Full-shell Majorana nanowires

A theoretical description

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Outline

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*.
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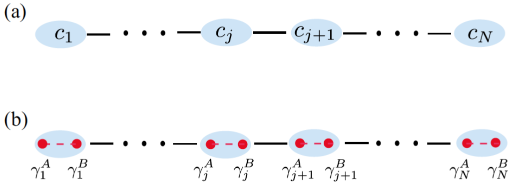
- Majorana representation:

$$c_j = \tfrac{1}{2} \left(\gamma_j^A + i\gamma_j^B \right), \quad c_j^\dagger = \tfrac{1}{2} \left(\gamma_j^A - i\gamma_j^B \right)$$



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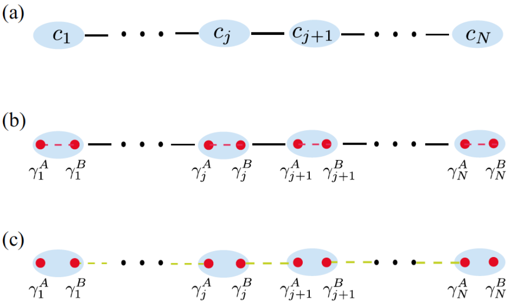
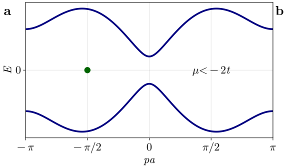
- Hamiltonian in terms of Majorana operators:

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



Kitaev chain energy dispersion

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



b

c

d

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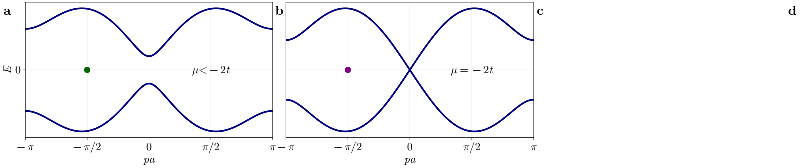

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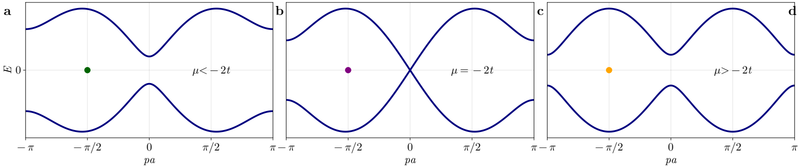

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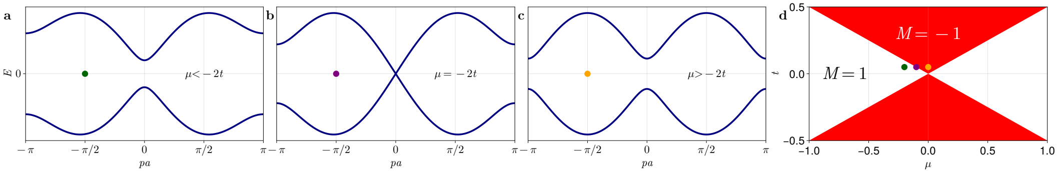

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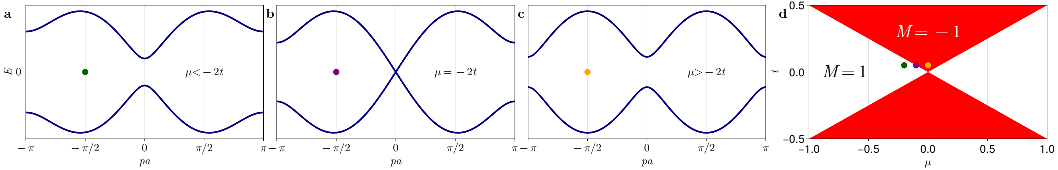

- Two distinct phases characterized by a $\mathbb{Z}_2$ invariant, $M = (-1)^{\nu}$.

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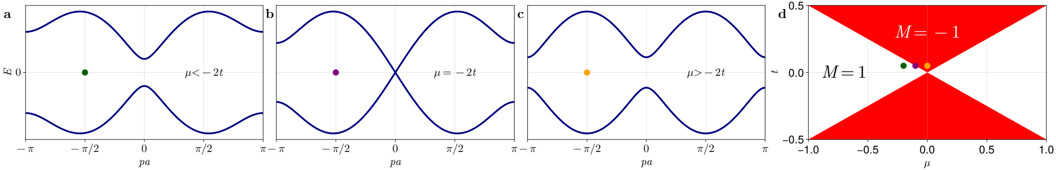

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- ν is the number of times the energy gap closes in the Brillouin zone.

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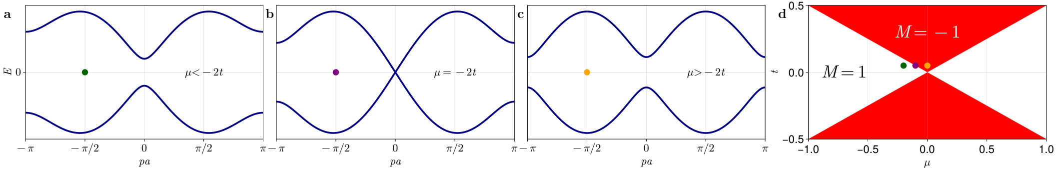

- Two distinct phases characterized by a $\mathbb{Z}_2$ invariant, $M = (-1)^{\nu}$.
- ν is the number of times the energy gap closes in the Brillouin zone.
- $M = 1 \Rightarrow$ no unpaired MZM. $M = -1 \Rightarrow$ unpaired MZM (bulk-boundary correspondance).

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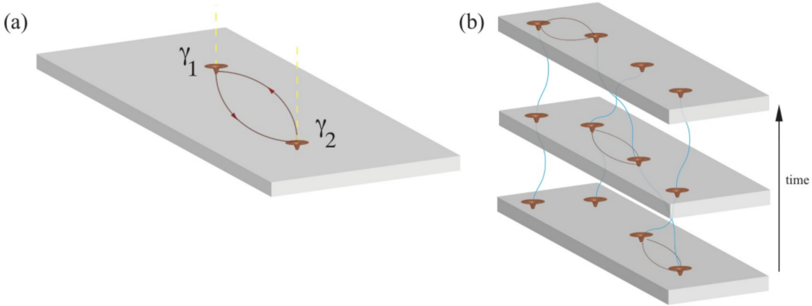
Majoranas for qubits



- MZM are non-Abelian anyons.
- Gap closing/reopening ⇒ topological protection.

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We need a $p-$wave superconductor!

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

L. Fu and C. L. Kane 2008, *Phys. Rev. Lett.*
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- Lutchyn and Oreg: proximitize semiconductors with strong spin-orbit coupling.

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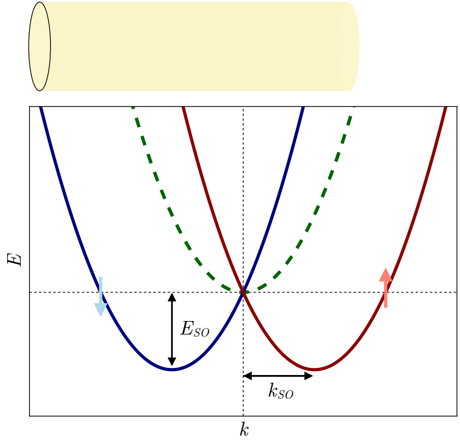
Rashba, Zeeman and helical bands



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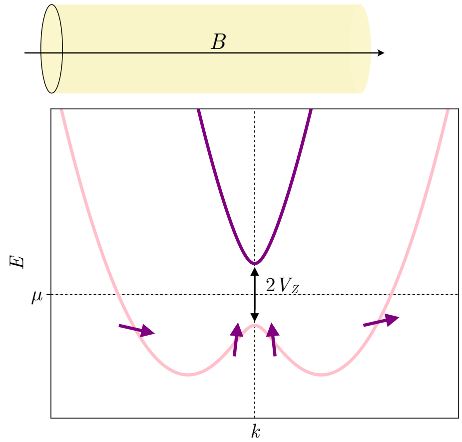

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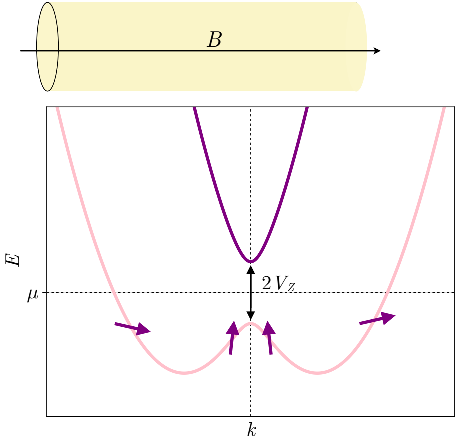

