Full-shell Majorana nanowires

A theoretical description

Carlos Payá

Instituto de Ciencia de Materiales de Madrid (ICMM), CSIC

January 10, 2024

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Outline

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1. Engeniering topologically protected edge states
2. Signals in the LDOS: CdGM analogs
3. Full 2D simulation: band bending and the solid-core model
4. Disorder-induced mode-mixing: a new mechanism for topology
5. Conclusions

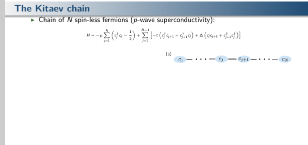
The Kitaev chain

- Chain of N spin-less fermions (p-wave superconductivity):

$$H = -\mu \sum_{j=1}^{N} \left(c_j^\dagger c_j - \frac{1}{2} \right) + \sum_{j=1}^{N-1} \left[-t \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) + \Delta \left(c_j c_{j+1} + c_{j+1}^\dagger c_j^\dagger \right) \right]$$

(a)

R. Aguado 2017, *Rivista del Nuovo Cimento.*
E. Prada *et al.* 2020, *Nature Reviews Physics.*
A. Y. Kitaev 2001, *Physics-Uspekhi.*



The simplest topological model.

1. Chain of fermions. Chem pot + hopping + superconducting pairing.
2. Majorana representation. γ^A and γ^B are Majorana operators.
3. Hamiltonian in terms of Majorana operators. Cases:
   - $\Delta = t = 0$: trivial. Just a chain of decoupled fermions.
   - $t = \Delta$, $\mu = 0$. Long-range coupling. Same site decoupled. Edge states disappear from the hamiltonian!
4. Unpaired Majorana follow non-Abelian statistics. When two MBS interact, the final state of the system depends on the order of the exchanges.

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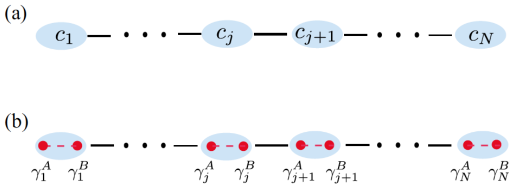

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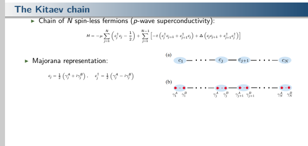

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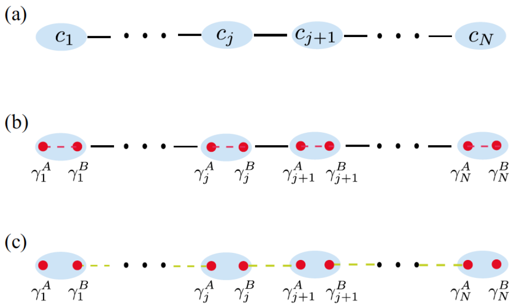
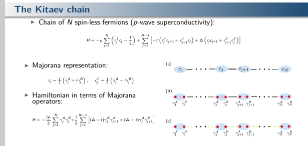
$$H = -\frac{i\mu}{2} \sum_{j=1}^{N} \gamma_j^A \gamma_j^B + \frac{i}{2} \sum_{j=1}^{N-1} \left[(\Delta + t)\gamma_j^B \gamma_{j+1}^A + (\Delta - t)\gamma_j^A \gamma_{j+1}^B \right]$$





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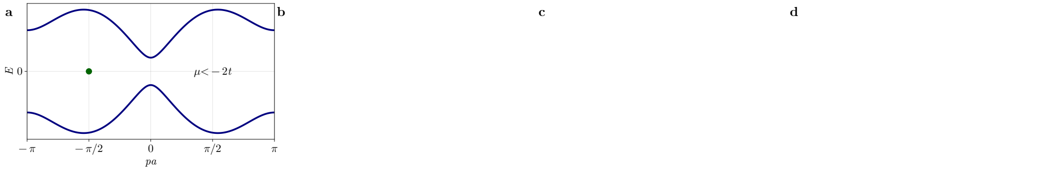
Kitaev chain energy dispersion

Let's consider periodic boundary conditions and solve the eigenvalue problem in momentum space:



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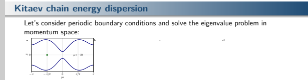

- We distinguish two regimes separated by a gap closing.
- In the open boundary conditions, they correspond to the presence or absence of MZM.
- It is an example of BDI topology.

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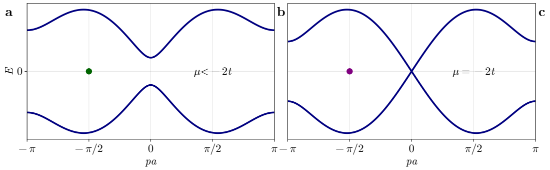

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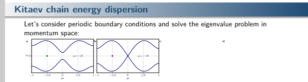

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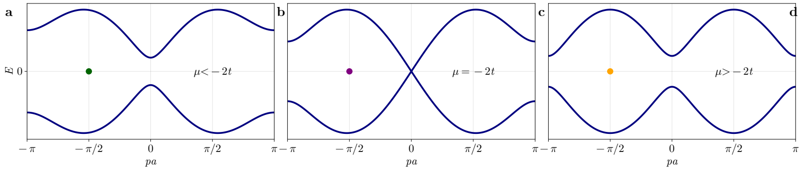

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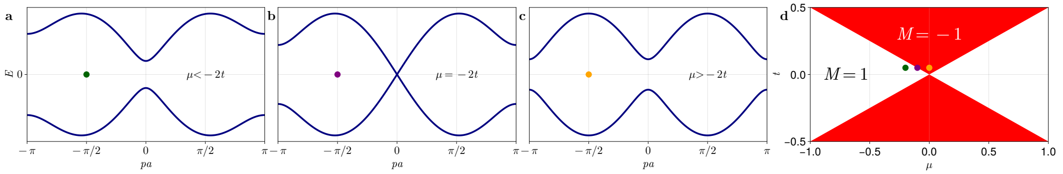

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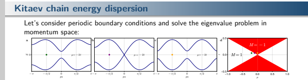

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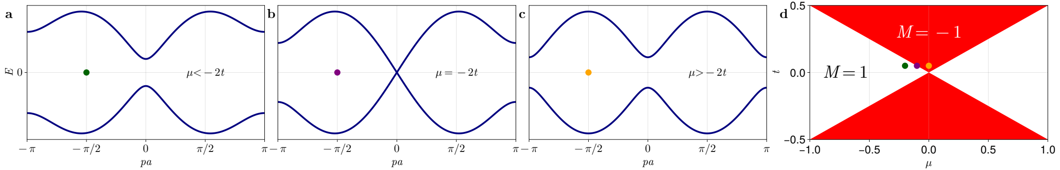

- Two distinct phases characterized by a $\mathbb{Z}_2$ invariant, $M = (-1)^\nu$.

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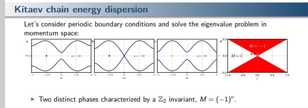

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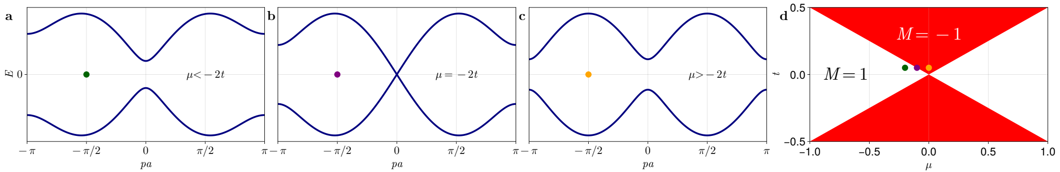

- Two distinct phases characterized by a $\mathbb{Z}_2$ invariant, $M=(-1)^\nu$.
- ν is the number of times the energy gap closes in the Brillouin zone.

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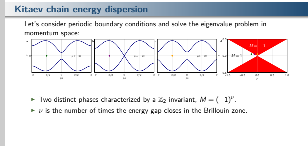

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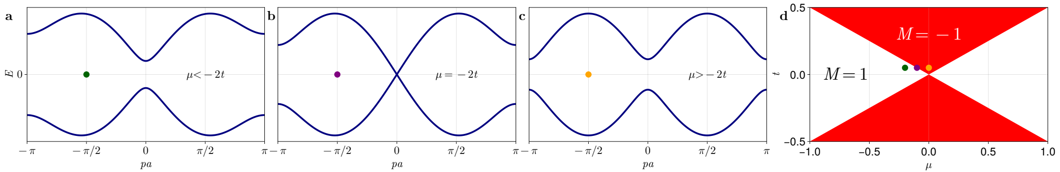

- Two distinct phases characterized by a $\mathbb{Z}_2$ invariant, $M = (-1)^\nu$.
- ν is the number of times the energy gap closes in the Brillouin zone.
- $M = 1 \Rightarrow$ no unpaired MZM. $M = -1 \Rightarrow$ unpaired MZM (bulk-boundary correspondance).

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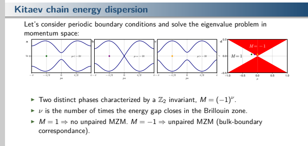

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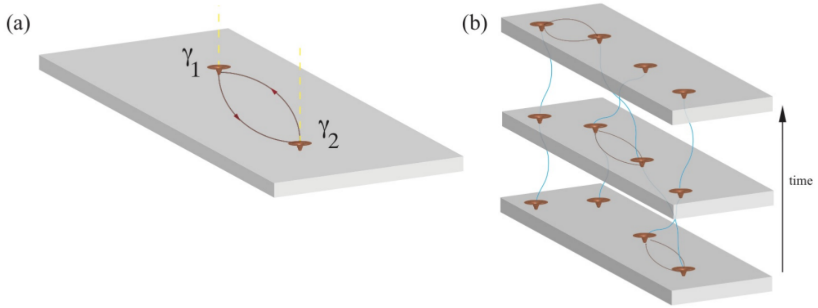
Majoranas for qubits



- MZM are non-Abelian anyons.
- Gap closing/reopening $\Rightarrow$ topological protection.

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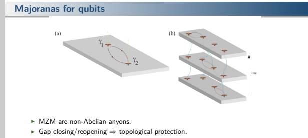
Full-shell Majorana nanowires
└Engeniering topologically protected edge states
└A toy model
└Majoranas for qubits



We need a $p-$wave superconductor!

- The superconducting pairing term in the Kitaev chain is spinless: $\Delta\left(c_j c_{j+1} + c_{j+1}^\dagger c_j^\dagger\right)$.

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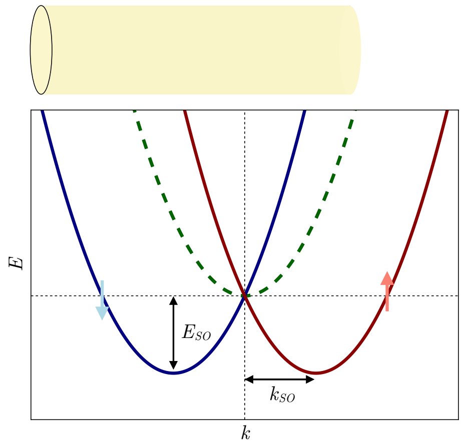
Rashba, Zeeman and helical bands



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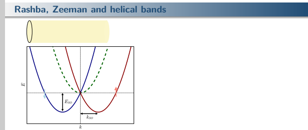

- SOC breaks spin degeneracy and shifts bands in energy and *k*-space.
- Zeeman field breaks time-reversal symmetry and splits bands in energy.
- When μ in the Zeeman gap, there is only one band with spin locked to momentum, i.e. helical.
- Add SC $\Rightarrow$ two gaps. One of them, Δ_1, can close and induce a topological transition.

