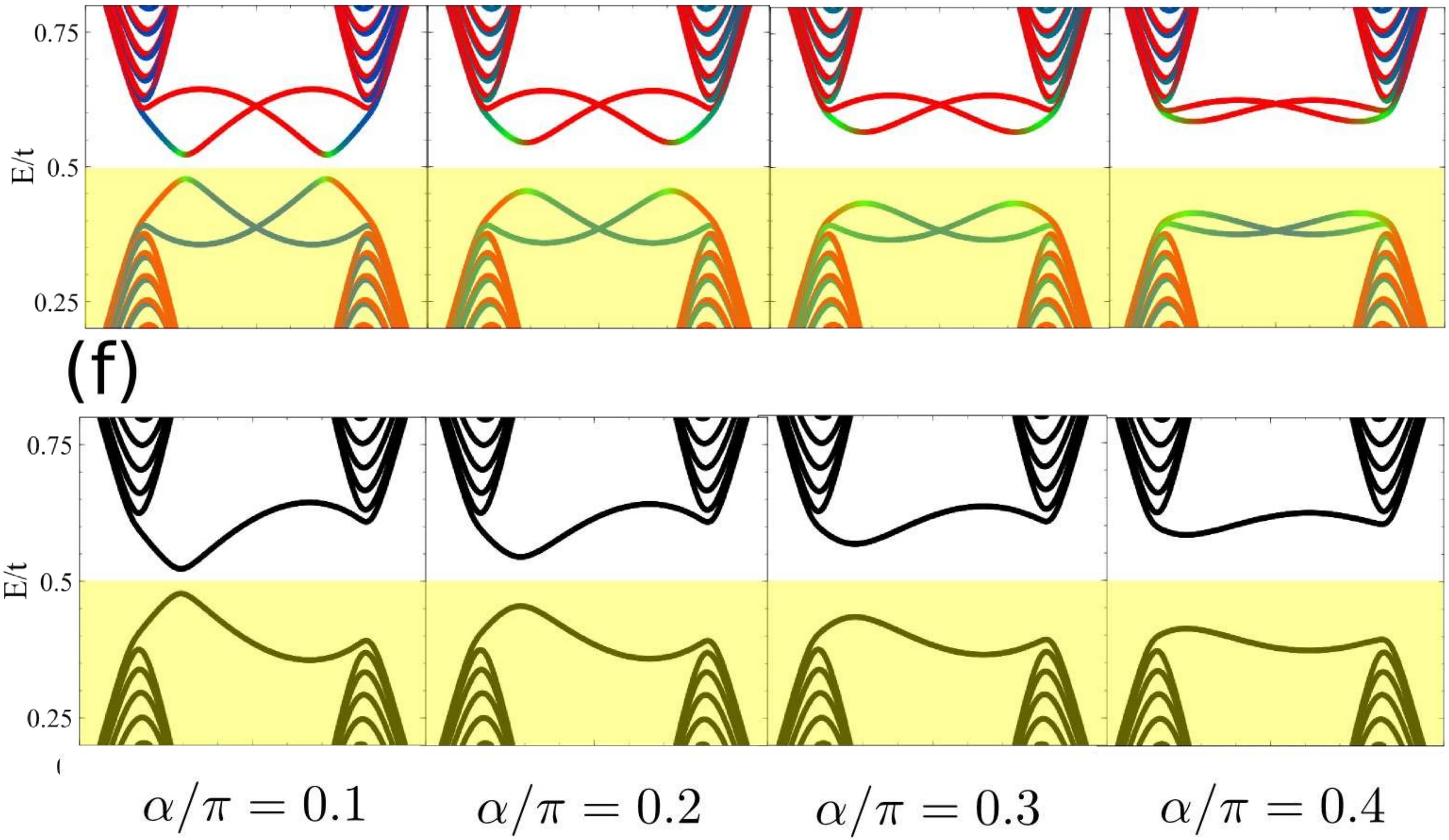
Magnetization anisotropy





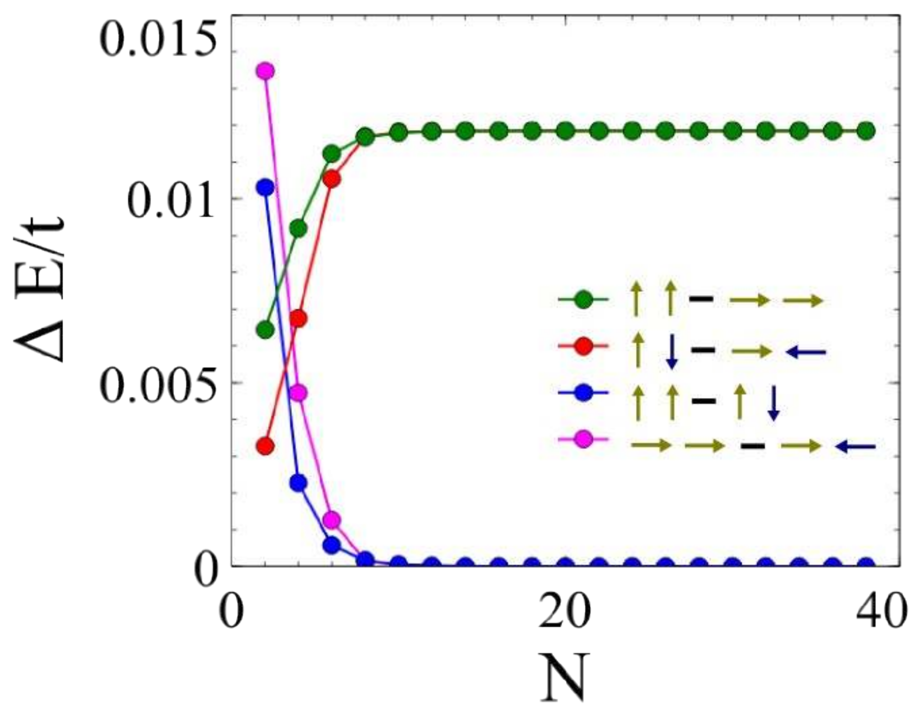
Dependence with the angle