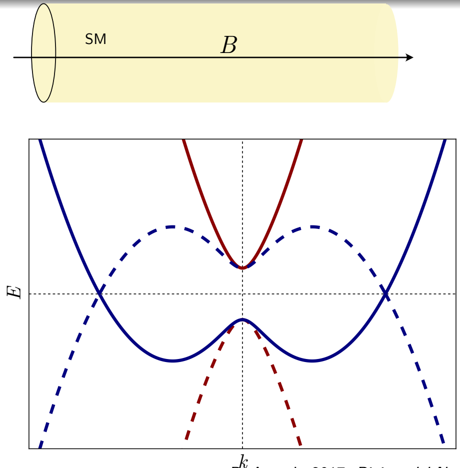

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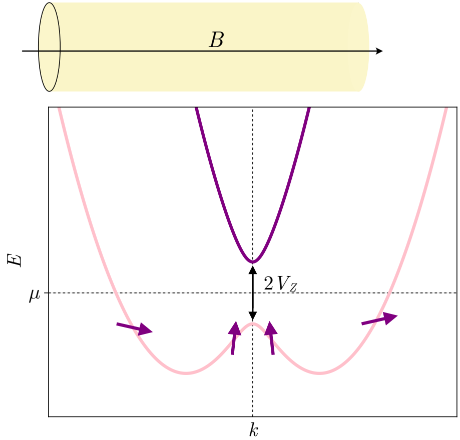

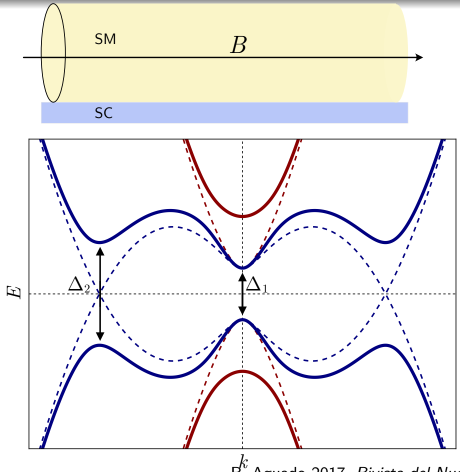

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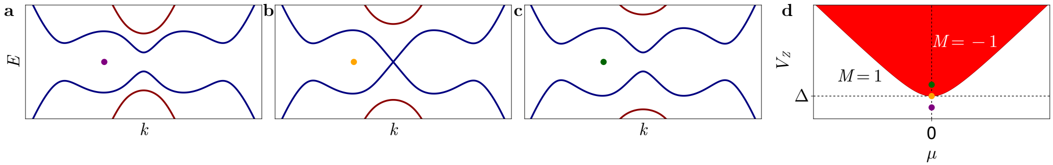
Topological phase transition



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

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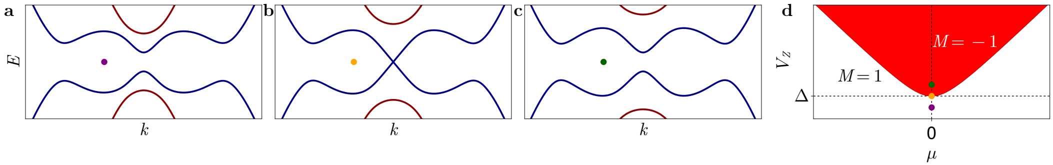

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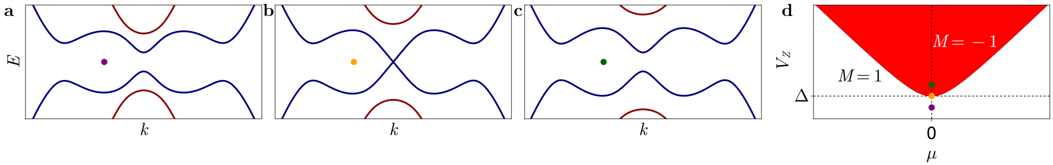

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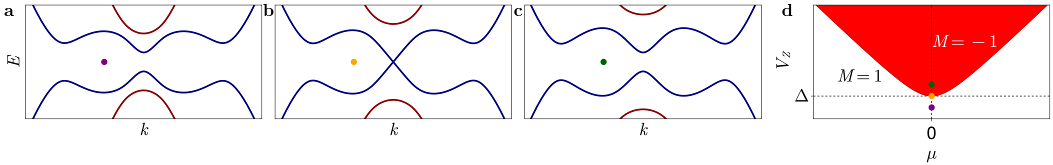

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- $V_Z \gtrsim \Delta$.
- Need high g-factor materials and high magnetic fields.

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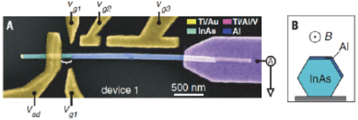
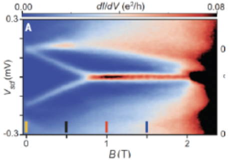
Searching for Majoranas

- Strong experimental interest.



Zero-bias anomalies in tunneling spectroscopy experiments

Mourik 2012, Albrecht 2016, Deng 2016



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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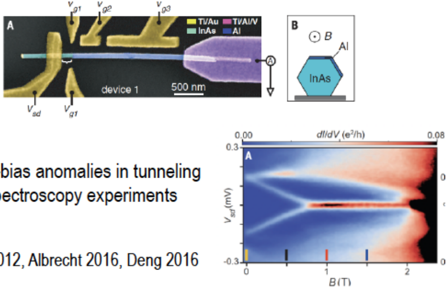

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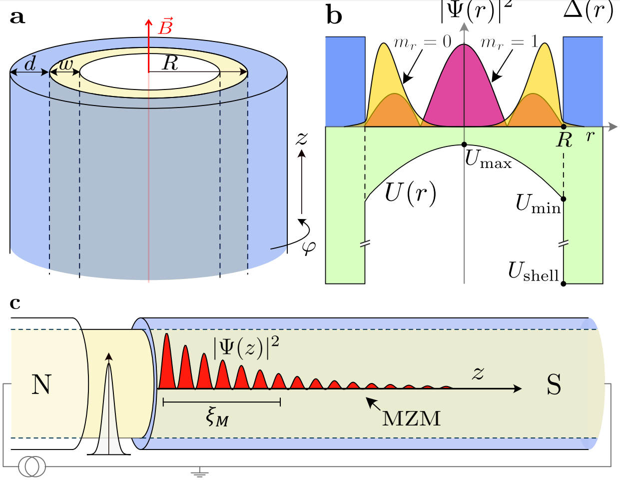
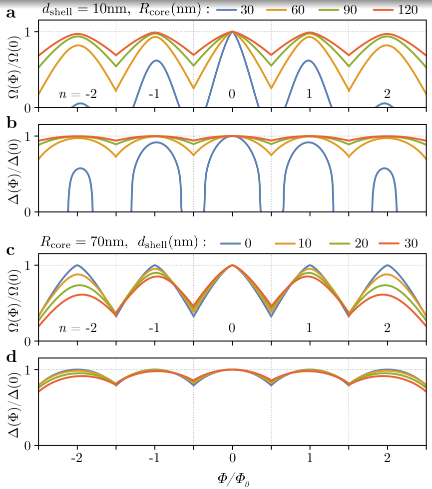
The full-shell nanowire



S. Vaitiekėnas *et al.* 2020, *Science*.
P. San-Jose *et al.* 2023, *Phys. Rev. B*.
C. Payá *et al.* 2023, *arXiv*.

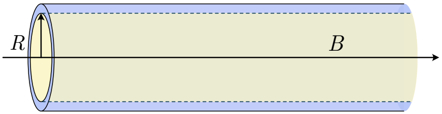
The Little-Parks effect



- Cylinder $\Leftrightarrow$ 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 $\Rightarrow$ 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. $\Phi \sim \Phi_0$.

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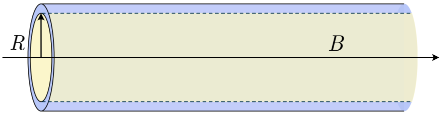

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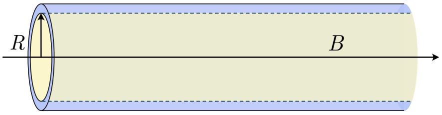
- Good generalized angular momentum $J_z = -i\partial_\varphi + \frac{1}{2}\sigma_z + \frac{1}{2}n\tau_z$:

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

S. Vaitiekėnas *et al.* 2020, *Science*.
P. San-Jose *et al.* 2023, *Phys. Rev. B*.
C. Payá *et al.* 2023, *arXiv*.

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.
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- $\Rightarrow$ Computationally affordable.