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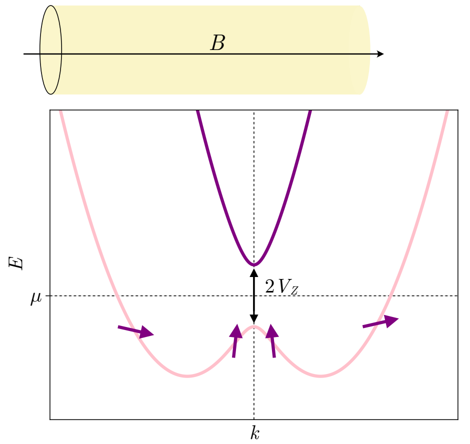

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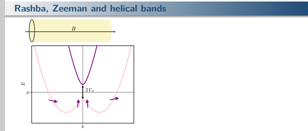

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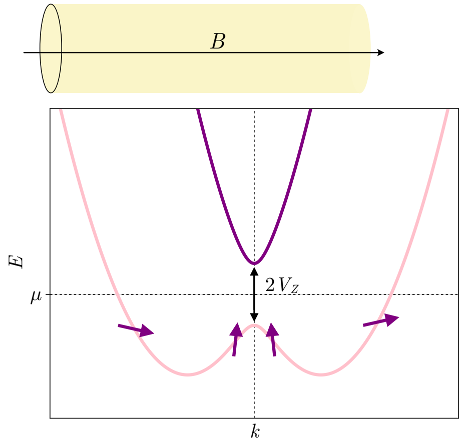

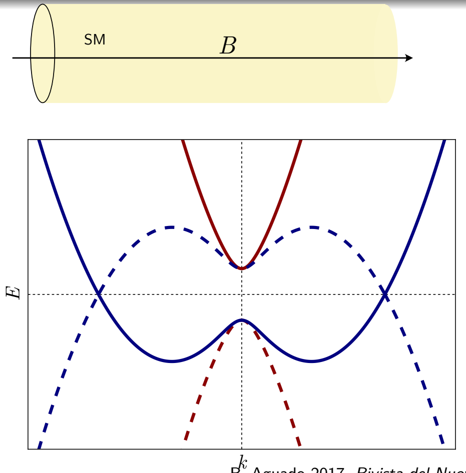

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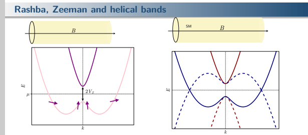

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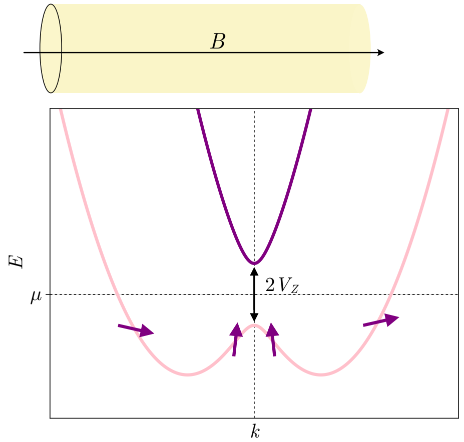

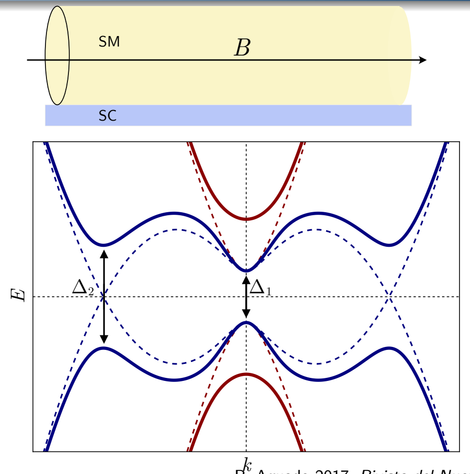

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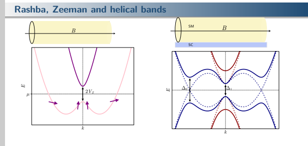

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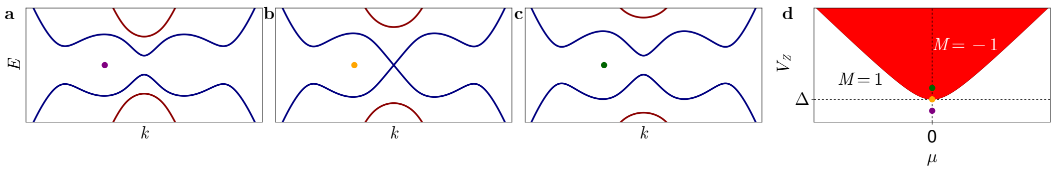
Topological phase transition



$$V_{Zc} = \sqrt{\Delta^2 + \mu^2}$$

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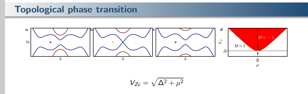

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- Disadvantage: need high magnetic fields and high g.
- High magnetic fields kill SC.

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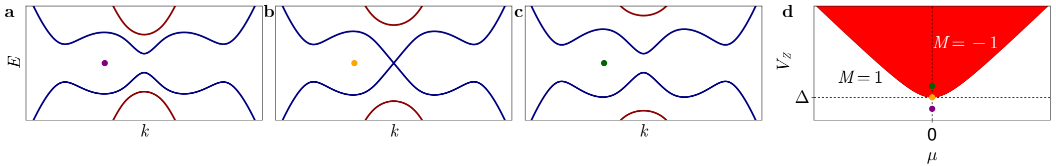

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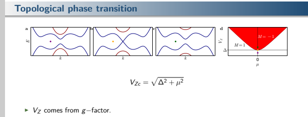

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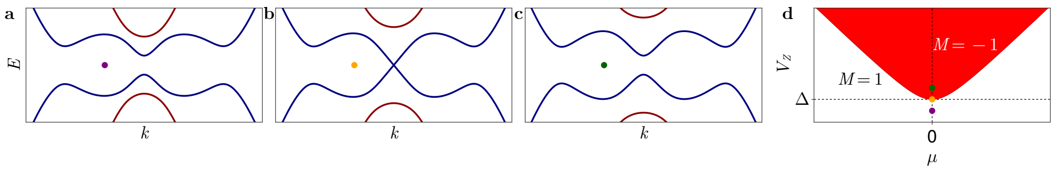

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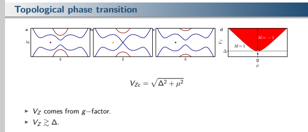
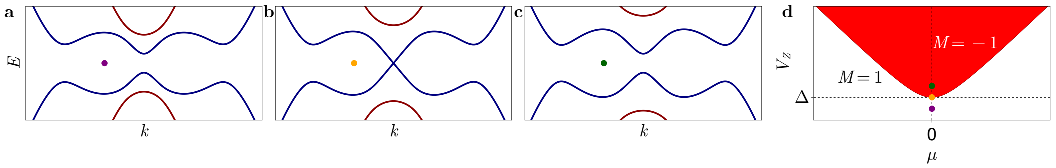


- Δ_1 closes at $k=0$ for $V_Z = V_{Zc}$.
- Disadvantage: need high magnetic fields and high g.
- High magnetic fields kill SC.

Topological phase transition



$$V_{Zc} = \sqrt{\Delta^2 + \mu^2}$$

- V_Z comes from $g-$factor.
- $V_Z \gtrsim \Delta$.

- Need high g-factor materials and high magnetic fields.

R. M. Lutchyn, J. D. Sau, and S. Das Sarma 2010, *Phys. Rev. Lett.*
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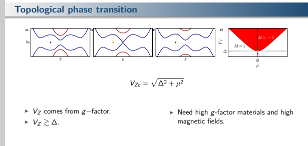

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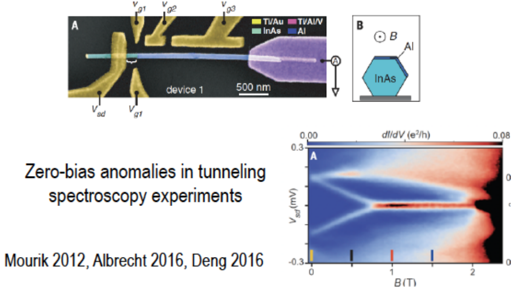
Searching for Majoranas

- Strong experimental interest.



Claims: V. Mourik *et al.* 2012, *Science*. S. M. Albrecht *et al.* 2016, *Nature*. M. T. Deng *et al.* 2016, *Science*.
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Searching for Majoranas

- Strong experimental interest.
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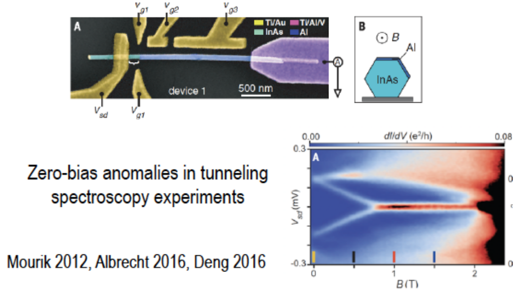

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2024-01-10

Full-shell Majorana nanowires
└Engeniering topologically protected edge states
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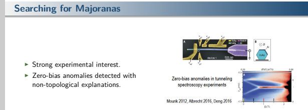

Searching for Majoranas

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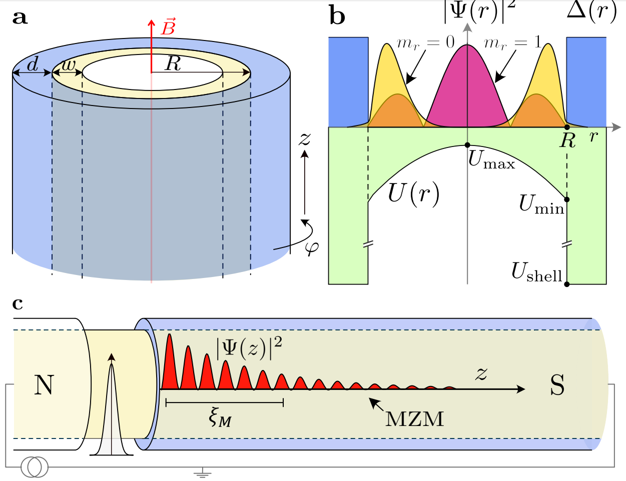
The full-shell nanowire



S. Vaitiekėnas *et al.* 2020, *Science*.
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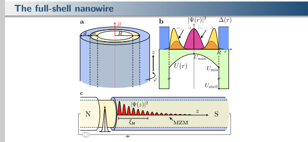
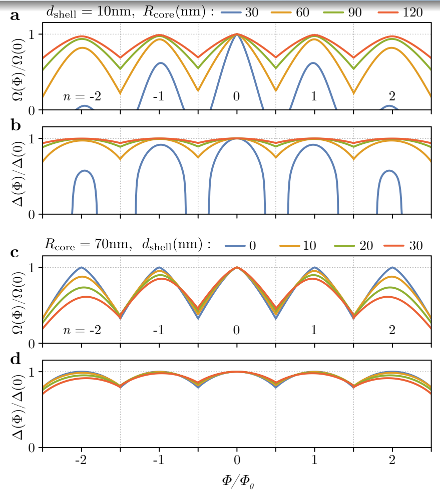
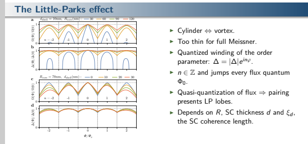


The Little-Parks effect

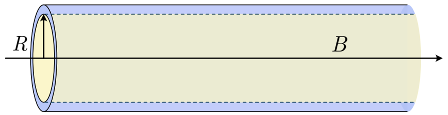


- Cylinder ⇔ vortex.
- Too thin for full Meissner.
- Quantized winding of the order parameter: $\Delta = |\Delta| e^{in\varphi}$.
- $n \in \mathbb{Z}$ and jumps every flux quantum Φ_0.
- Quasi-quantization of flux ⇒ pairing presents LP lobes.
- Depends on R, SC thickness d and ξ_d, the SC coherence length.