Evolution of the band structures with the quantization angle

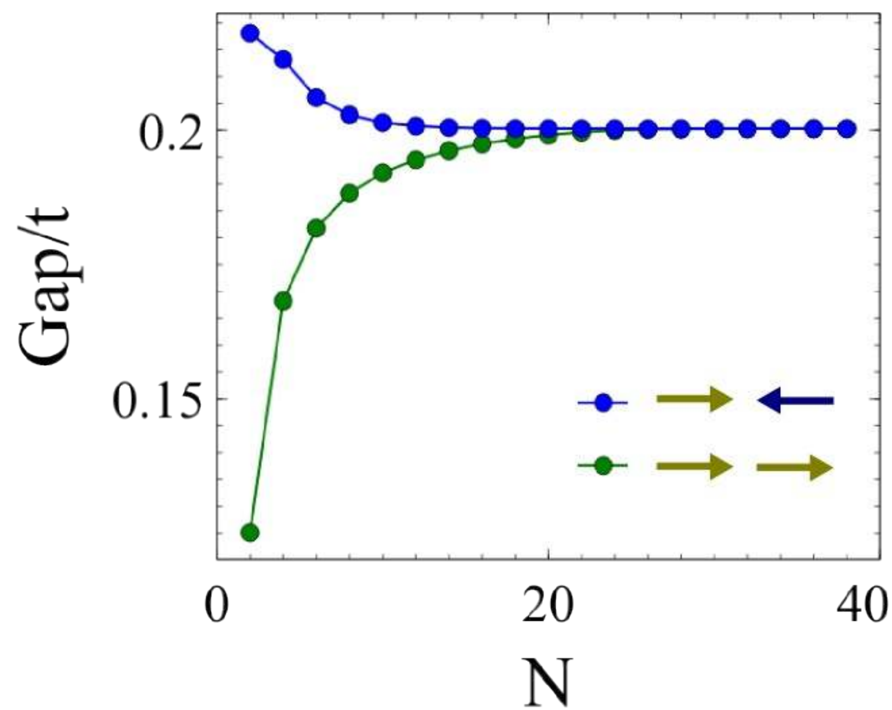


Dependence with width

Energy differences