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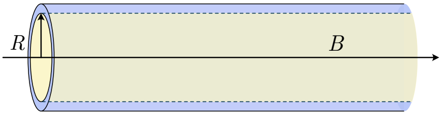

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S. Vaitiekėnas *et al.* 2020, *Science*.
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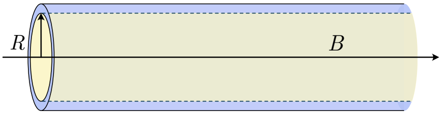

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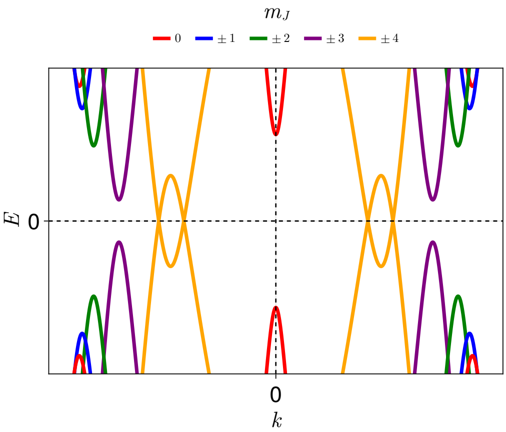
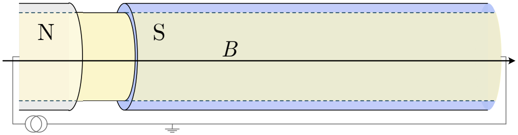
- $\Rightarrow$ Computationally affordable.
- Easier to understand physics.
- SOC and chemical potential non-tunable.

S. Vaitiekėnas *et al.* 2020, *Science*.
P. San-Jose *et al.* 2023, *Phys. Rev. B*.
C. Payá *et al.* 2023, *arXiv*.

The CdGM analog states





C. Payá *et al.* 2023, *arXiv*.
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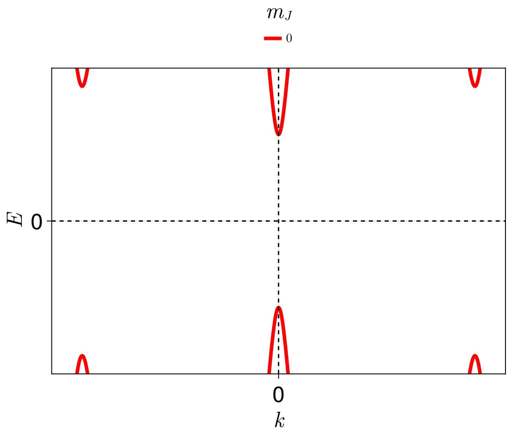

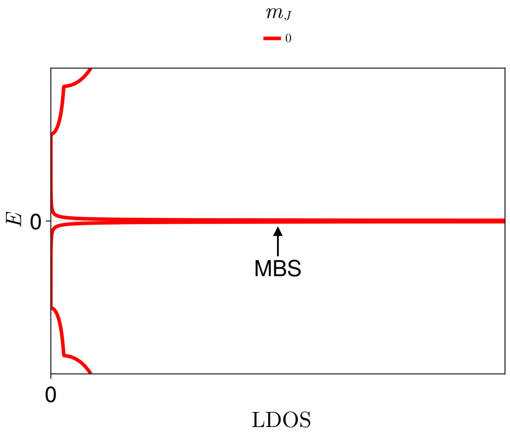

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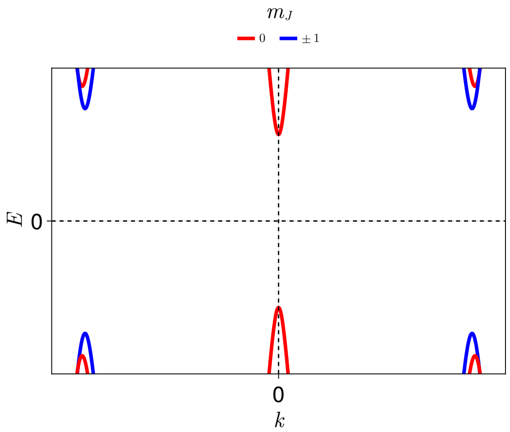

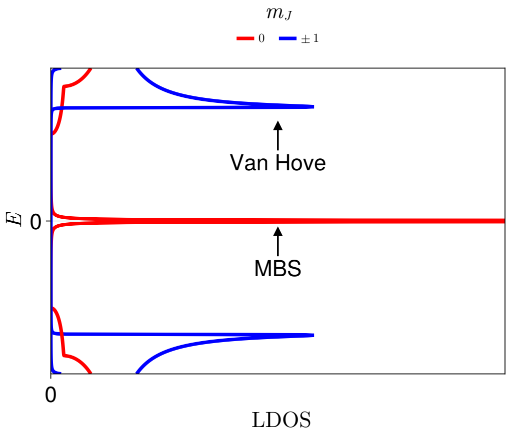

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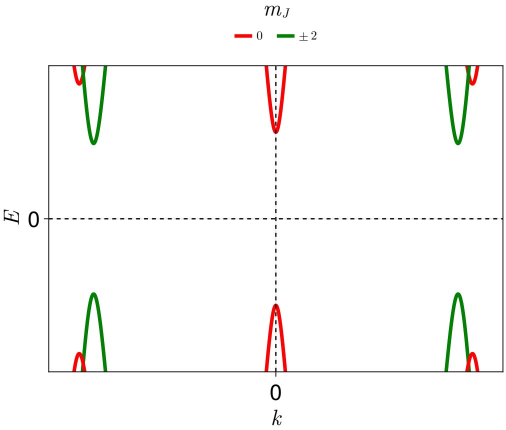

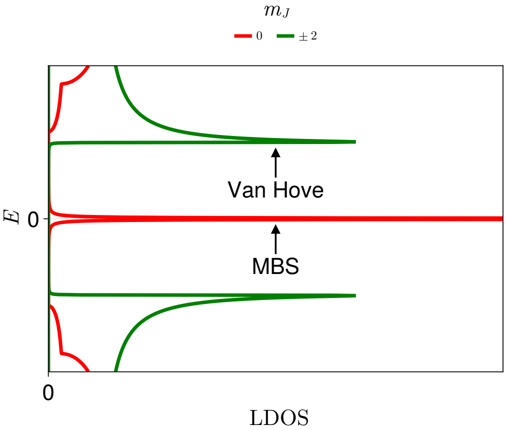

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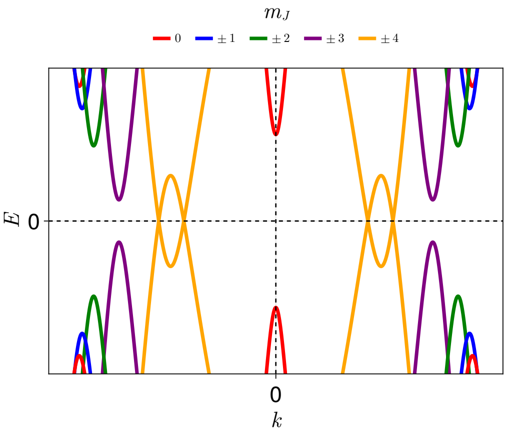