W. A. Little and R. D. Parks 1962, *Phys. Rev. Lett.*
R. D. Parks and W. A. Little 1964, *Phys. Rev.*



The full-shell nanowire: analytical hollow-core model



- **Effective** Zeeman field:

$$V_Z = \phi\left(\frac{1}{4mR^2} + \frac{\alpha}{2R}\right)$$

- $\phi = n - \frac{\Phi}{\Phi_0}$, magnetic flux.
- n number of fluxoids.
- No need for $g-$factor. $\Phi \sim \Phi_0$.

S. Vaitiekėnas *et al.* 2020, *Science*.
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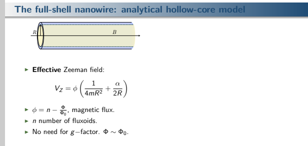

- Zeeman field for the hollow-core model.
- n integer part of flux.

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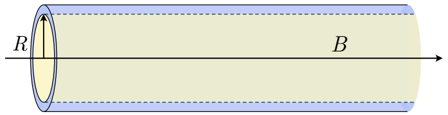

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- Good generalized angular momentum $J_z = -i\partial_\varphi + \frac{1}{2}\sigma_z + \frac{1}{2}n\tau_z$:

$$m_J = \begin{cases} \mathbb{Z} + 1/2, & \text{if } n \text{ even} \\ \mathbb{Z}, & \text{if } n \text{ odd} \end{cases}$$

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P. San-Jose *et al.* 2023, *Phys. Rev. B*.
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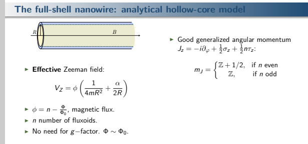

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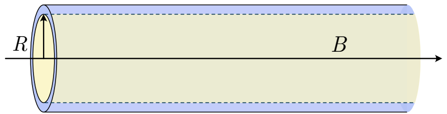

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- $\Rightarrow$ Computationally affordable.

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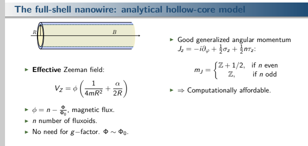

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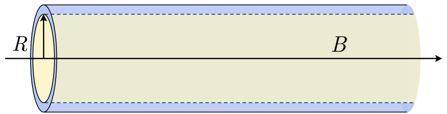

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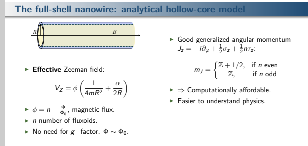

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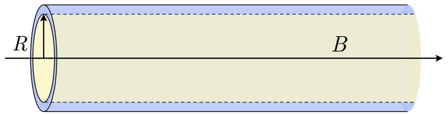

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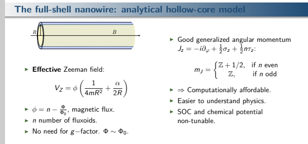

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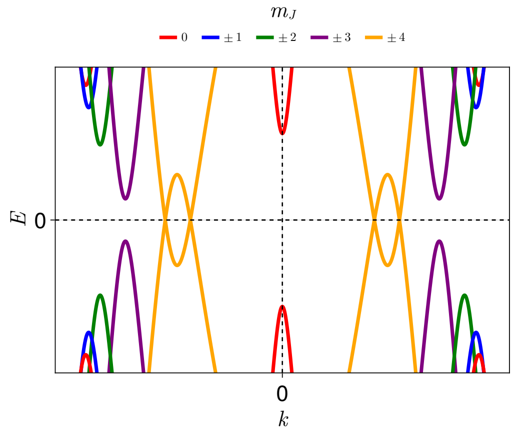
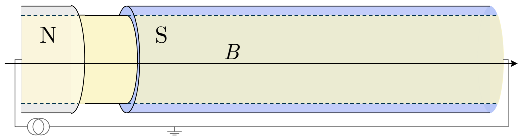
The CdGM analog states





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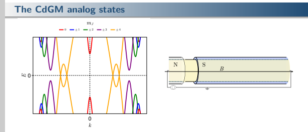

- Each minimum in the bands corresponds to a van Hove peak in the LDOS.
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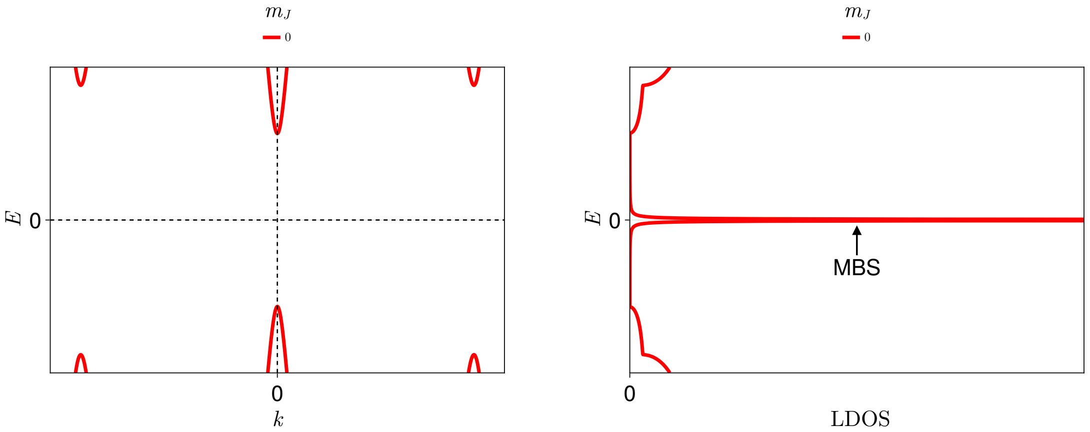

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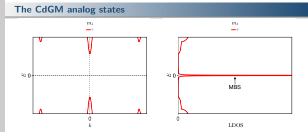

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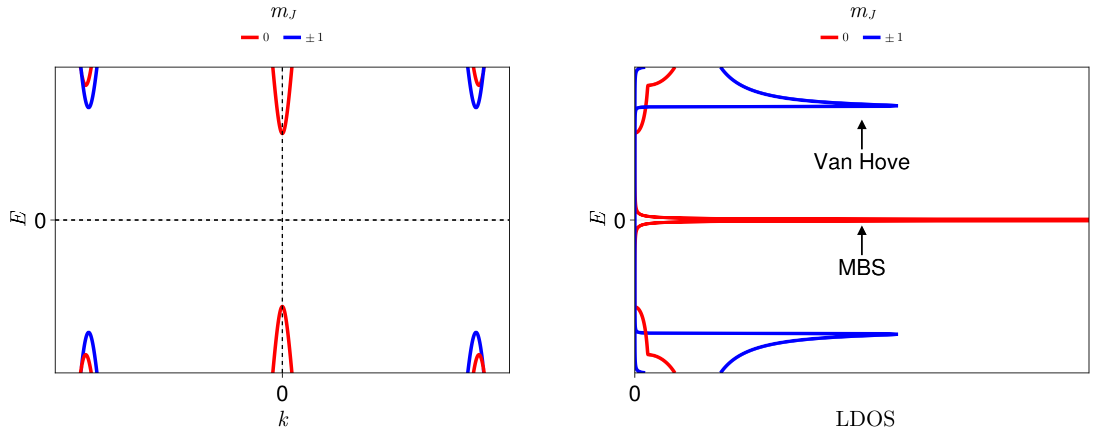

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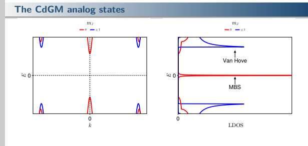

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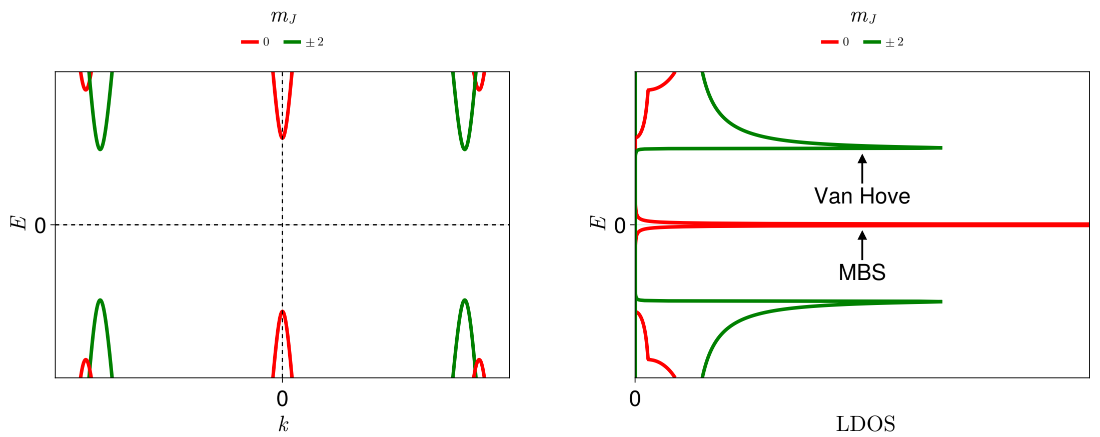

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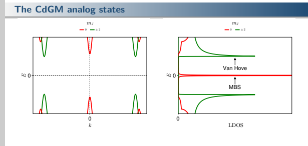

