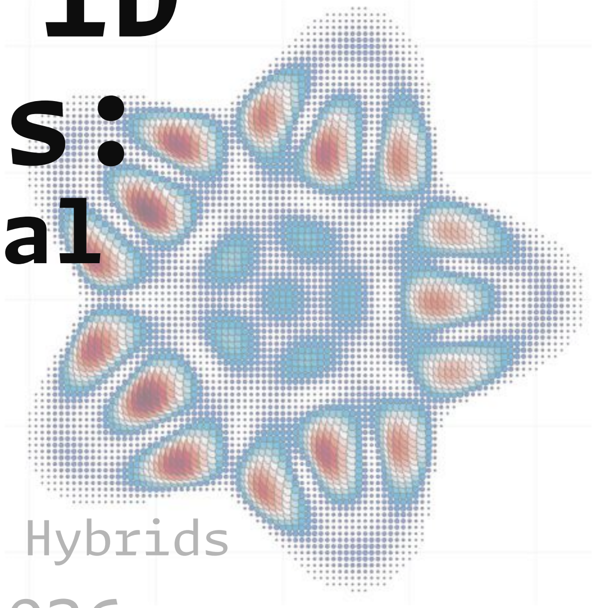
Realistic Modeling of 1D Hybrid Superconductors:
from equations to experimental simulations

Carlos Payá



International Workshop on Superconductor-Semiconductor Hybrids

Villard-de-Lans, France – 5 February 2026

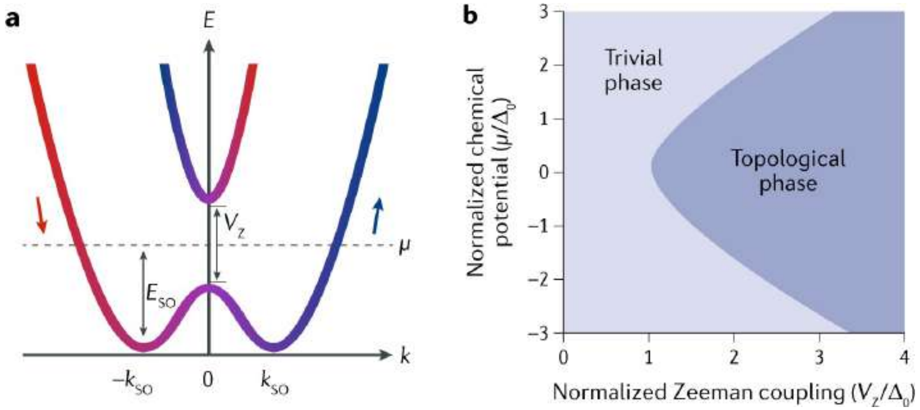
CSIC QUDYMA icmm

Our team


Madrid
Elsa Prada
Ramón Aguado
Pablo San-Jose
Thesis supervisors
Quantica.jl
icmm

Toy models are not enough

$$H = \frac{p_x^2}{2m} - \mu + V_Z + \alpha p_x \sigma_y + \Delta \tau_x$$



R. M. Lutchyn *et al. Nature Reviews Materials* 3, 52-68 (2018)

But actual devices…

Disorder Inhomogeneities 3D (multiband)

1) Full *ab initio* models

2) Elaborated models, close to the experiment but in touch with theory

A multi-level pipeline

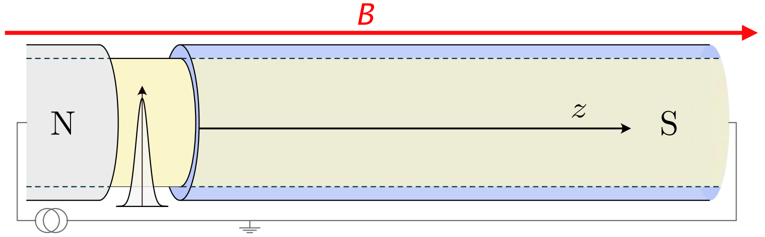
Analytics → Tight-binding → Computational implementation