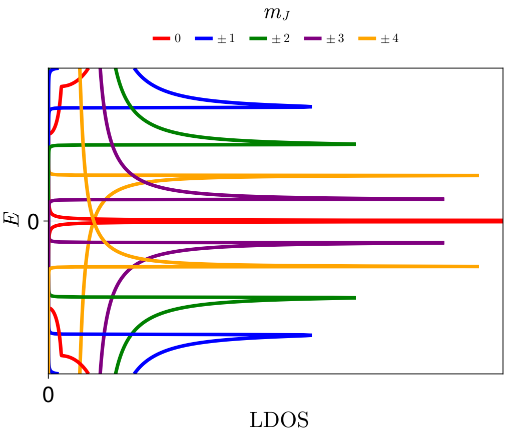

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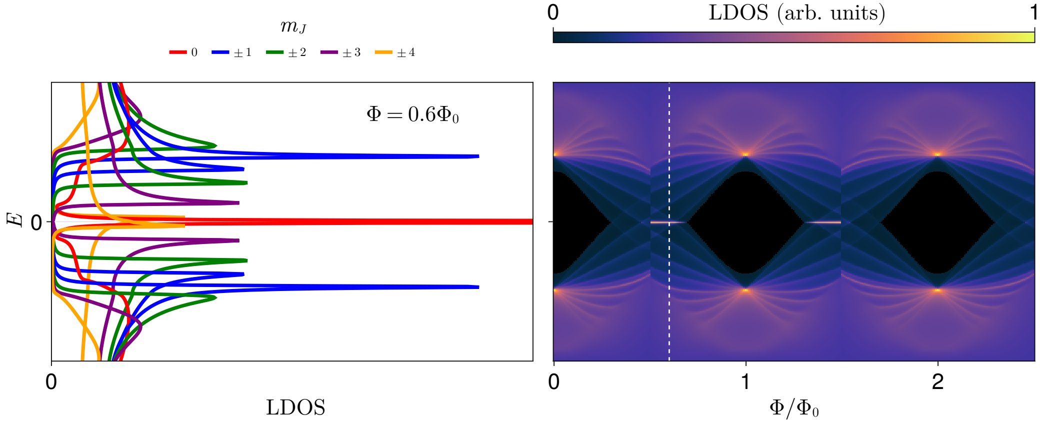
LDOS vs. flux



C. Payá *et al.* 2023, *arXiv*.
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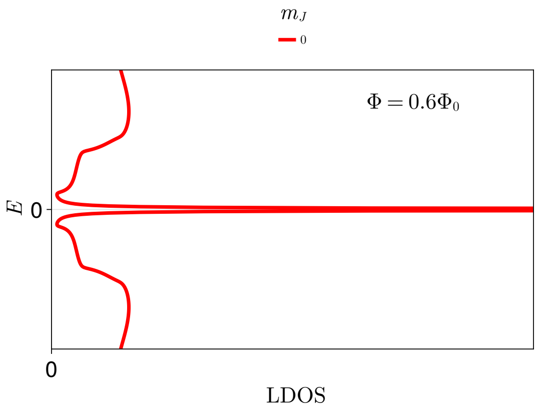
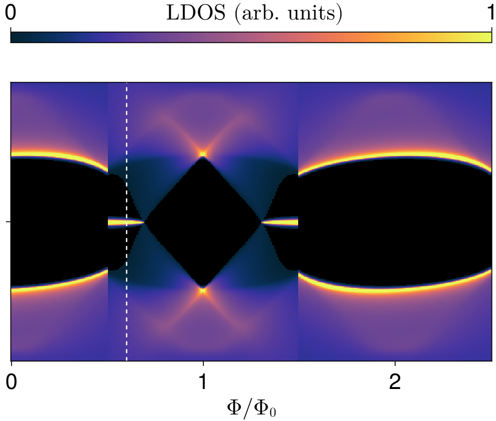
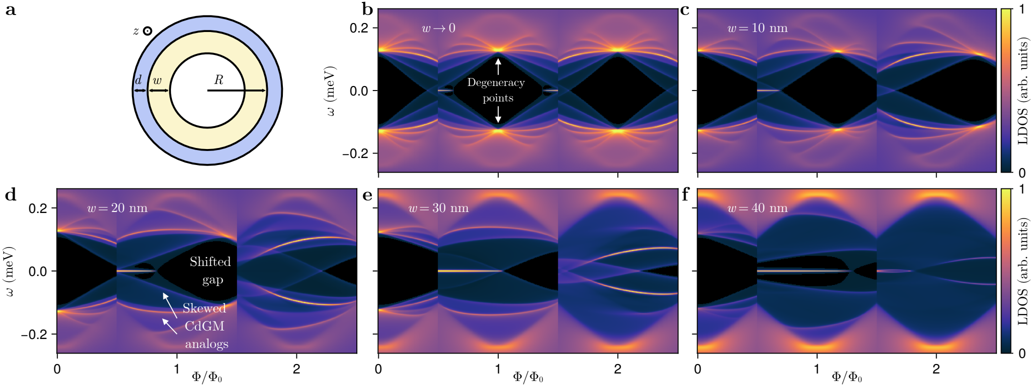




C. Payá *et al.* 2023, *arXiv*.
P. San-Jose *et al.* 2023, *Phys. Rev. B*.

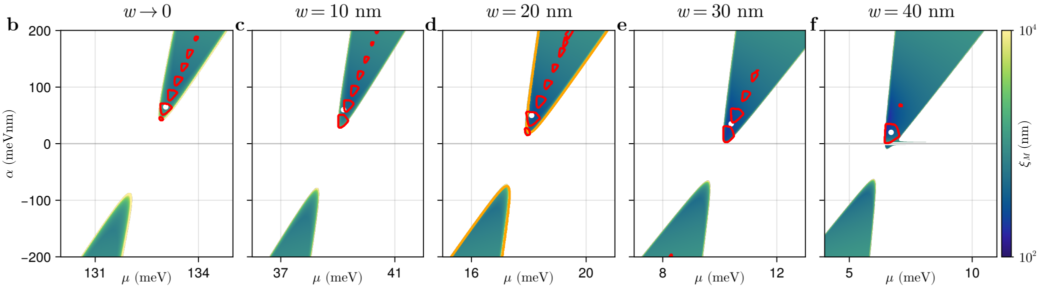
The tubular-core model



- $\frac{\Phi_{dp}}{\Phi_0} = \left(\frac{R_{LP}}{R_{av}}\right)^2$, 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*.