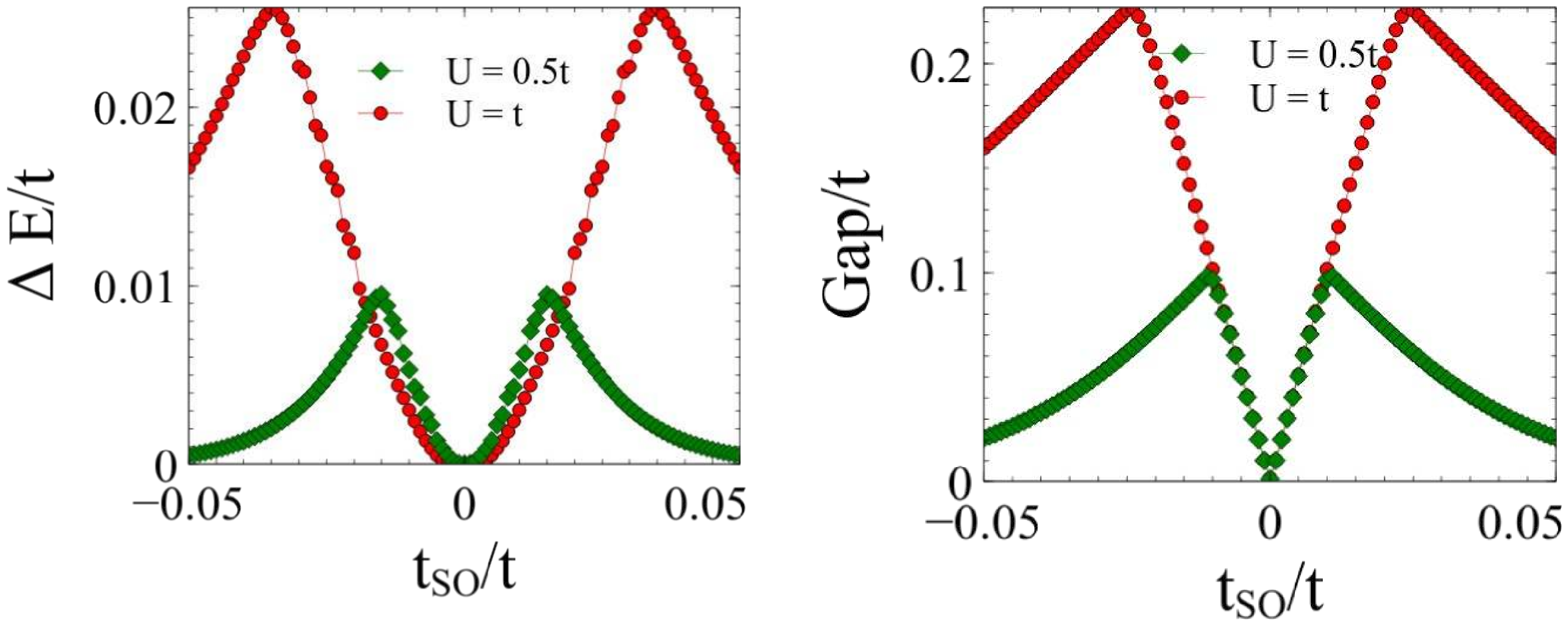


Gap



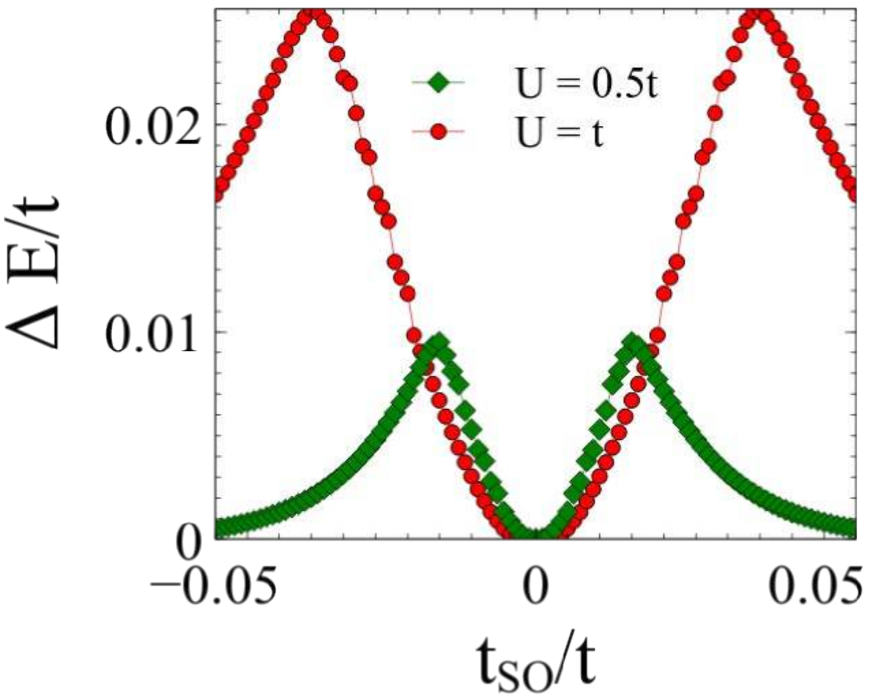
At large width the edges decouple (FE and AF are equivalent)