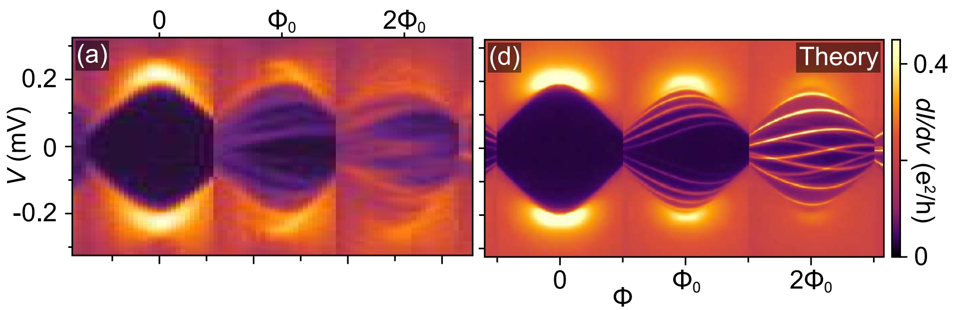
Full-shell Hybrid Nanowires

Theory of Caroli-de Gennes-Matricon analogs in full-shell hybrid nanowires
P. San-Jose, **CP**, C. M. Marcus, S. Vaitiekėnas, E. Prada
Phys. Rev. B 107, 155423 (2023)

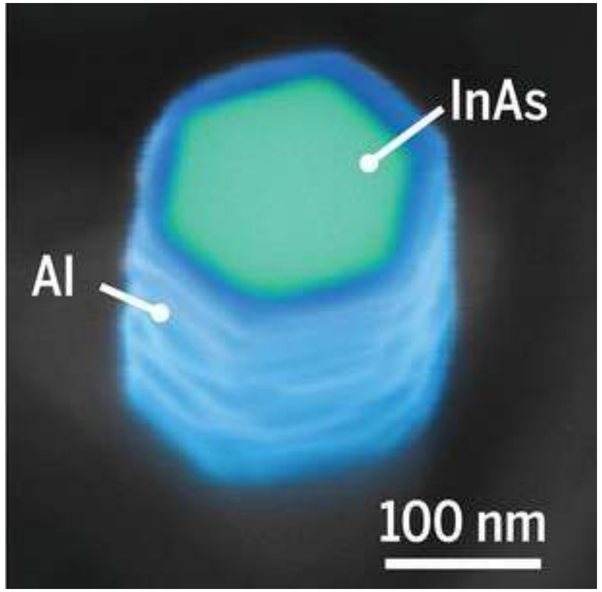
Phenomenology of Majorana zero modes in full-shell hybrid nanowires
CP, S. D. Escribano, A. Vezzosi, F. Peñaranda, R. Aguado, P. San-Jose, E. Prada
Phys. Rev. B 109, 155428 (2024)

Caroli-de Gennes-Matricon Analogs in Full-Shell Hybrid Nanowires
M. T. Deng, **CP**, P. San-Jose, E. Prada, C. M. Marcus, S. Vaitiekėnas
Phys. Rev. Lett. 134, 206302 (2025)