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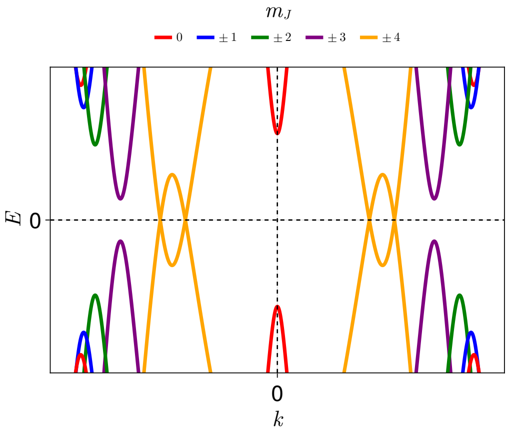
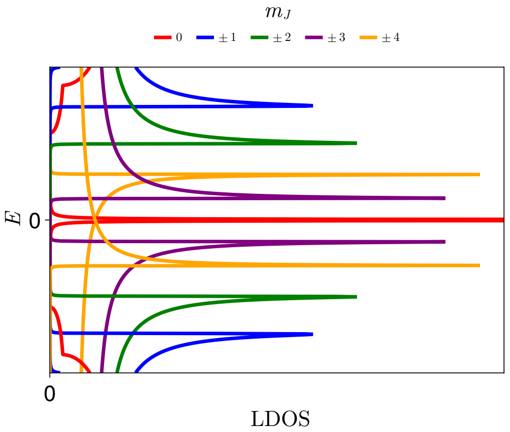
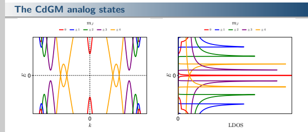
The CdGM analog states



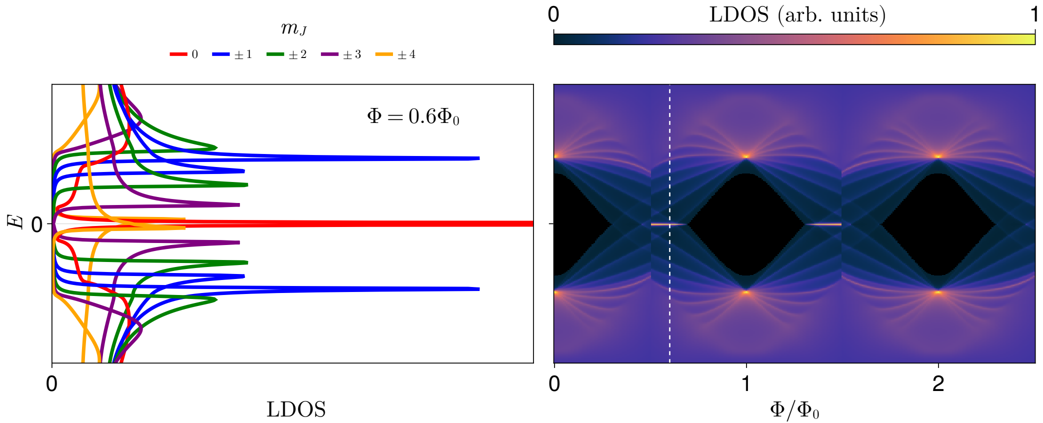


C. Payá *et al.* 2023, *arXiv*.
P. San-Jose *et al.* 2023, *Phys. Rev. B.*



- Each minimum in the bands corresponds to a van Hove peak in the LDOS.
- These Van Hove peaks are CdGM analogs.
- LP switched off for clarity.
- Turn on and see LDOS against flux.

LDOS vs. flux



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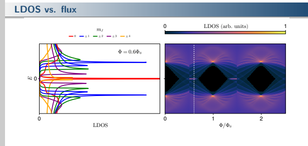
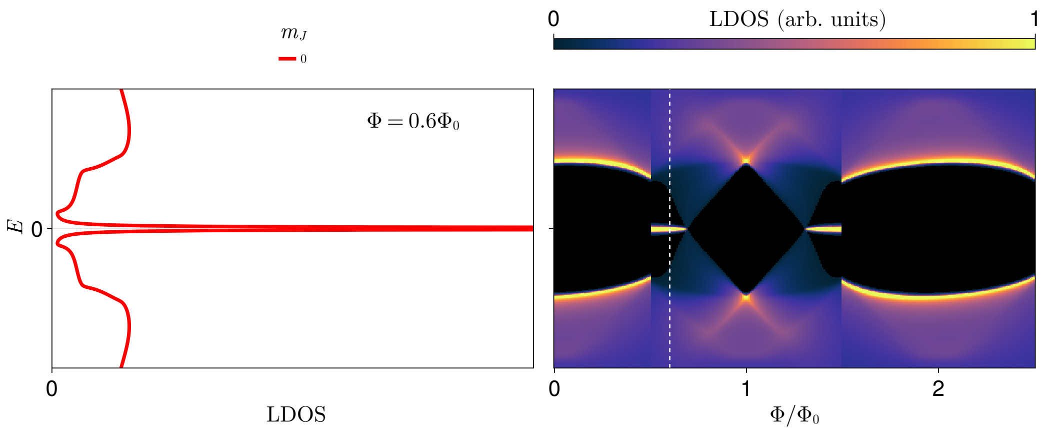


- LP effect turned on.
- Left: LDOS cut for white line in LDOS v flux.
- Lots of states over MZM.
- Taking only $m_J = 0$, minigap is huge.

LDOS vs. flux



C. Payá *et al.* 2023, *arXiv*.
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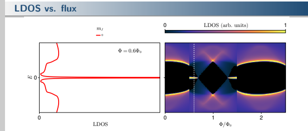

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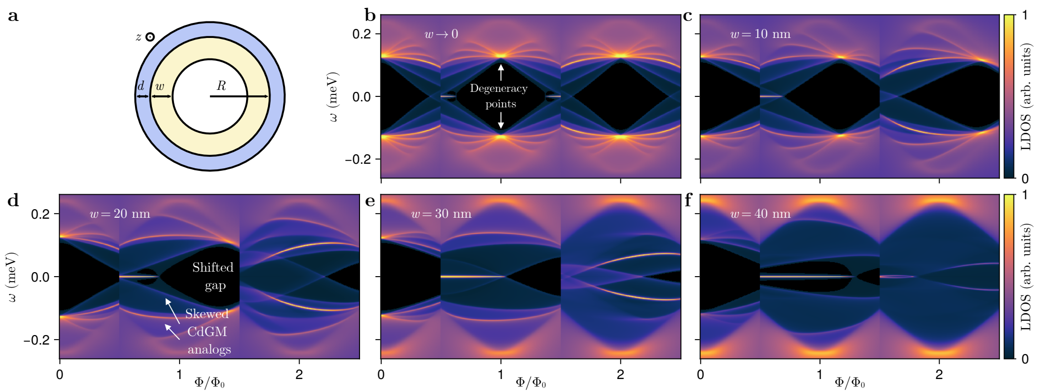
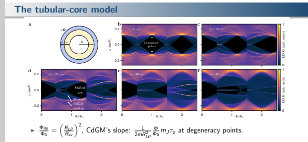
The tubular-core model



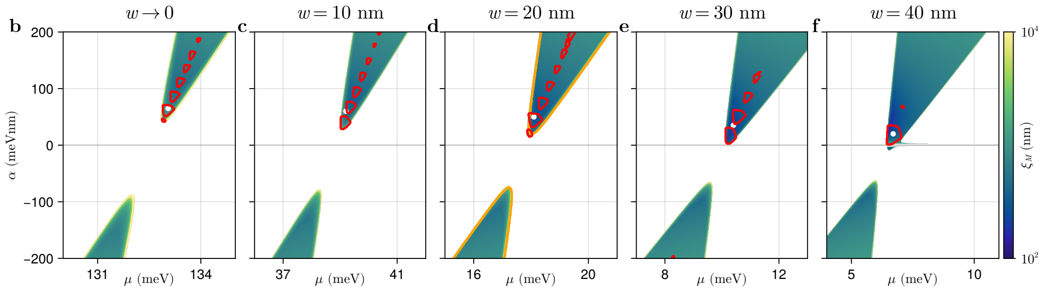
- $\frac{\Phi_{dp}}{\Phi_0} = \left(\frac{R_{LP}}{R_{av}}\right)^2$, CdGM's slope: $\frac{1}{2mR_{LP}^2}\frac{\Phi}{\Phi_0}m_J\tau_z$ at degeneracy points.

C. Payá *et al.* 2023, *arXiv*.



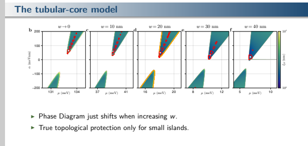
- Increase *w* and keep "equivalent" parameters.
- Notice DP. It shifts towards higher fluxes.
- Leading to a shifted gap and skewed CdGM analogs.
- Sometimes there is true topological minigap! Why? ⇒ competition between MBS and CdGMs.

The tubular-core model



- Phase Diagram just shifts when increasing *w*.
- True topological protection only for small islands.

C. Payá *et al.* 2023, *arXiv*.



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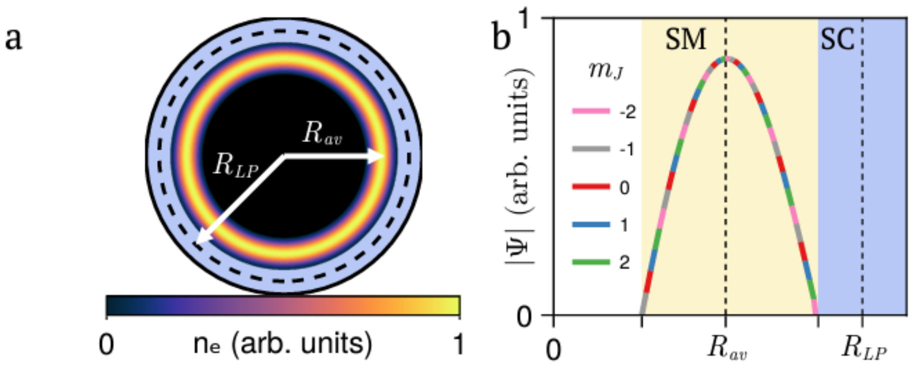
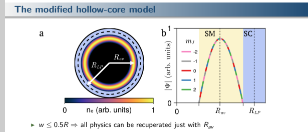
The modified hollow-core model



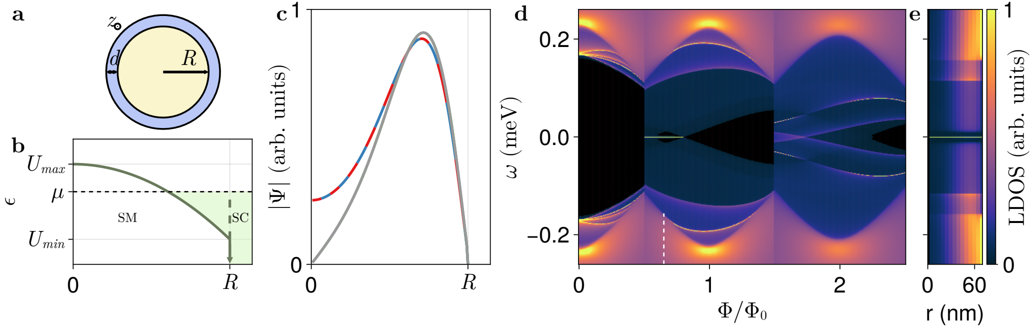
- $w \leq 0.5R \Rightarrow$ all physics can be recuperated just with R_{av}

C. Payá *et al.* 2023, *arXiv*.



- PD have the same shape for all w.
- Up to $w = 0.5R$, they can be fitted to a $w \to 0$ model (orange in $w = 20$ nm).