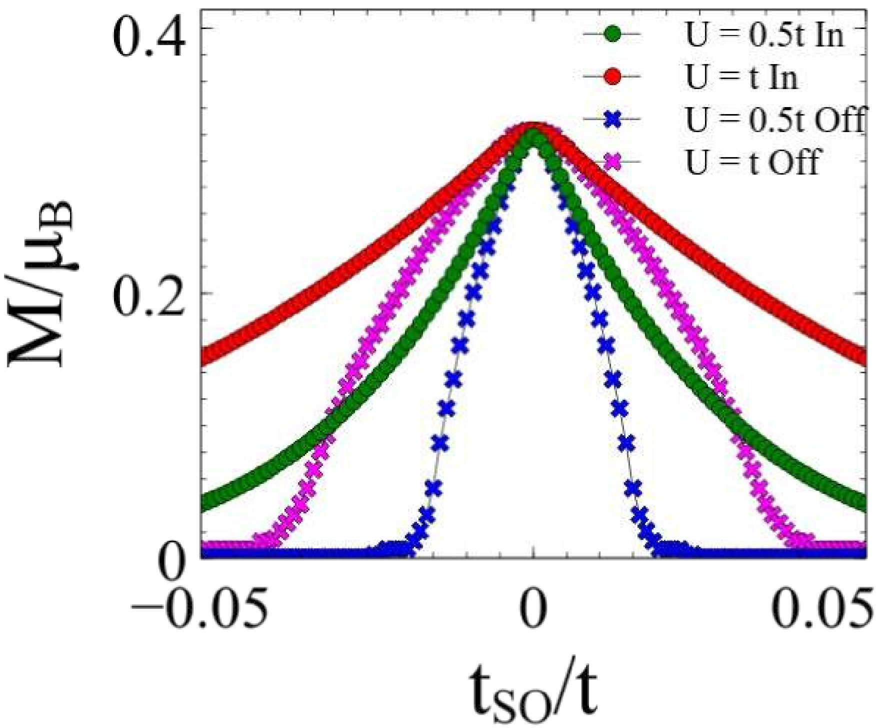
Evolution with SOC



Two regimens of gap opening
→ Bulk (lineal driven by SOC)
→ Edge (non lineal, anisotropic driven)