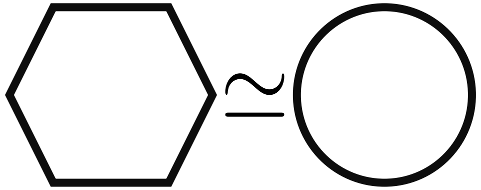


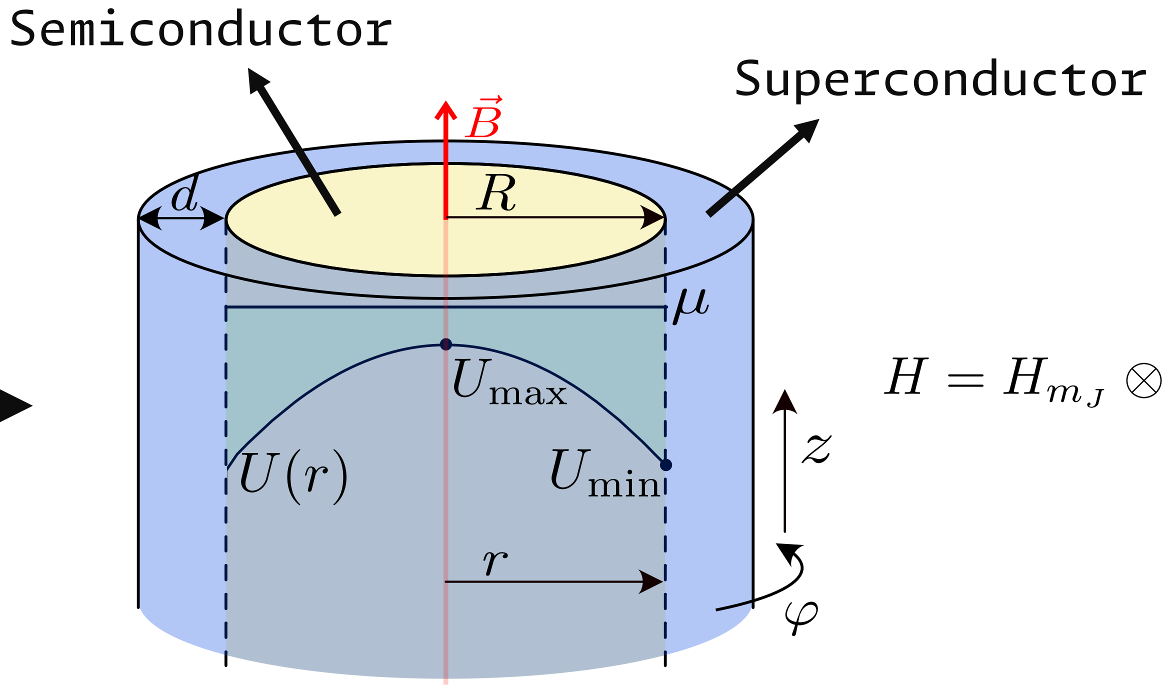


Modelling the device



S. Vaitiekėnas *et al.* *Science* 367, 1442 (2020)



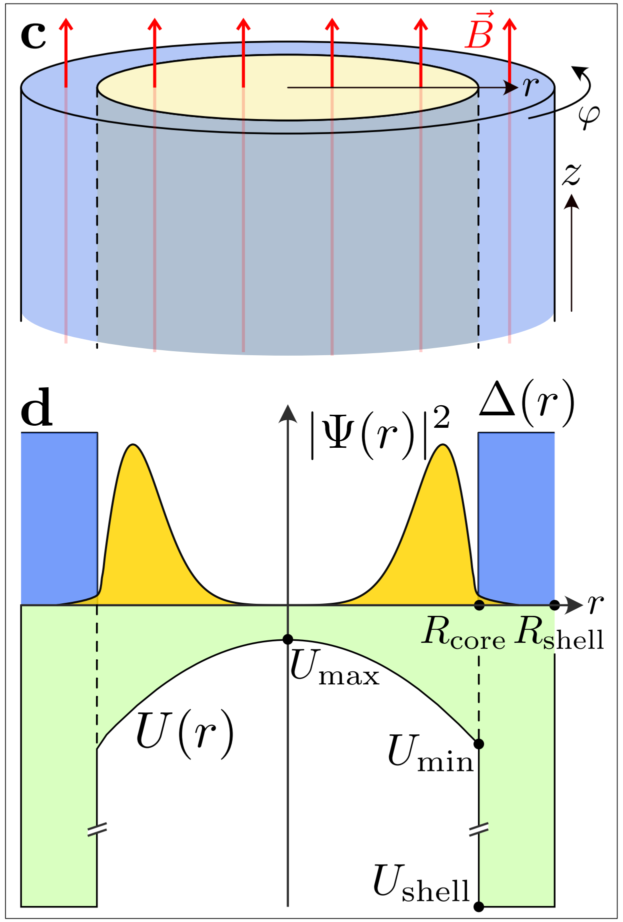


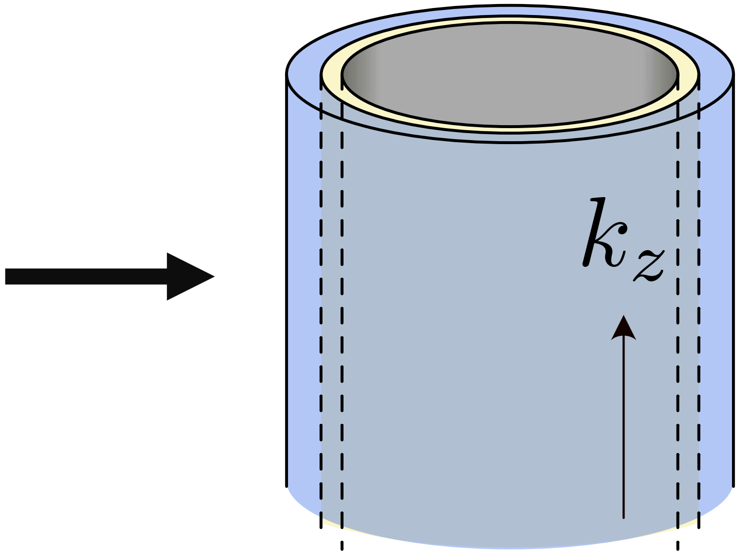
$$H = H_{m_J} \otimes I_{m_J}$$

- Cylindrical symmetry
- Charge at interface
- SOC induced by band bending

P. San-Jose, **CP**, *et al. Phys. Rev. B* 107, 155423
CP *et al. Phys. Rev. B* 109, 115428

Modelling the device





$r \to R$

P. San-Jose, **CP**, *et al. Phys. Rev. B* 107, 155423
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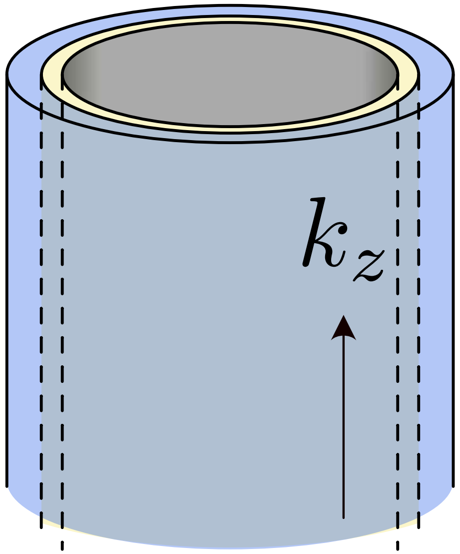
Modelling the device



Rashba wire

$$H_{\rm SM} = \frac{(\vec{p} + eA_\varphi \hat{\varphi})^2}{2m^*} - \mu + \alpha \hat{r} \cdot [\vec{\sigma} \times (\vec{p} + eA_\varphi \hat{\varphi})] + V_{\rm Z} \sigma_z$$