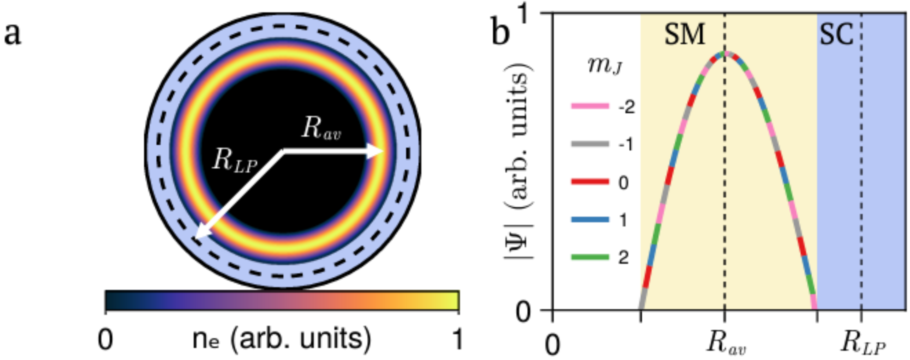
The tubular-core model



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

C. Payá *et al.* 2023, *arXiv*.

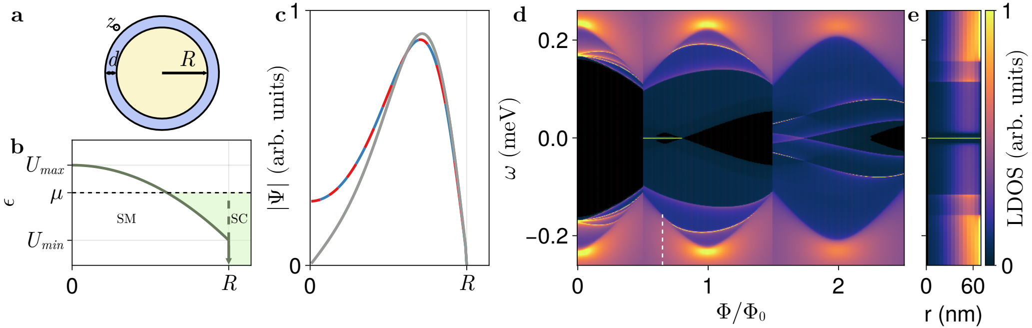
The modified hollow-core model



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

C. Payá *et al.* 2023, *arXiv*.

A solid core simulation: first radial mode



C. Payá *et al.* 2023, ***arXiv***.

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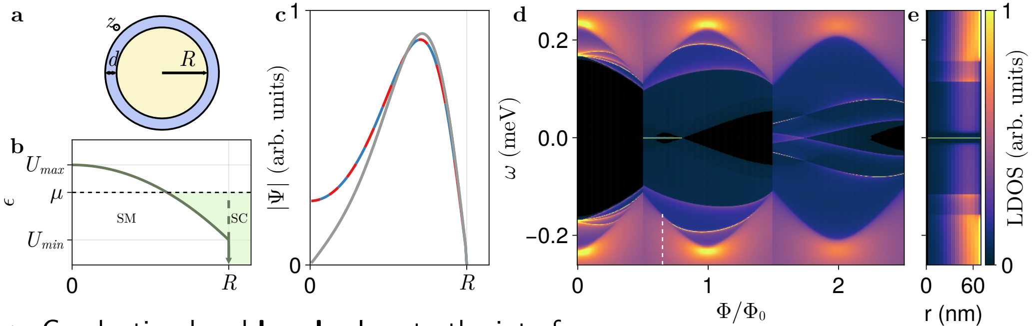
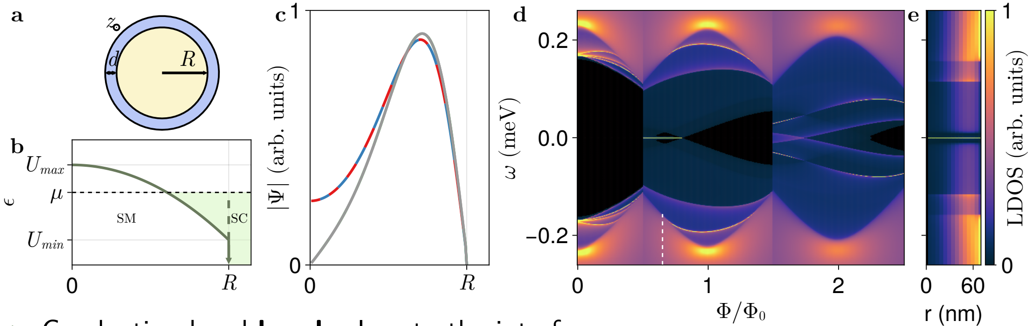


- Conduction band **bends** close to the interface.

C. Payá *et al.* 2023, ***arXiv***.

A solid core simulation: first radial mode



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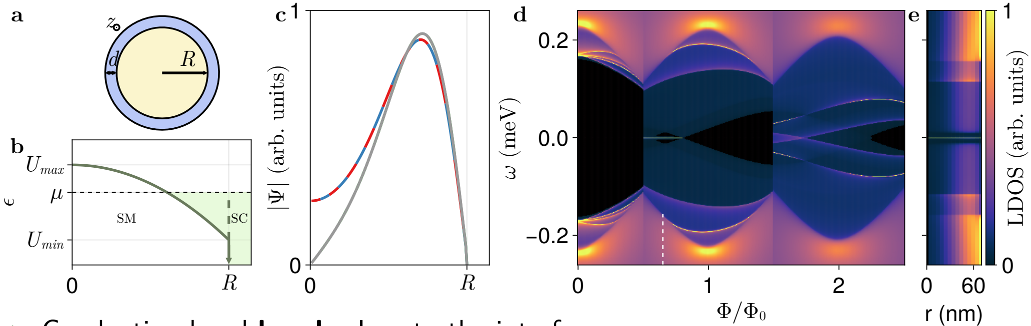
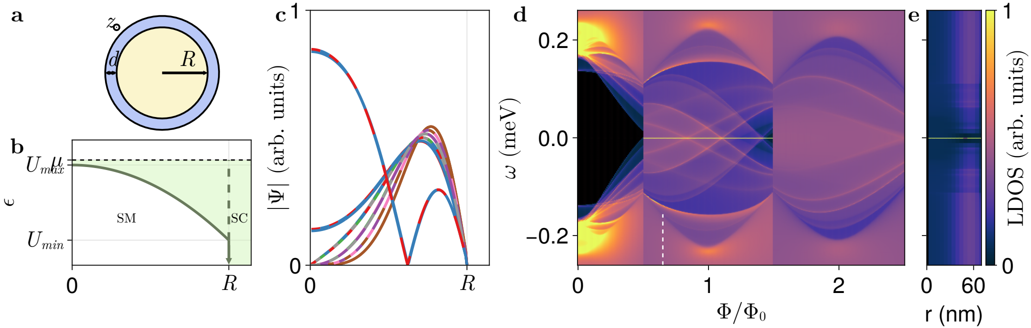


- Conduction band **bends** close to the interface.
- Different boundary conditions: WF can extend to $r = 0$.
- If all WF are in first radial mode, physics similar to the tubular-core.

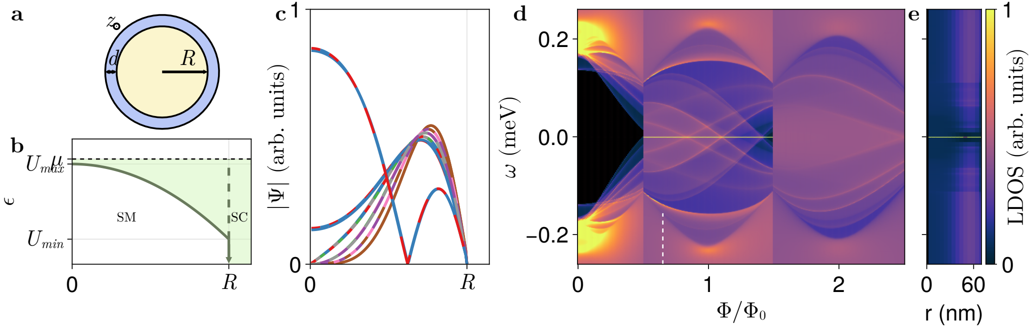
C. Payá *et al.* 2023, *arXiv*.

A solid core simulation: second radial mode



C. Payá *et al.* 2023, ***arXiv***.

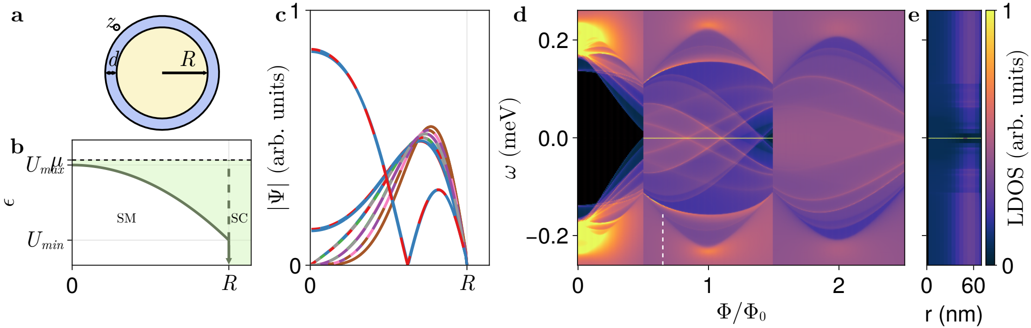
A solid core simulation: second radial mode



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

C. Payá *et al.* 2023, *arXiv*.

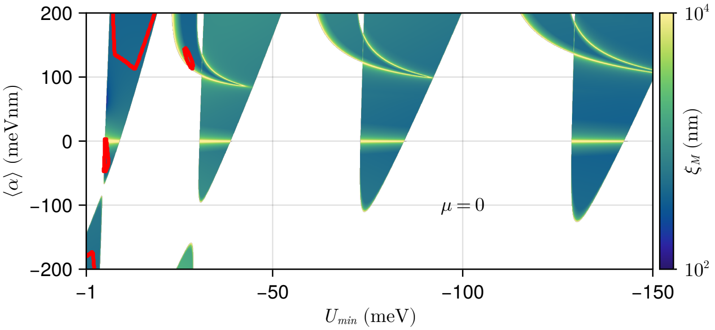
A solid core simulation: second radial mode



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

C. Payá *et al.* 2023, ***arXiv***.

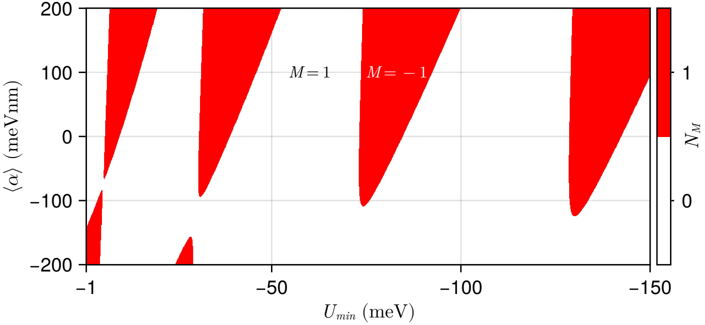
More radial modes in the Phase Diagram



- 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*.

Topological invariant



- N_M is the number of MBS.

C. Payá *et al.* 2023, *arXiv*.

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*.