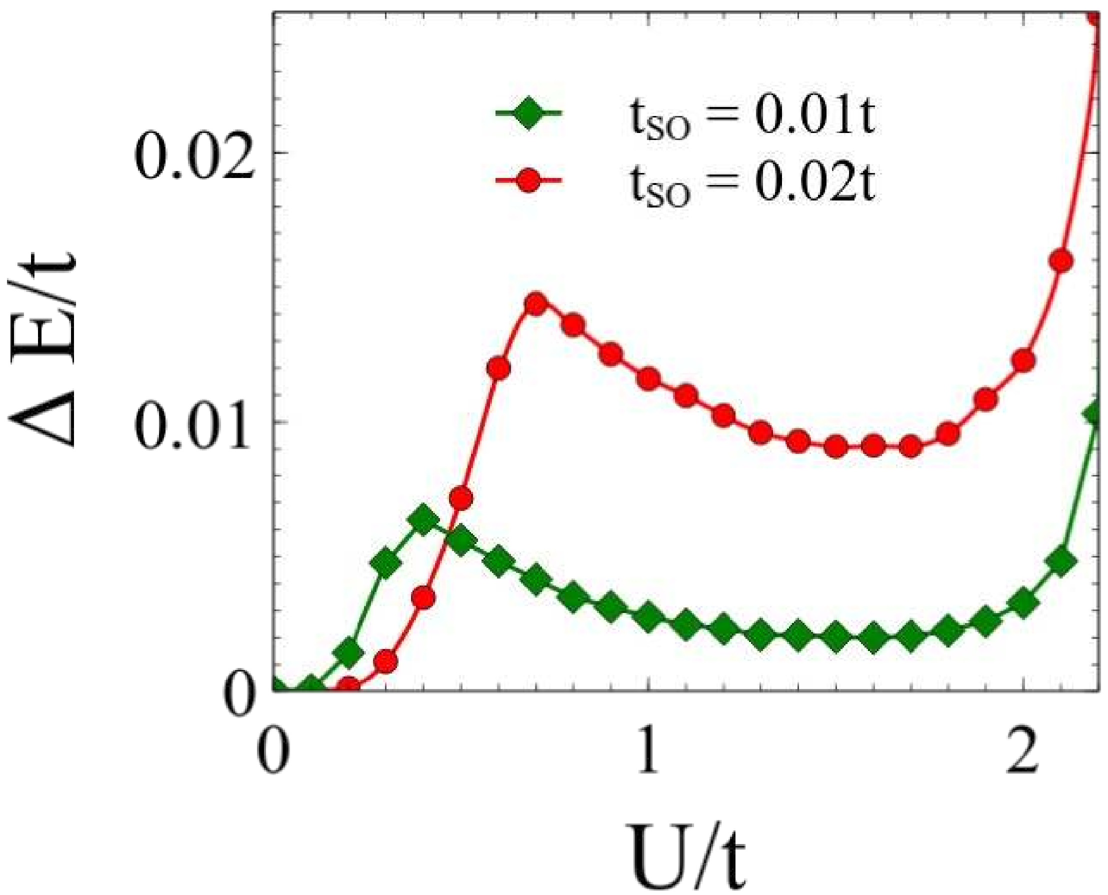
Evolution with SOC





SOC quenches the magnetism
Off-plane solution suffers more quenching

Evolution with U



Conclusion

- Interaction destroys gapless edge states in QSH zig-zag ribbons
- On-site interaction and SOC creates a colossal magnetic anisotropy on the edges
- Stanene edges would be a realistic system realizing this phenomenology

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Graphene	0.1 μeV	2.7 eV
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Mean field Hubbard calculation

$$H_{int} = U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

Mean field decoupling

$$0 \approx \langle [A - \langle A \rangle][B - \langle B \rangle] \rangle = \langle A \rangle \langle B \rangle + AB - A\langle B \rangle - B \langle A \rangle$$

By Wick theorem we have two contraction (and a constant term)

$$H^{MF}_{int} = H_H + H_F + H_{DC}$$

Mean field Hubbard calculation

So in general we have two operators

$$H_{int}^{MF} = H_H + H_F + H_{DC}$$

$$H_H = U[\langle c_{i\uparrow}^\dagger c_{i\uparrow}\rangle c_{i\downarrow}^\dagger c_{i\downarrow} + c_{i\uparrow}^\dagger c_{i\uparrow}\langle c_{i\downarrow}^\dagger c_{i\downarrow}\rangle]$$

$$H_F = -U[\langle c_{i\downarrow}^\dagger c_{i\uparrow}\rangle c_{i\downarrow}^\dagger c_{i\uparrow} + c_{i\uparrow}^\dagger c_{i\downarrow}\langle c_{i\uparrow}^\dagger c_{i\downarrow}\rangle]$$

But in a collineal calculation we neglect the local exchange term!!!

$$H_{MF} = U[\langle n_{i\uparrow(\alpha)}\rangle n_{i\downarrow(\alpha)} + n_{i\uparrow(\alpha)}\langle n_{i\downarrow(\alpha)}\rangle - \langle n_{i\uparrow(\alpha)}\rangle\langle n_{i\downarrow(\alpha)}\rangle]$$