Diffusive superconductor

$$\Sigma_{\rm SC}(\omega) = \Gamma \frac{\tau_x - u(\omega)\tau_0}{\sqrt{1 - u^2(\omega)}}$$

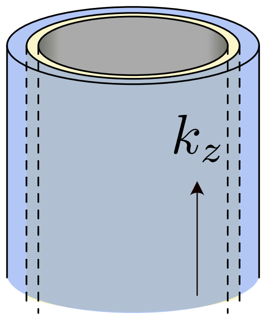
BdG formalism, Nambu basis $\left(\Psi_\uparrow, \Psi_\downarrow, \Psi_\downarrow^\dagger, -\Psi_\uparrow^\dagger\right)$

$$\vec{\sigma} \otimes \vec{\tau}$$

$$H_{m_J} = \langle m_J | H(\varphi) | m_J \rangle$$

P. San-Jose, **CP**, *et al. Phys. Rev. B* 107, 155423
CP *et al. Phys. Rev. B* 109, 115428

Doubly connected SC: Little-Parks modulation

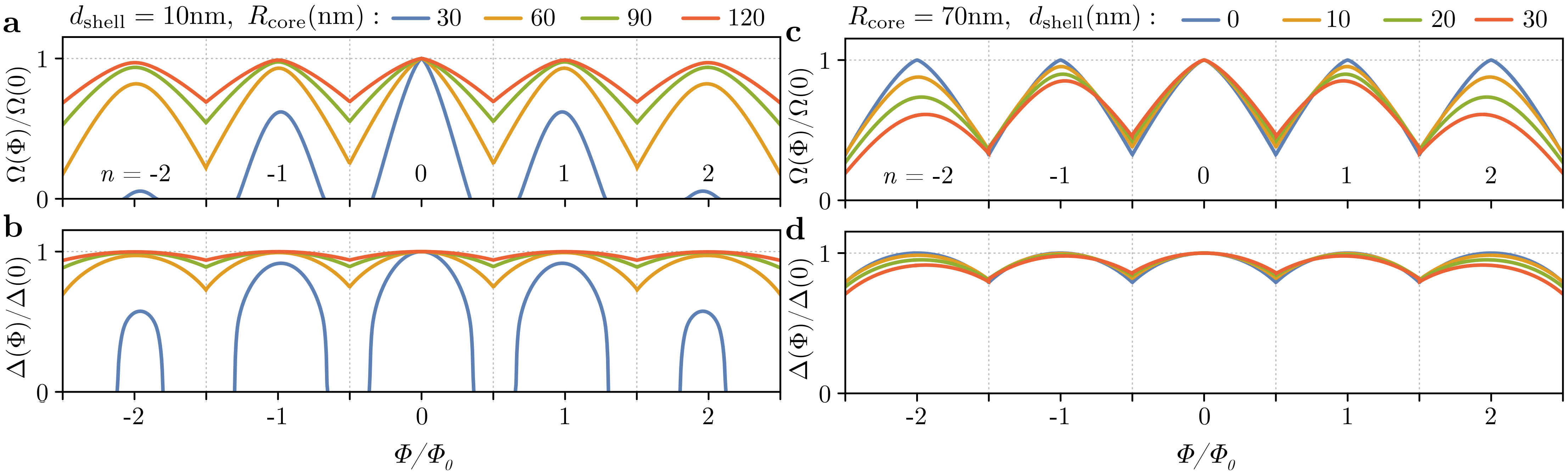


Modulation of the SC pairing with magnetic field

$$\Delta = |\Delta|\, e^{in\varphi} \qquad n = \frac{\Phi'}{\Phi_0}, \Phi = \Phi' + \oint \Lambda \vec{J} d\vec{l}$$