Topology through mode-mixing

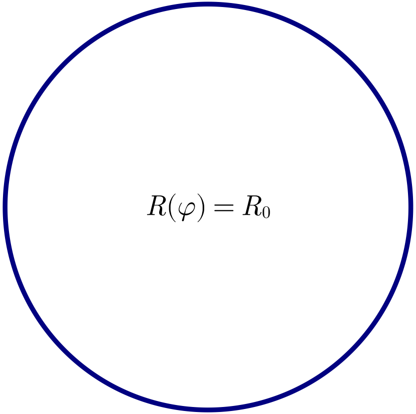
- A $\pm m_J$ crossing is parabolic $\epsilon \sim k_z^2$.
- It can be shown that any mode-mixing term $M \sim \mathbb{I}, \sigma_z, \tau_z$:

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

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

C. Payá *et al.* 2023, *arXiv*.

Shaping the wave-function with radial harmonics



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

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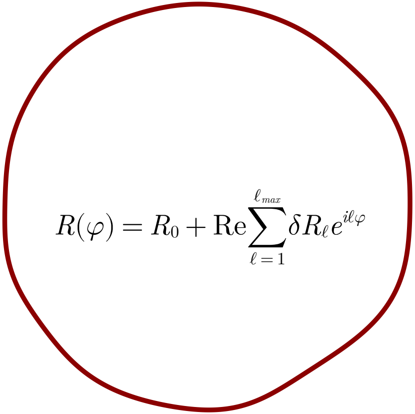

$$R(\varphi) = R_0 + \mathrm{Re}\sum_{\ell=1}^{\ell_{max}} \delta R_\ell e^{i\ell\varphi}$$

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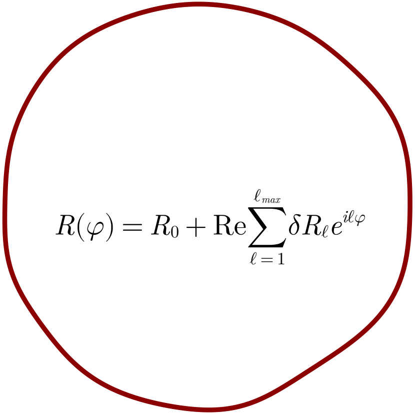

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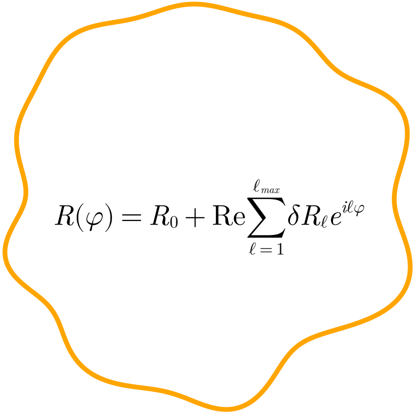

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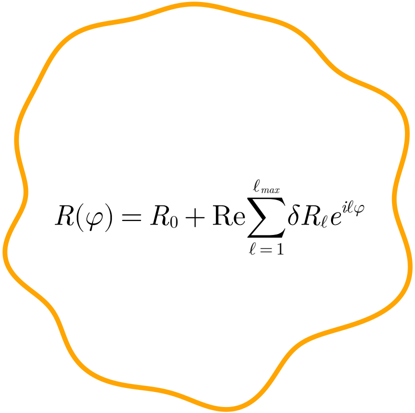


$$R(\varphi) = R_0 + \mathrm{Re}\sum_{\ell=1}^{\ell_{max}} \delta R_\ell e^{i\ell\varphi}$$

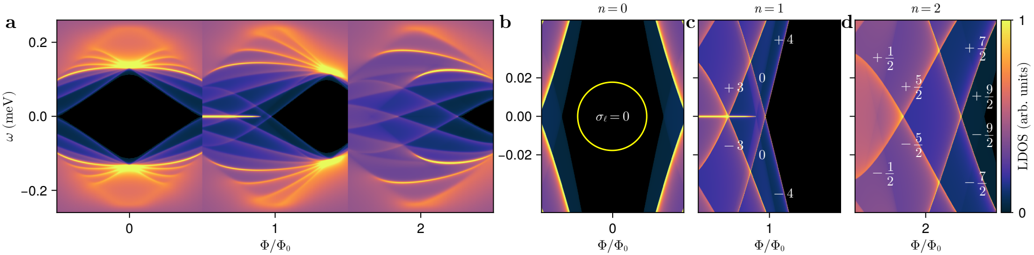
$$\langle m_J|H|m_J+\ell\rangle = h_{m_J,m_J+\ell}(\ell,\delta R_\ell)$$

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

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

C. Payá *et al.* 2023, *arXiv*.

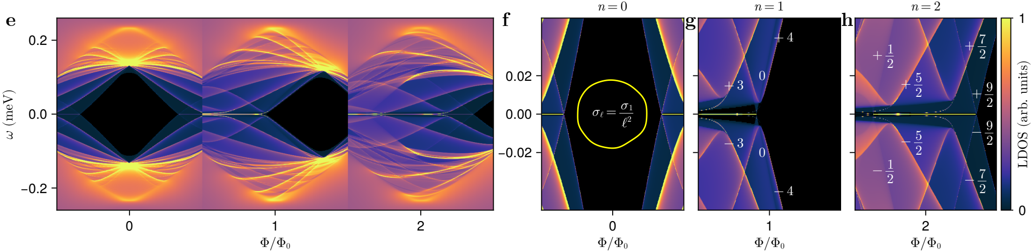
Effects on the LDOS



- Unperturbated cylinder.
- No topological protection.

C. Payá *et al.* 2023, *arXiv*.

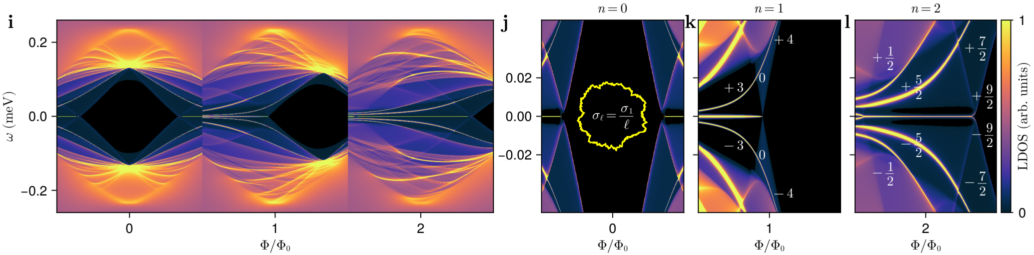
Effects on the LDOS



- Smooth distortion $\sim$ 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*.

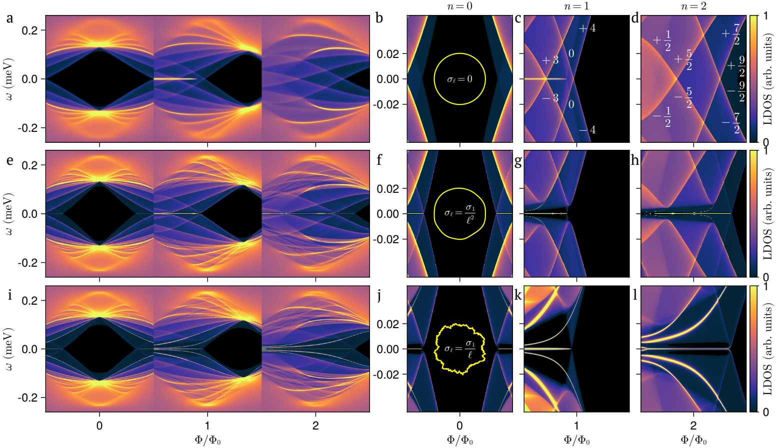
Effects on the LDOS



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

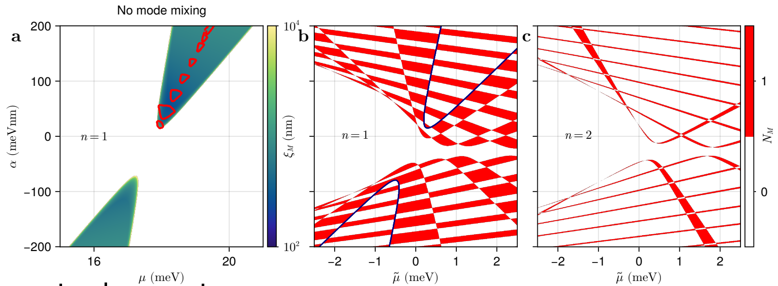
C. Payá *et al.* 2023, *arXiv*.