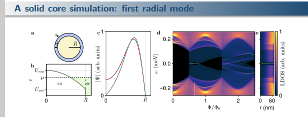
A solid core simulation: first radial mode



C. Payá *et al.* 2023, ***arXiv***.

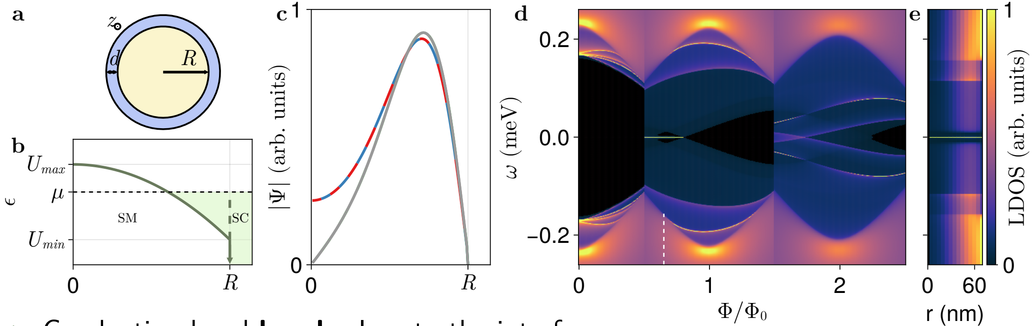
2024-01-10

Full-shell Majorana nanowires
└Full 2D simulation: band bending and the solid-core model
└Role of the radial modes
└A solid core simulation: first radial mode



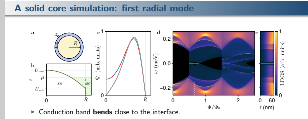
- Solid-core: boundary conditions change.
- Realistic simulation: conduction band-bending.
- If all states in first radial mode, similar to tubular-core.

A solid core simulation: first radial mode



- Conduction band **bends** close to the interface.

C. Payá *et al.* 2023, *arXiv*.



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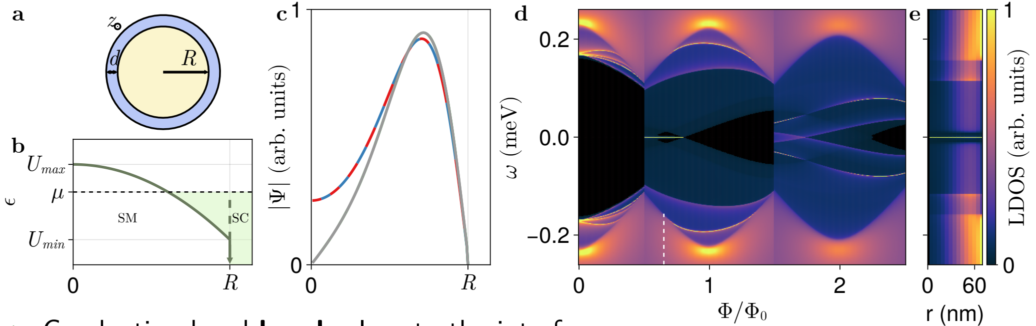

- Conduction band **bends** close to the interface.
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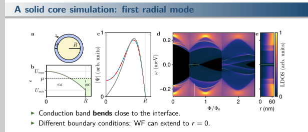
C. Payá *et al.* 2023, *arXiv*.



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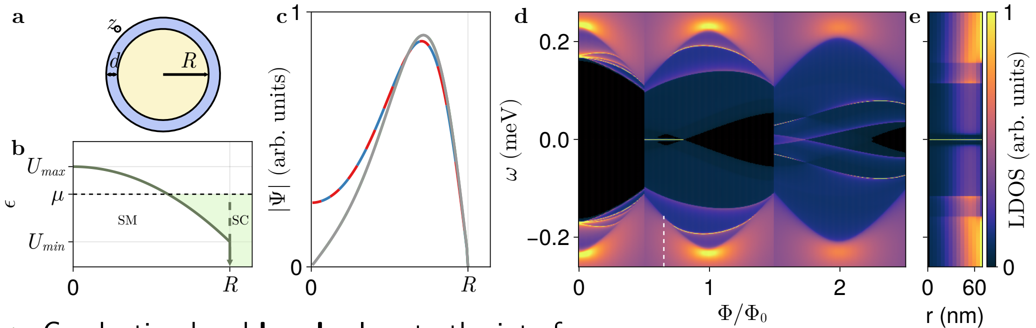
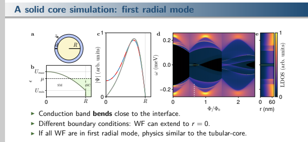


- Conduction band **bends** close to the interface.
- Different boundary conditions: WF can extend to $r = 0$.
- If all WF are in first radial mode, physics similar to the tubular-core.

C. Payá *et al.* 2023, *arXiv*.



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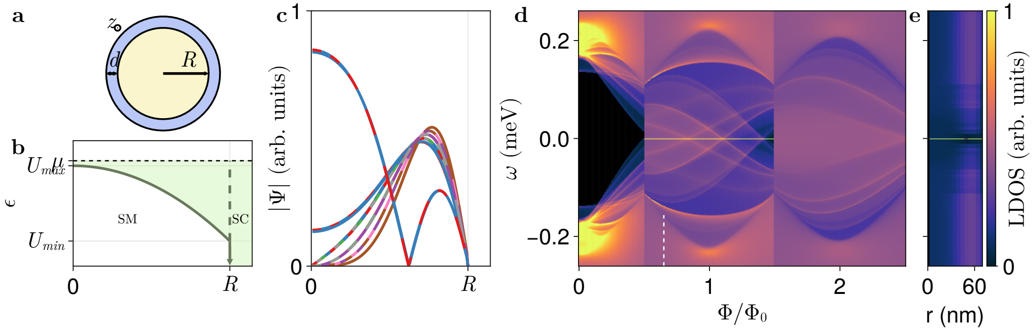
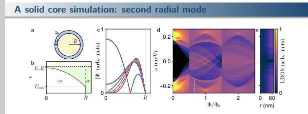
A solid core simulation: second radial mode

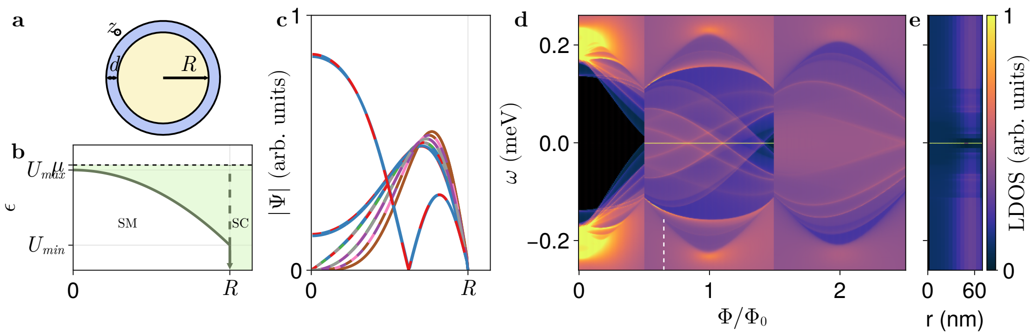


C. Payá *et al.* 2023, *arXiv*.



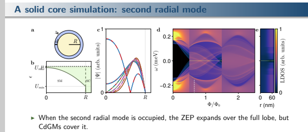
- MBS second radial mode is the first to enter ⇒ extends through all first lobe.
- But all m_J in first radial mode enter before.
- LDOS is covered with CdGM.
- No true topological protection anywhere.
- Intuition: larger radial modes have smaller average radius.

A solid core simulation: second radial mode



- When the second radial mode is occupied, the ZEP expands over the full lobe, but CdGMs cover it.

C. Payá *et al.* 2023, *arXiv*.



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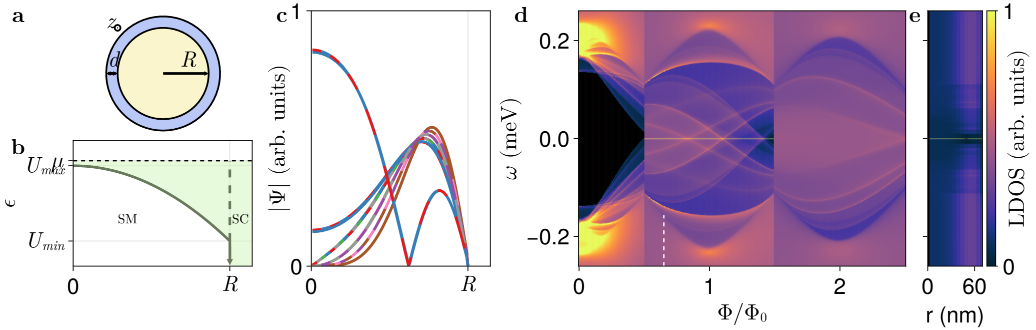
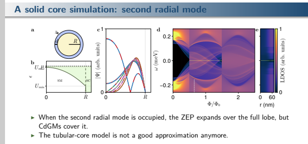


- When the second radial mode is occupied, the ZEP expands over the full lobe, but CdGMs cover it.
- The tubular-core model is not a good approximation anymore.

C. Payá *et al.* 2023, *arXiv*.



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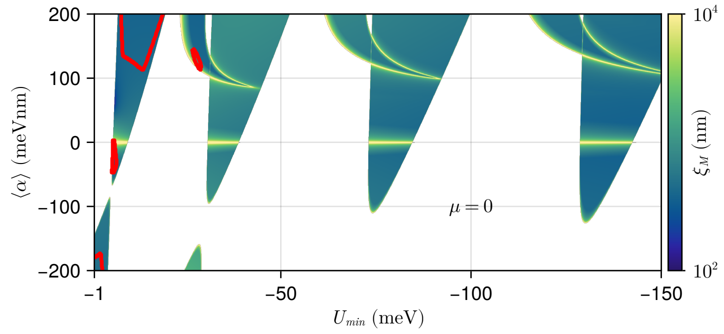
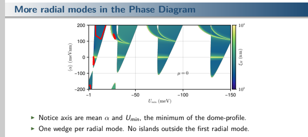
More radial modes in the Phase Diagram



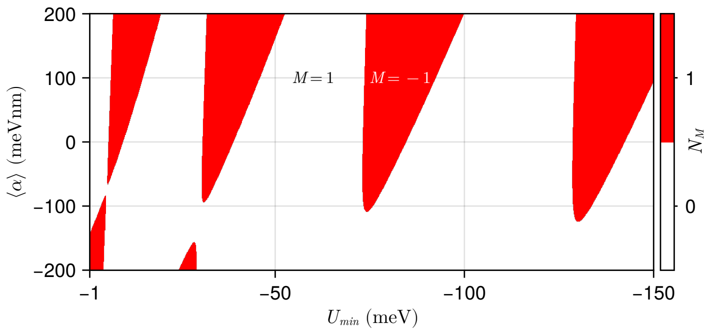
- Notice axis are mean α and U_{min}, the minimum of the dome-profile.
- One wedge per radial mode. No islands outside the first radial mode.