Diffusive SC $\Rightarrow \Delta \neq \Omega$

supercurrent



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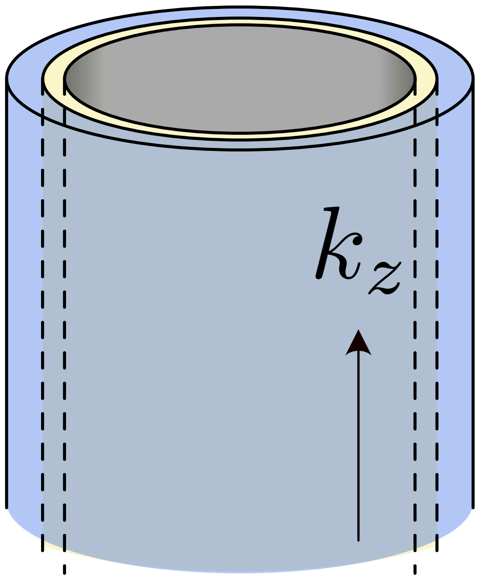
Doubly connected SC: Little-Parks modulation



$$\Sigma_{\mathrm{SC}}(\omega) = \Gamma \frac{\tau_x - u(\omega)\tau_0}{\sqrt{1-u^2(\omega)}}$$

Usadel $$u(\omega) = \frac{\omega}{\Delta(\Lambda)} + \frac{\Lambda}{\Delta(\Lambda)} \frac{u(\omega)}{\sqrt{1-u^2(\omega)}}$$

Depairing $$\Lambda(\Phi) \propto \frac{\xi_d^2}{(R+d/2)^2}\left(n - \frac{\Phi}{\Phi_0}\right)^2 + \frac{d^2}{(R+d/2)^2}\left(\frac{\Phi^2}{\Phi_0^2} + \frac{n^2}{3}\right)$$

Magnetic flux

$$n = \lfloor \frac{\Phi}{\Phi_0} \rceil$$

Geometry treated as paramagnetic impurities

(Abrikosov-Gor'kov, 1961)

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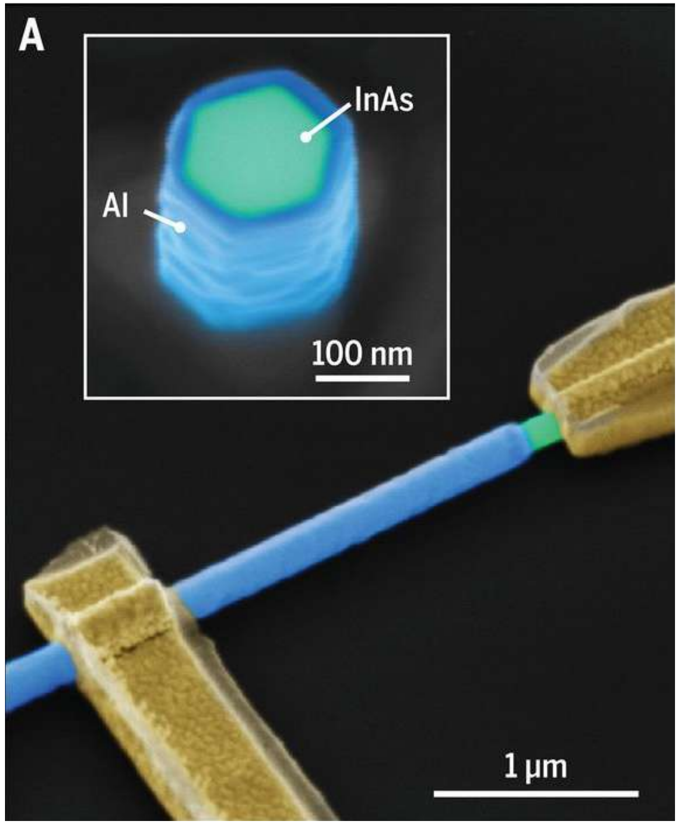
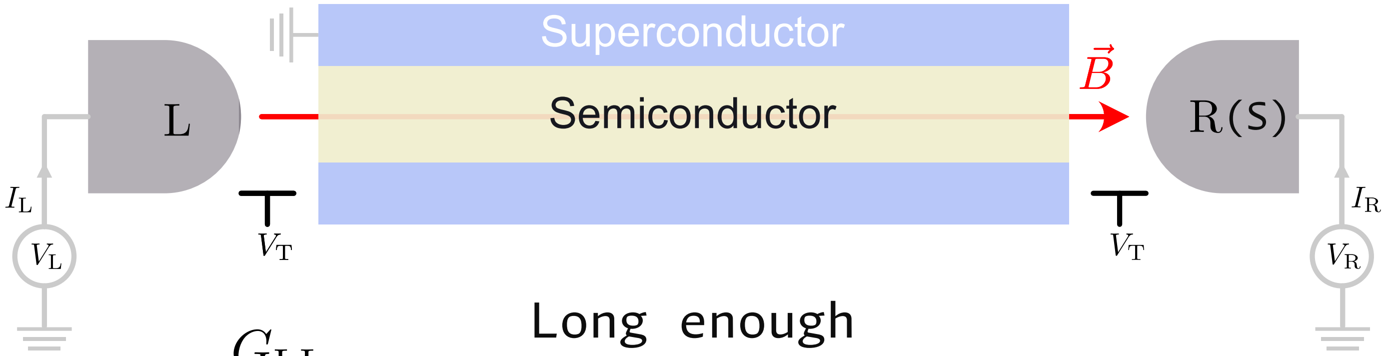
Modelling the setup