Effects on the LDOS



C. Payá *et al.* 2023, ***arXiv***.

Tubular-core



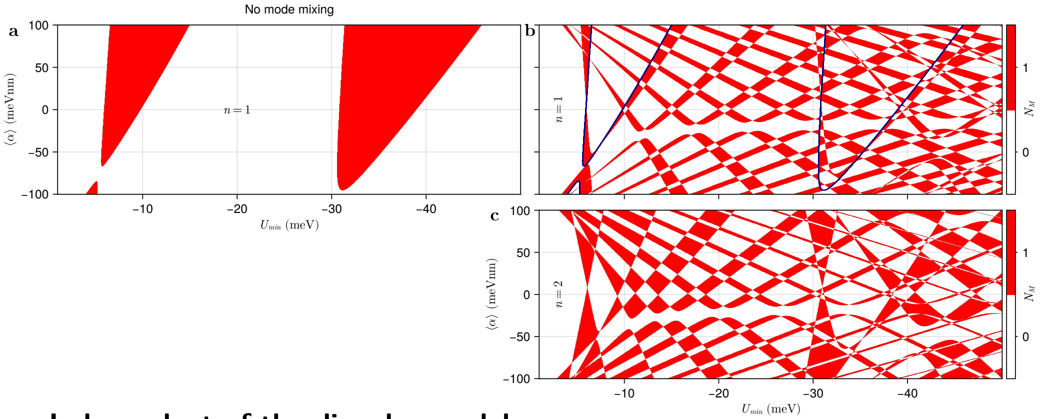
- Follows a simple equation:

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

- **Valid for any disorder model.**

C. Payá *et al.* 2023, *arXiv*.

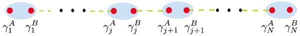
Solid-core



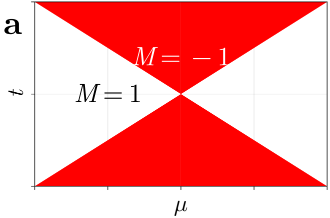
- **Independent of the disorder model.**

C. Payá *et al.* 2023, *arXiv*.

Summary


γ_1^A γ_1^B γ_j^A γ_j^B γ_{j+1}^A γ_{j+1}^B γ_N^A γ_N^B

Summary



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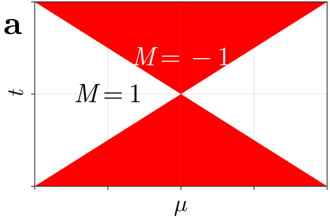

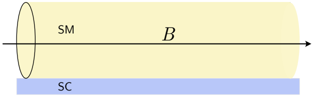

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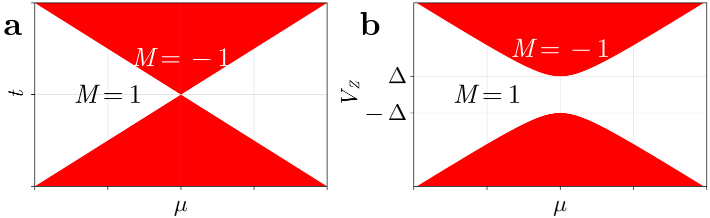

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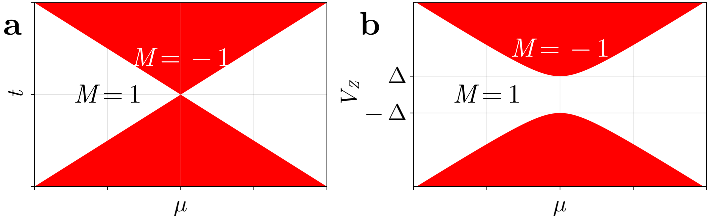
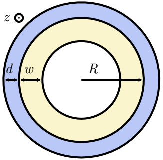
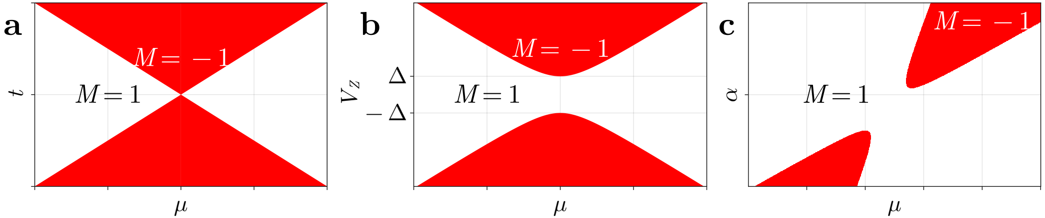
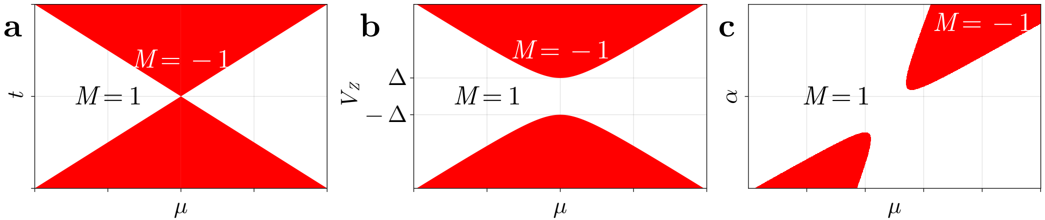


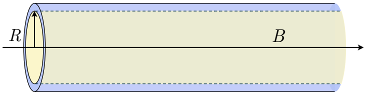


Summary

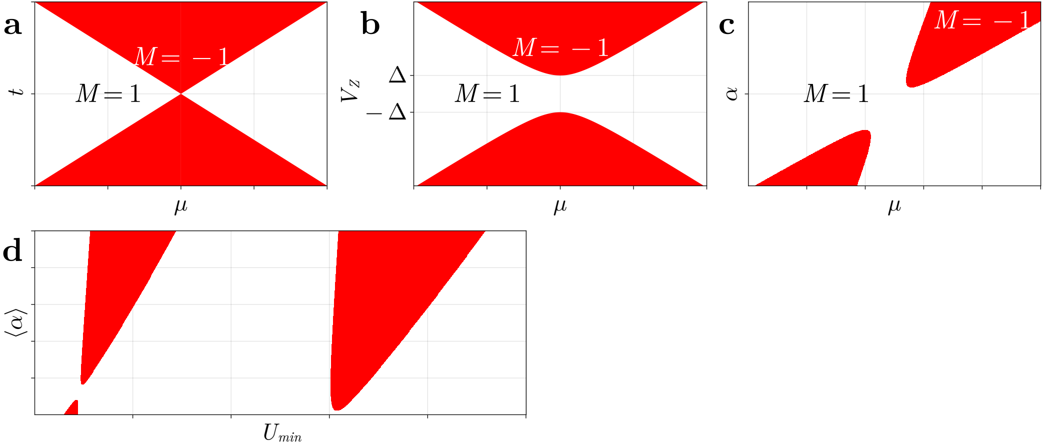


Summary

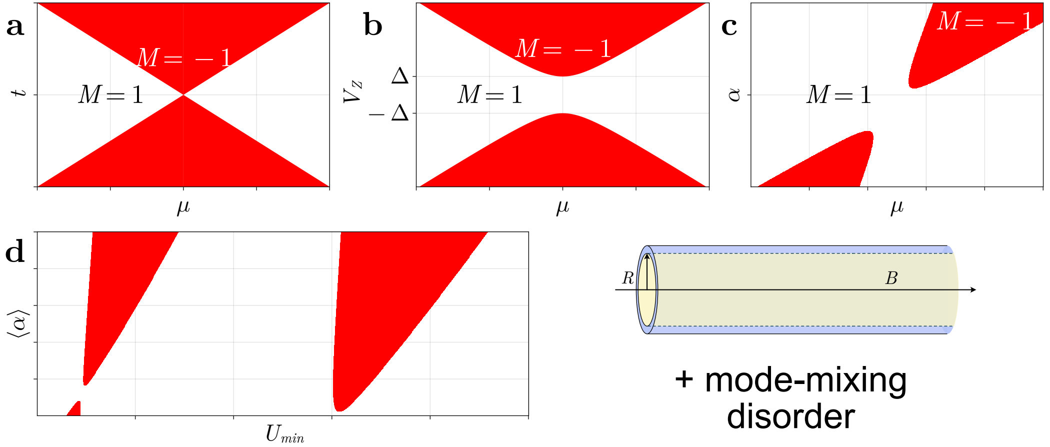




Summary


a
$M = -1$
$M = 1$
t
μ
b
$M = -1$
$M = 1$
V_Z
Δ
$-\Delta$
μ
c
$M = -1$
$M = 1$
α
μ
d
$\langle\alpha\rangle$
U_{min}