C. Payá *et al.* 2023, *arXiv*.



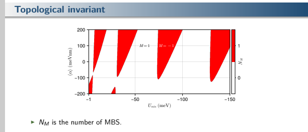
- At $\langle\alpha\rangle = 0$, singularity. No topology possible.
- Begins at $U_{min} = -1$ meV bc. mean α is not well defined at $U_{min} = 0$.

Topological invariant



- N_M is the number of MBS.

C. Payá *et al.* 2023, ***arXiv***.



- N_M calculated with Pfaffian.
- Pfaffian is a generalization of the determinant for antisymmetric matrices.

Where is topology in the Hamiltonian?

Hamiltonian

$$\langle m_J|H|m_J\rangle = H_{K,m_J}\tau_z + V_Z\sigma_z + A_{m_J} + C_{m_J}\sigma_z\tau_z + \alpha k_z\sigma_y\tau_z$$

- *σ_i, τ_i Pauli matrices in spin and electron-hole space.*
- *H_{K,m_J} is the kinetic term (+ effective chemical potential).*
- *V_Z is the effective Zeeman term.*
- *A_{m_J} and C_{mJ} is the coupling of J_z with the magnetic field and the spin.*
- *$\alpha k_z\sigma_y\tau_z$ allows topological transitions when $m_J = 0$.*

S. Vaitiekėnas *et al.* 2020, *Science.*
C. Payá *et al.* 2023, *arXiv.*

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$\alpha k_z\sigma_y\tau_z$ allows topological transitions when $m_J = 0$.

- This hamiltonain is for the MHC, but the structure is valid for the SCM.
- H_K contains μ, the effective chemical potential renormalized by α.
- V_Z is the effective Zeeman term shown before.
- $\alpha k_z\sigma_y\tau_z$ is the term that provides helical bands.

Topology through mode-mixing

- A $\pm m_J$ crossing is parabolic $\epsilon \sim k_z^2$.
- It can be shown that any mode-mixing term $M \sim \mathbb{I}, \sigma_z, \tau_z$:

$$\langle m_J | M | -m_J \rangle \sim \alpha k_z.$$

- $\Rightarrow$ **mode-mixing acts as $p-$wave pairing between $m_J \leftrightarrow -m_J$ states.**

C. Payá *et al.* 2023, *arXiv*.

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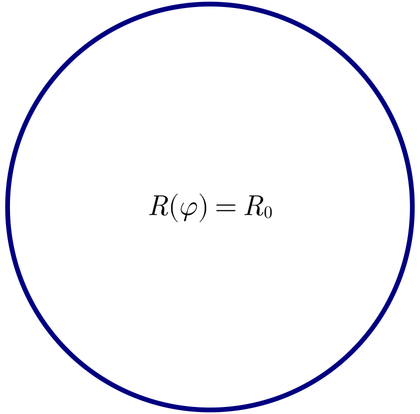
$\Rightarrow$ mode-mixing acts as $p-$wave pairing between $m_J \leftrightarrow -m_J$ states.

- Bands have to cross at $k_z = 0$.
- Demonstration only requires diagonality in spin and electron-hole space.
- Actual size of the minigaps depend on the model.

Shaping the wave-function with radial harmonics

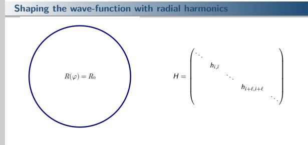


$$H = \begin{pmatrix} \ddots & & & & \\ & h_{i,i} & & & \\ & & \ddots & & \\ & & & h_{i+\ell,i+\ell} & \\ & & & & \ddots \end{pmatrix}$$

C. Payá *et al.* 2023, *arXiv*.

2024-01-10

Full-shell Majorana nanowires
└Disorder-induced mode-mixing: a new mechanism for topology
└The topological transition mechanism
└Shaping the wave-function with radial harmonics



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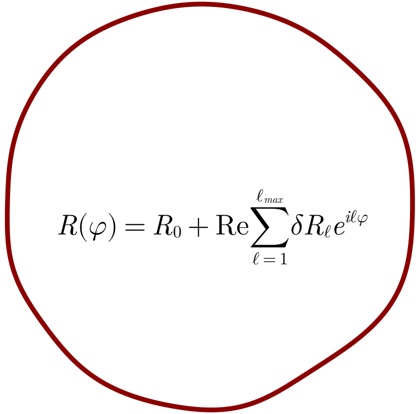
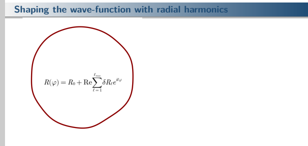


$$R(\varphi) = R_0 + \mathrm{Re}\sum_{\ell=1}^{\ell_{max}} \delta R_\ell e^{i\ell\varphi}$$

C. Payá *et al.* 2023, *arXiv*.



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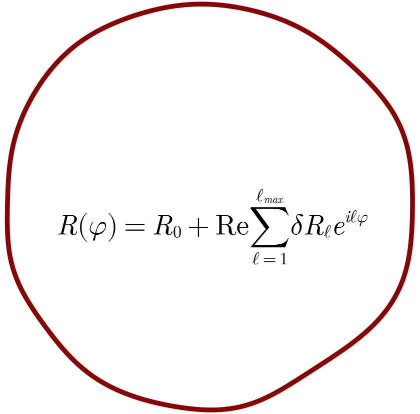

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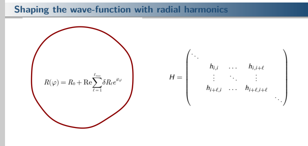
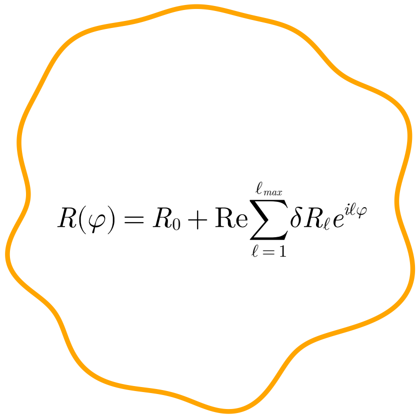
C. Payá *et al.* 2023, *arXiv*.



Shaping the wave-function with radial harmonics



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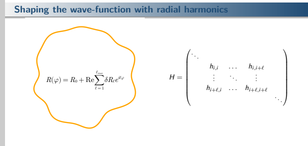

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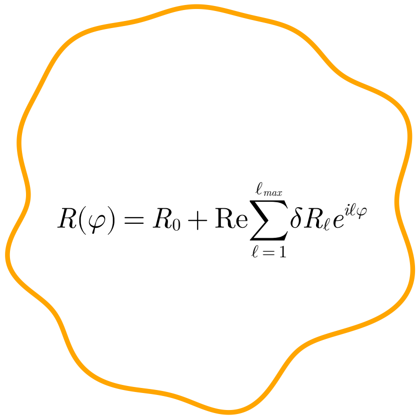


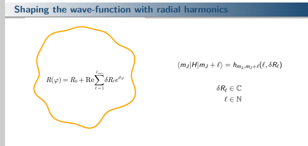
$$R(\varphi) = R_0 + \mathrm{Re}\sum_{\ell=1}^{\ell_{max}} \delta R_\ell e^{i\ell\varphi}$$

$$\langle m_J | H | m_J + \ell \rangle = h_{m_J, m_J+\ell}(\ell, \delta R_\ell)$$

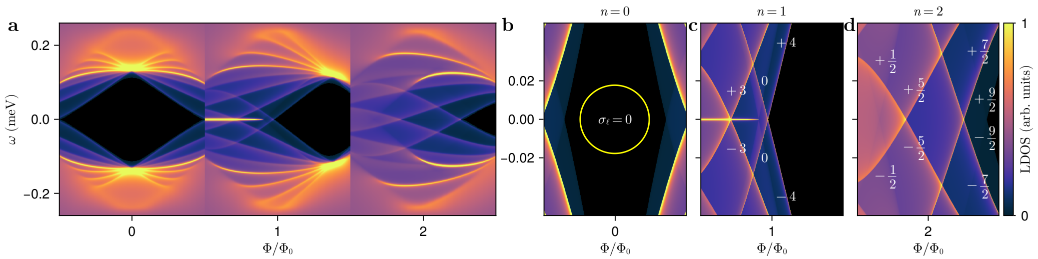
$$\delta R_\ell \in \mathbb{C}$$

$$\ell \in \mathbb{N}$$

C. Payá *et al.* 2023, *arXiv*.

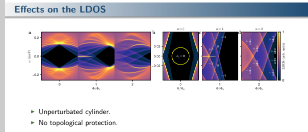


Effects on the LDOS



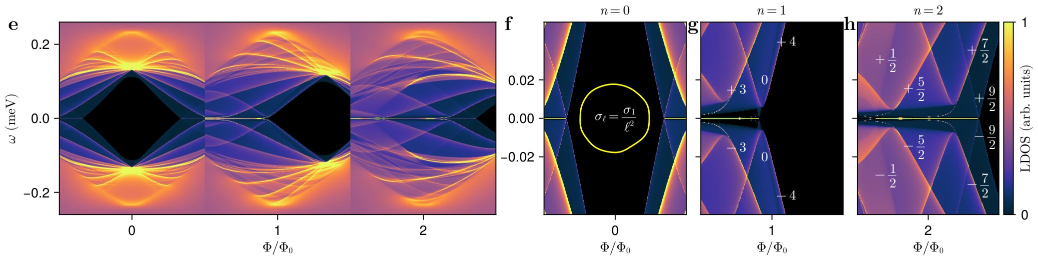
- Unperturbated cylinder.
- No topological protection.

C. Payá *et al.* 2023, *arXiv*.



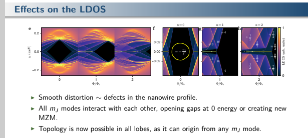
- m_J is tracked even if it's not well defined just by continuity of the CdGMs.
- Smooth model ensures non-divergent second derivative.
- Non-smooth model ensures only non-divergent first derivative.

Effects on the LDOS



- Smooth distortion ∼ defects in the nanowire profile.
- All m_J modes interact with each other, opening gaps at 0 energy or creating new MZM.
- Topology is now possible in all lobes, as it can origin from any m_J mode.