S. Vaitiekėnas *et al.* *Science* 367, 1442 (2020)

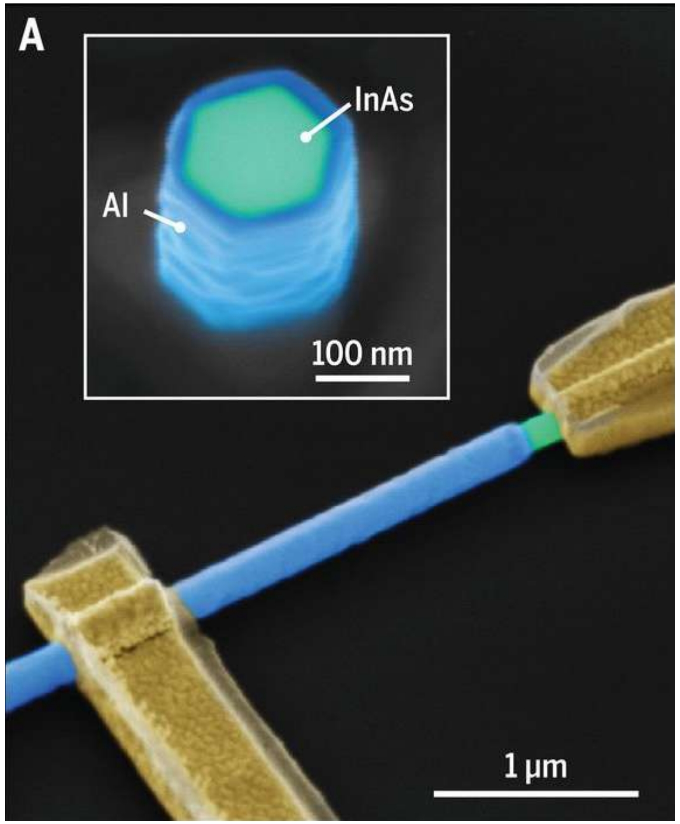


G_{LL}

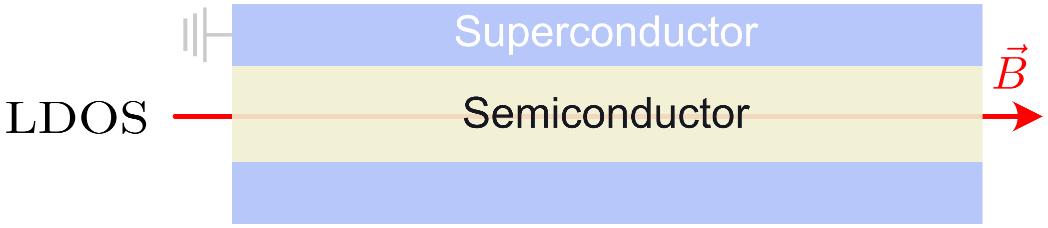
Long enough
Semi-infinite

P. San-Jose, **CP**, *et al.* *Phys. Rev. B* 107, 155423
CP *et al.* *Phys. Rev. B* 109, 115428

Modelling the setup



S. Vaitiekėnas *et al.* *Science* 367, 1442 (2020)



Long enough
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CP *et al.* *Phys. Rev. B* 109, 115428