Summary


a
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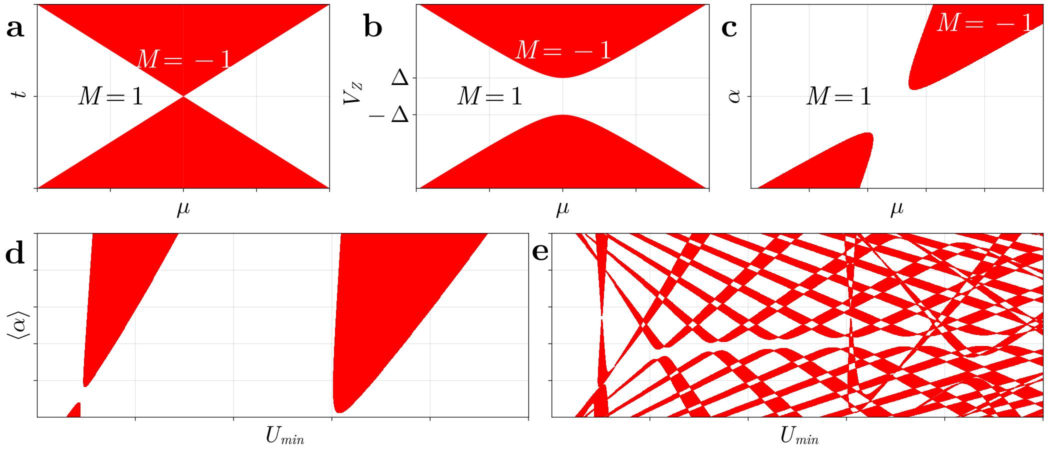
$M = -1$
$M = 1$
t
μ
V_Z
Δ
$-\Delta$
α
$\langle\alpha\rangle$
U_{min}
R
B
+ mode-mixing
disorder

Summary


a
$M=-1$
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t
μ
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$M=1$
V_Z
Δ
$-\Delta$
μ
c
$M=-1$
$M=1$
α
μ
d
$\langle\alpha\rangle$
U_{min}
e
U_{min}

Conclusions

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  1. Majorana zero modes appear at odd LP lobes coexist with CdGM analog states.

C. Payá *et al.* 2023, *arXiv*.

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  6. Generic disorder generates new MZMs and opens topological minigaps.

C. Payá *et al.* 2023, *arXiv*.

Conclusions

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.

C. Payá *et al.* 2023, *arXiv*.

Full-shell Majorana nanowires

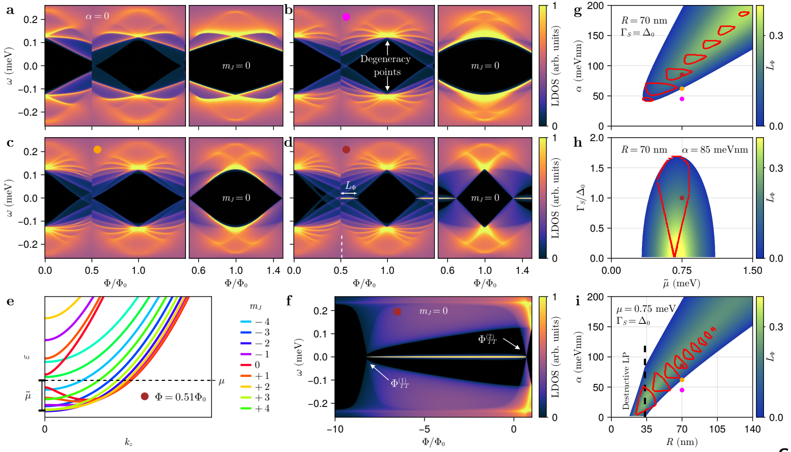
A theoretical description

Carlos Payá

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

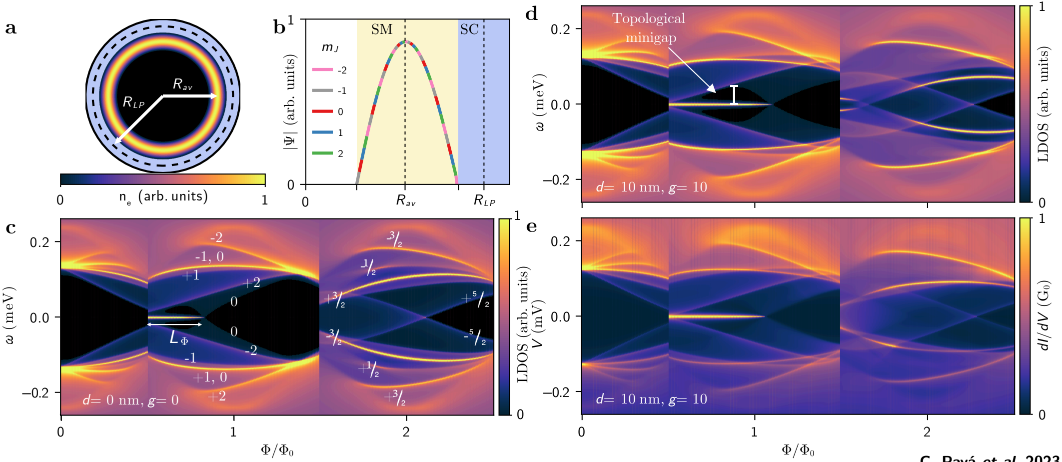
January 10, 2024

Hollow-core results



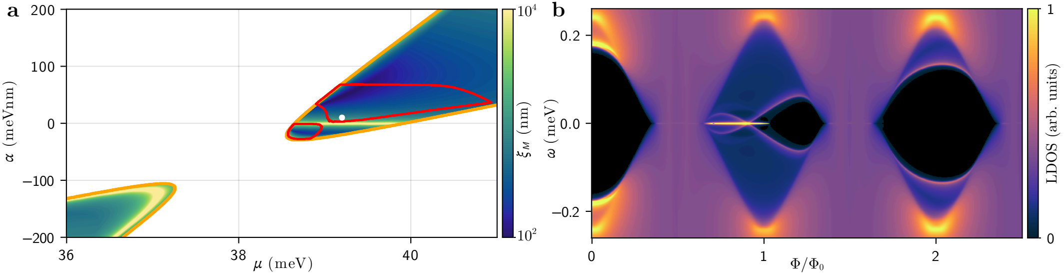
C. Payá *et al.* 2023, ***arXiv***.

Modified hollow-core results



C. Payá *et al.* 2023, *arXiv*.

Destructive Litle-Parks



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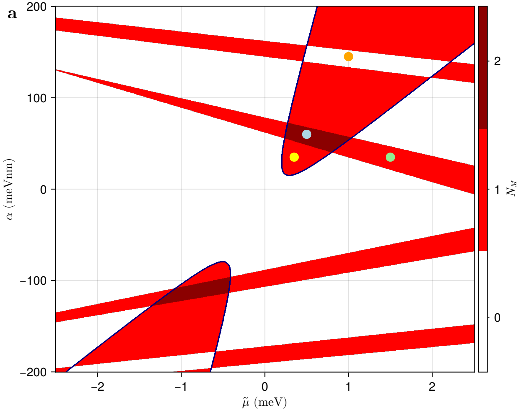
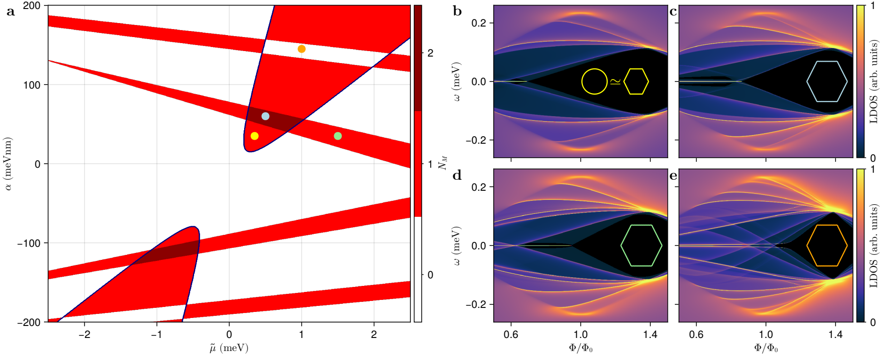
Hexagonal wave-function



- 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*.

Hexagonal wave-function



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

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