C. Payá *et al.* 2023, *arXiv*.



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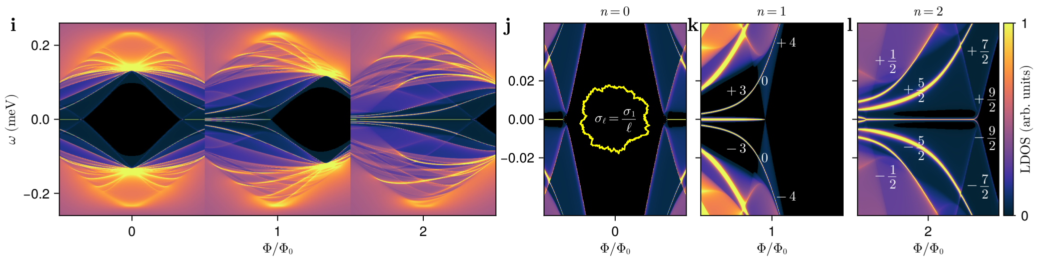
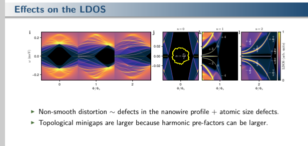


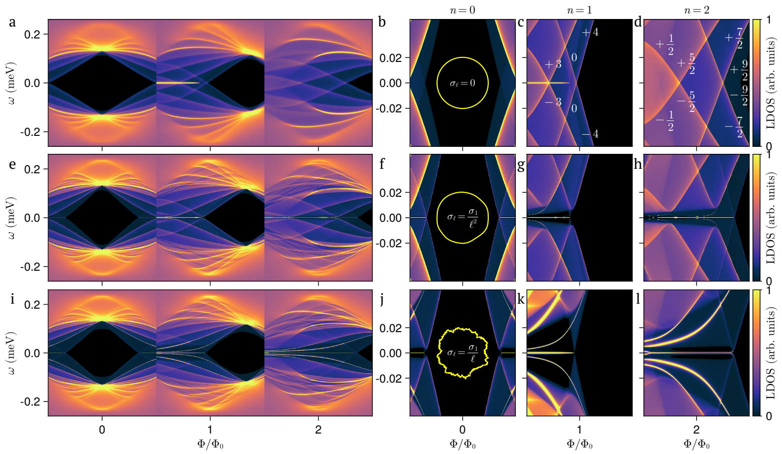
- Non-smooth distortion $\sim$ defects in the nanowire profile + atomic size defects.
- Topological minigaps are larger because harmonic pre-factors can be larger.

C. Payá *et al.* 2023, *arXiv*.



- m_J is tracked even if it's not well defined just by continuity of the CdGMs.
- Smooth model ensures non-divergent second derivative.
- Non-smooth model ensures only non-divergent first derivative.

Effects on the LDOS



C. Payá *et al.* 2023, ***arXiv.***

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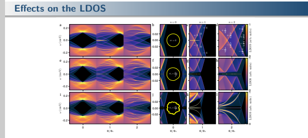
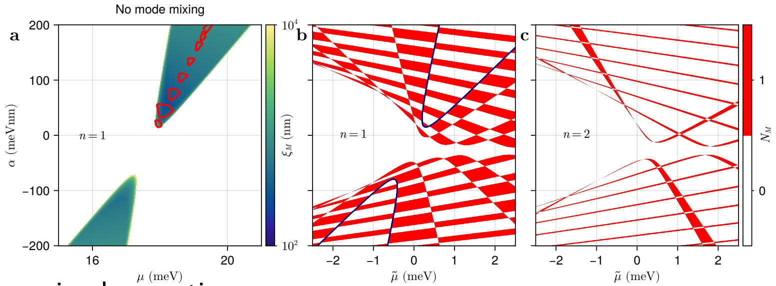
Full-shell Majorana nanowires
└Disorder-induced mode-mixing: a new mechanism for topology
└A nanowire with generic disorder
└Effects on the LDOS



- Remind MZM thickness is artificial.

Tubular-core

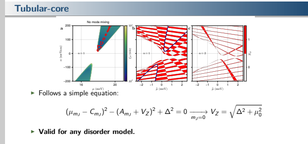


- Follows a simple equation:

$$(\mu_{m_J} - C_{m_J})^2 - (A_{m_J} + V_Z)^2 + \Delta^2 = 0 \xrightarrow[m_J=0]{} V_Z = \sqrt{\Delta^2 + \mu_0^2}$$

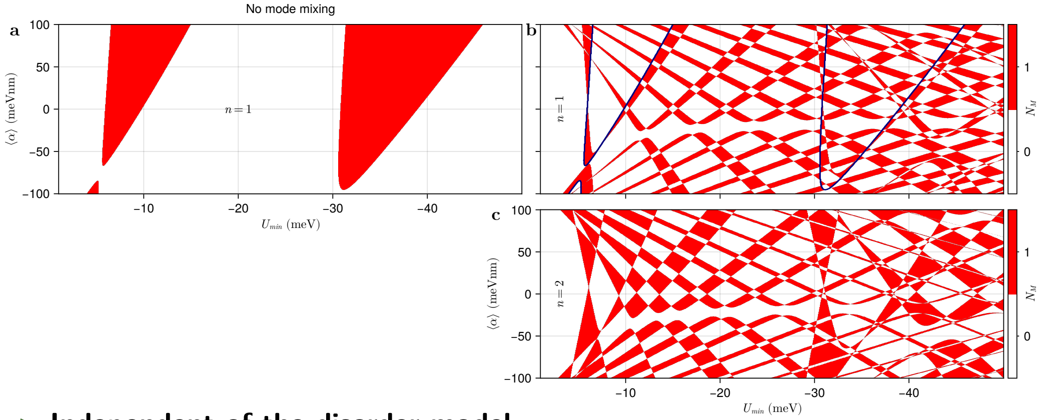
- **Valid for any disorder model.**

C. Payá *et al.* 2023, *arXiv*.



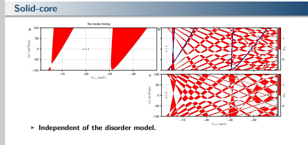
- The mode-mixing PD is just a continuation of the original Lutchyn-Oreg PD.
- No need for islands. All CdGM crossings are now gapped.
- However, minigaps depend on the disorder model.

Solid-core



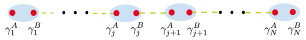
- **Independent of the disorder model.**

C. Payá *et al.* 2023, *arXiv*.



- Even if there is topology in the second lobe, minigaps there are probably quite small.
- Advantage of mode-mixing: topology is not confined to a region of the phase-diagram.

Summary



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Full-shell Majorana nanowires
└─Conclusions
└─Summary
└─Summary

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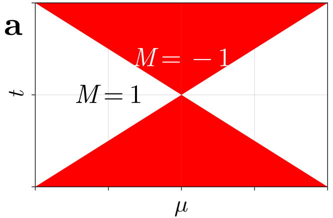

Full-shell Majorana nanowires
└Conclusions
  └Summary
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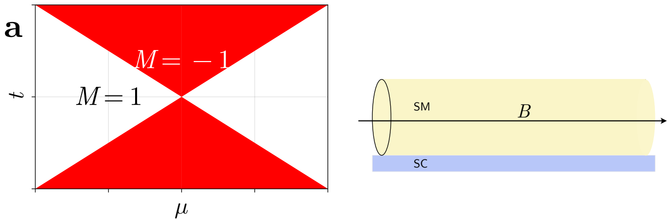

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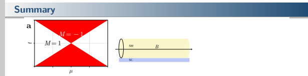

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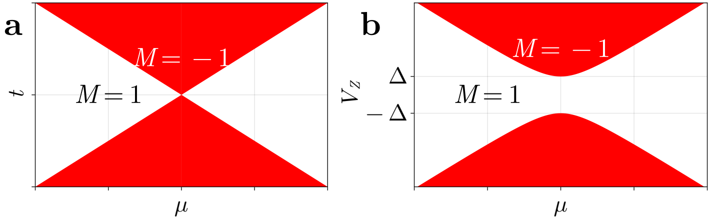

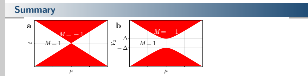

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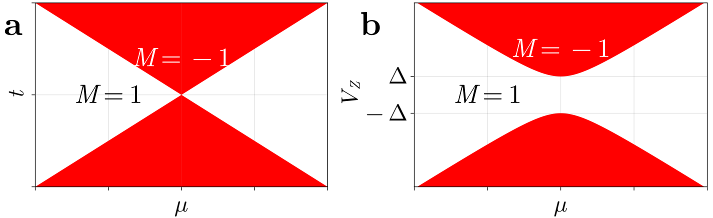

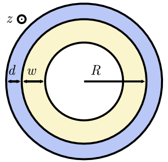

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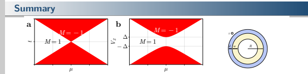

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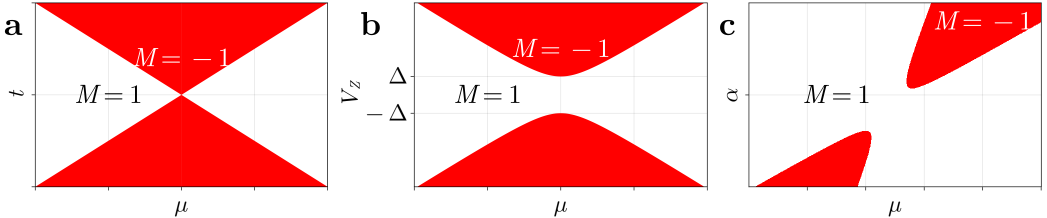

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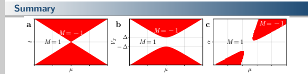

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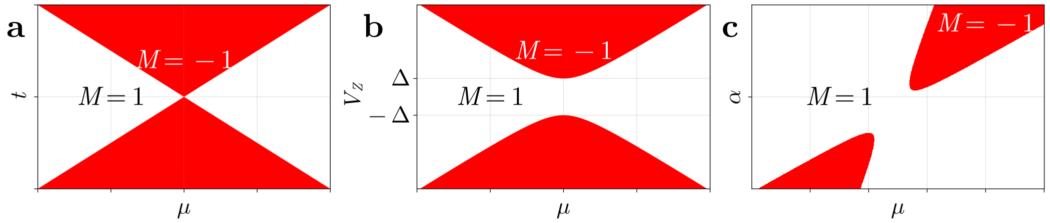

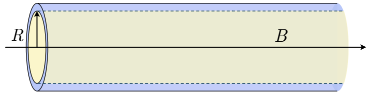

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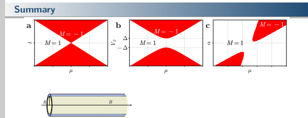

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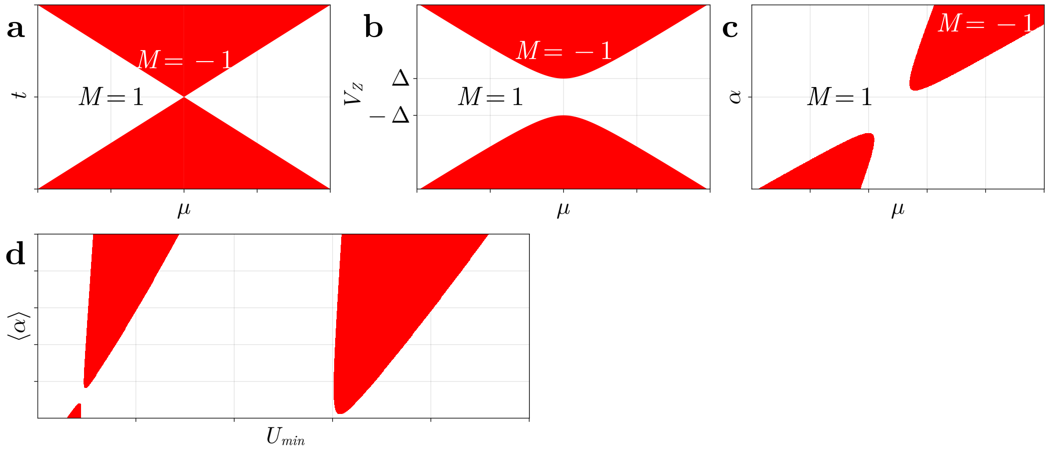