Quantica.jl: our tight-binding toolkit

Pablo San-Jose

Quantica.jl

Build Hamiltonian

↓

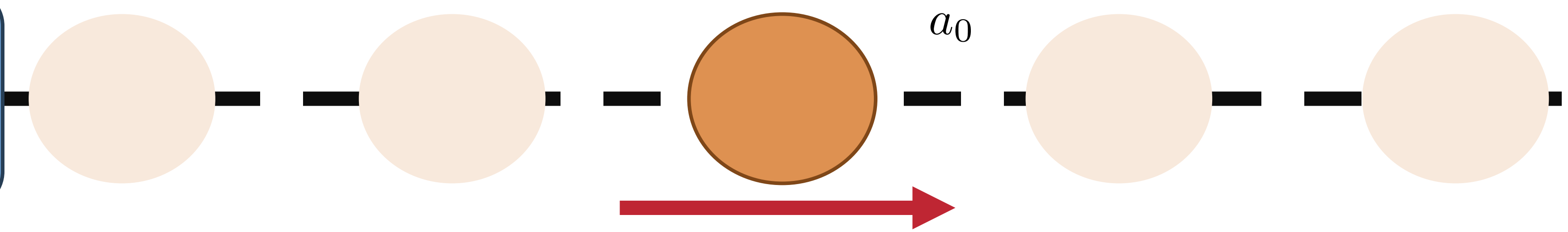
Compute Green's functions

↓

Calculate observables

Quantica.jl: our tight-binding toolkit

Build Hamiltonian



Lattice

+

Model

Quantica.jl

```julia
lat = LatticePresets.linear(; a0 = 5)
```

```
julia> lat
Lattice{Float64,2,1} : 1D lattice in 1D space
  Bravais vectors : [[5.0]]
  Sublattices     : 1
    Names         : (:A,)
    Sites         : (1,) --> 1 total per unit cell
```

Quantica.jl: our tight-binding toolkit

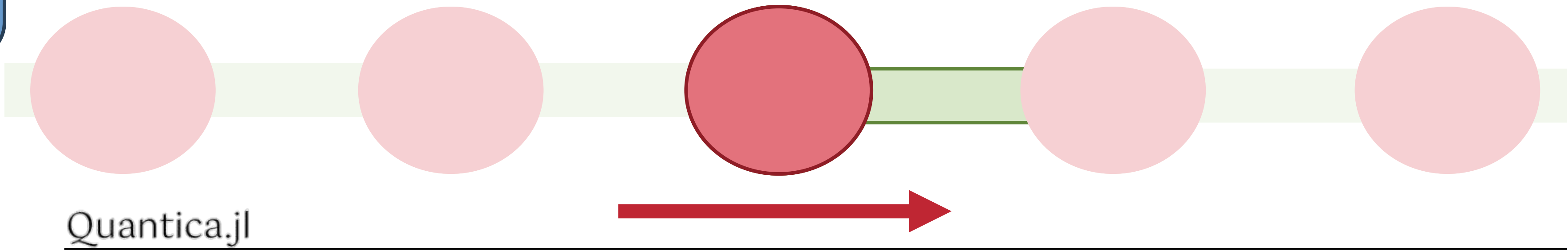
Build Hamiltonian

Lattice

+

Model

$\sim r, p^0$ onsite + hopping $\sim r, p$



Quantica.jl

```
@onsite((r; params...) -> o(r; params...); sites...)
```

```
zeeman = @onsite((; B = 0, g = 10) ->
           0.5 * g * μB * B * σzτ0
    )
```

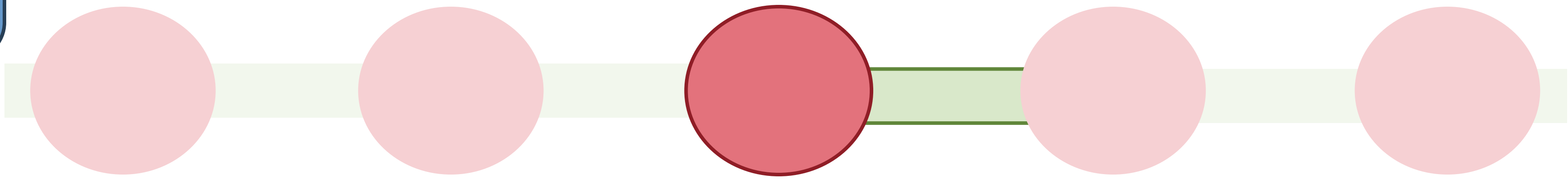
```
@hopping((r, dr; params...) -> t(r; params...); hops...)
```

```
rashba = @hopping((r, dr; α = 0) ->
           α * im * dr[1] / (2 * a0^2) * σyτz
    )
```