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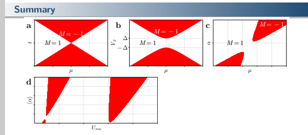

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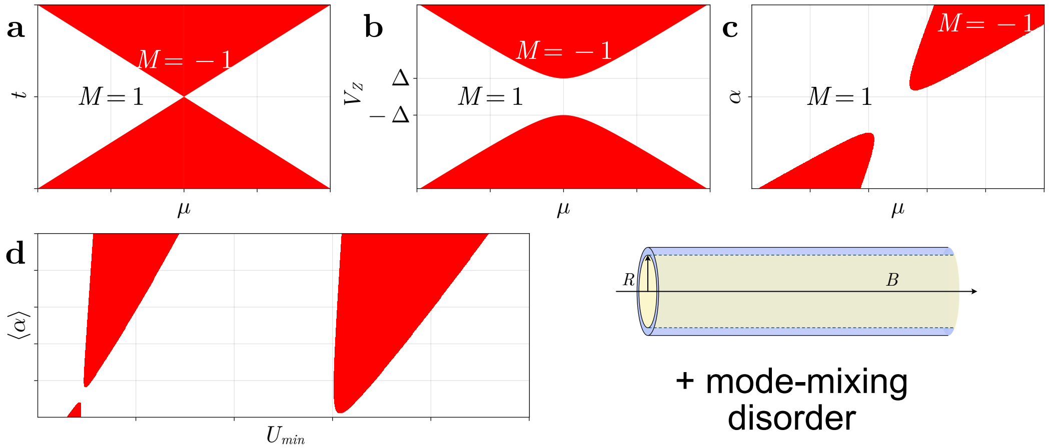

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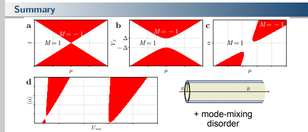

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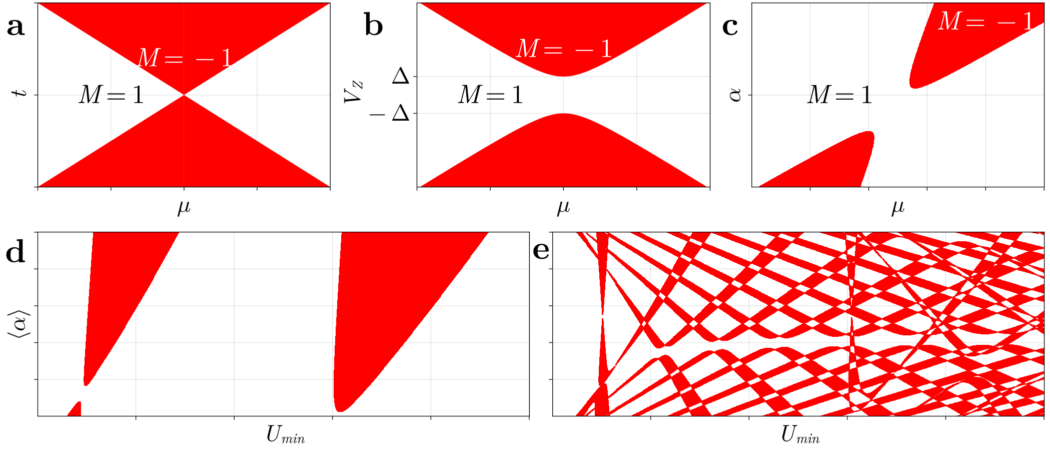

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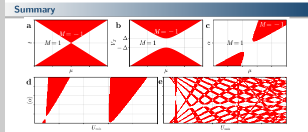

Conclusions

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C. Payá *et al.* 2023, *arXiv*.

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Take home message

Majorana physics of full-shell nanowires is very rich. For pristine configurations, the tubular-core model is the optimal candidate but, in the presence of mode-mixing, half of the parameter space is suitable for topologically protected Majorana bound states.

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Full-shell Majorana nanowires
A theoretical description

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January 10, 2024

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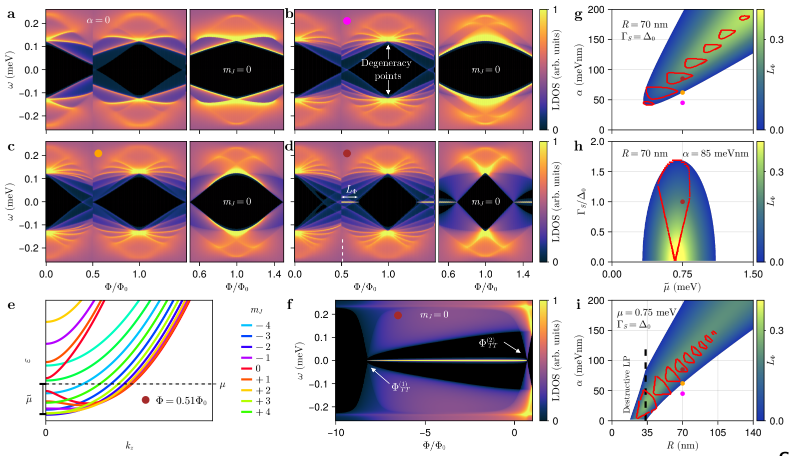
Hollow-core results



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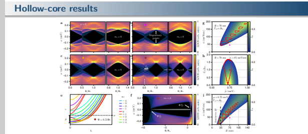
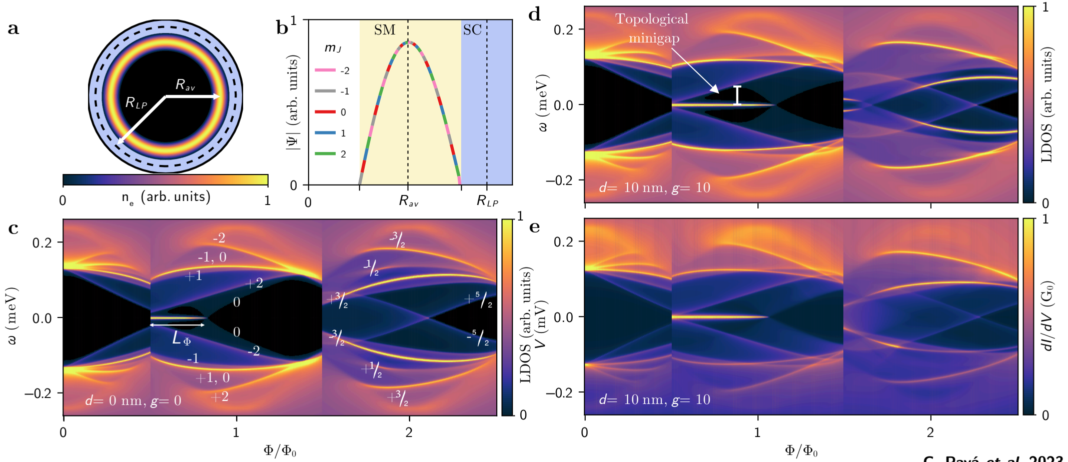


Modified hollow-core results



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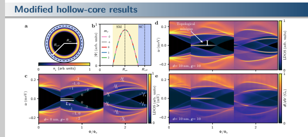
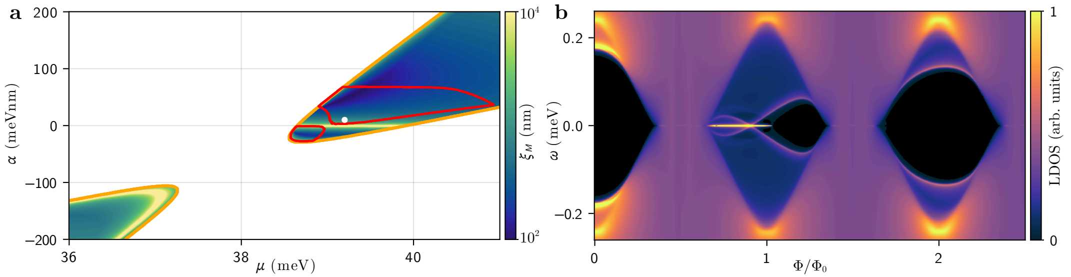


Destructive Litle-Parks



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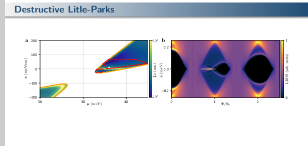
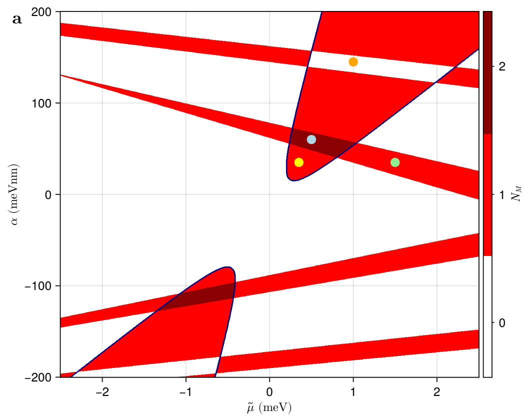
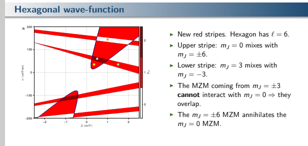


Hexagonal wave-function



- New red stripes. Hexagon has $\ell = 6$.
- Upper stripe: $m_J = 0$ mixes with $m_J = \pm 6$.
- Lower stripe: $m_J = 3$ mixes with $m_J = -3$.
- The MZM coming from $m_J = \pm 3$ **cannot** interact with $m_J = 0 \Rightarrow$ they overlap.
- The $m_J = \pm 6$ MZM annihilates the $m_J = 0$ MZM.

C. Payá *et al.* 2023, *arXiv*.



- $m_J \neq 0$ stripes are just a continuation of $m_J = 0$ (difficult to see in just one slide).
- In blue, original $m_J = 0$ PD border.

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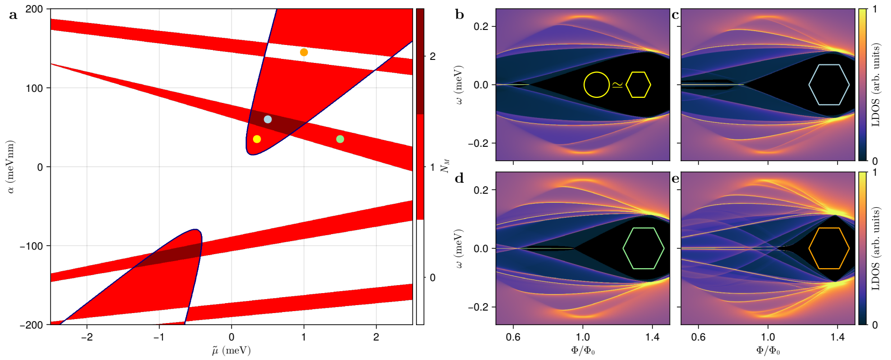
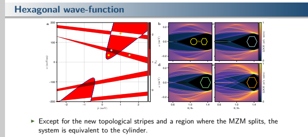


- Except for the new topological stripes and a region where the MZM splits, the system is equivalent to the cylinder.

C. Payá *et al.* 2023, *arXiv*.



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