Quantica.jl: our tight-binding toolkit

Build Hamiltonian

Hamiltonian



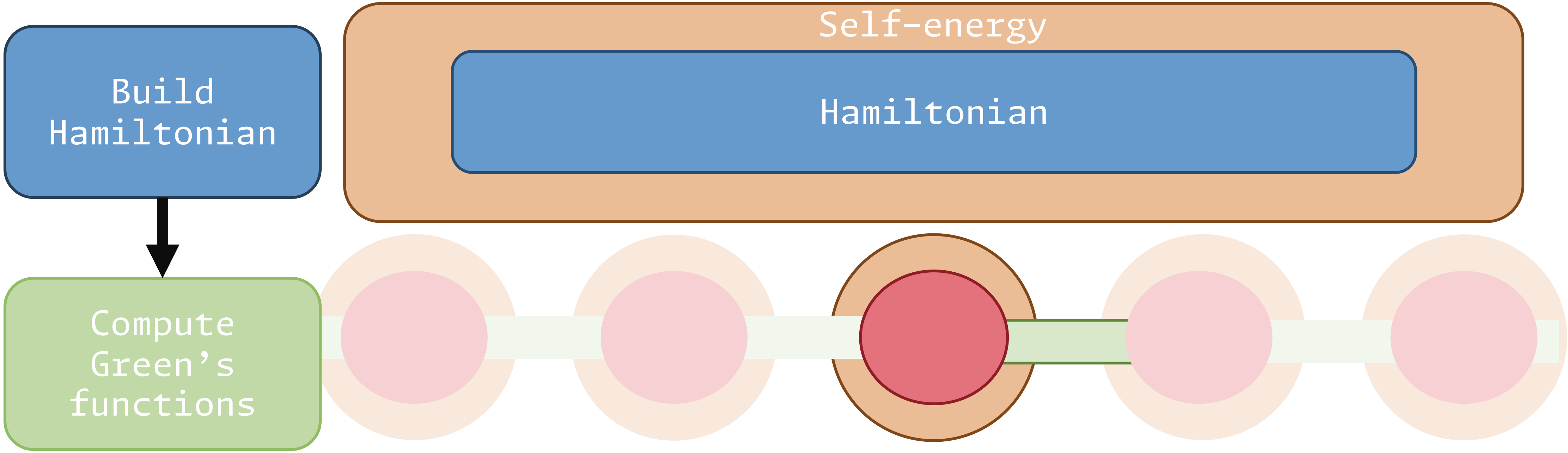
$$H(\phi) = \sum_{dn} H_{dn} e^{-i\phi dn}$$

Quantica.jl

```
hSM = lat |> hamiltonian(kinetic + rashba + zeeman + kinetic_gauge + rashba_gauge; orbitals = 4)
```

```
julia> hSM(π/4; B = 0.3)
4×4 SparseArrays.SparseMatrixCSC{ComplexF64, Int64} with 16 stored entries:
 39.0567+2.58552e-15im      0.0-2.82843im           0.0+0.0im               0.0+0.0im
     0.0+2.82843im      36.5218+2.58552e-15im       0.0+0.0im               0.0+0.0im
     0.0+0.0im              0.0+0.0im          -36.678-2.58552e-15im        0.0+2.82843im
     0.0+0.0im              0.0+0.0im               0.0-2.82843im      -39.5809-2.58552e-15im
```

Quantica.jl: our tight-binding toolkit

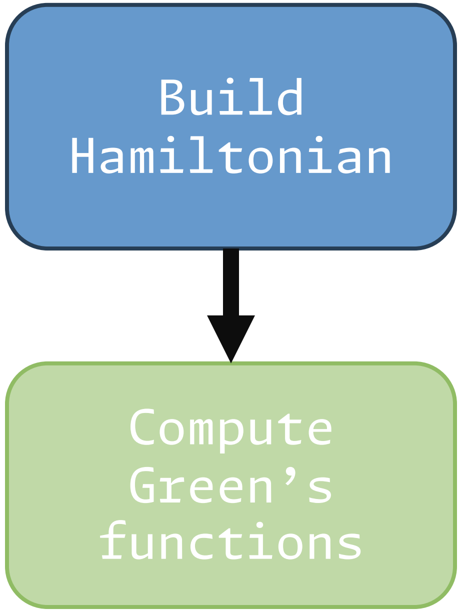


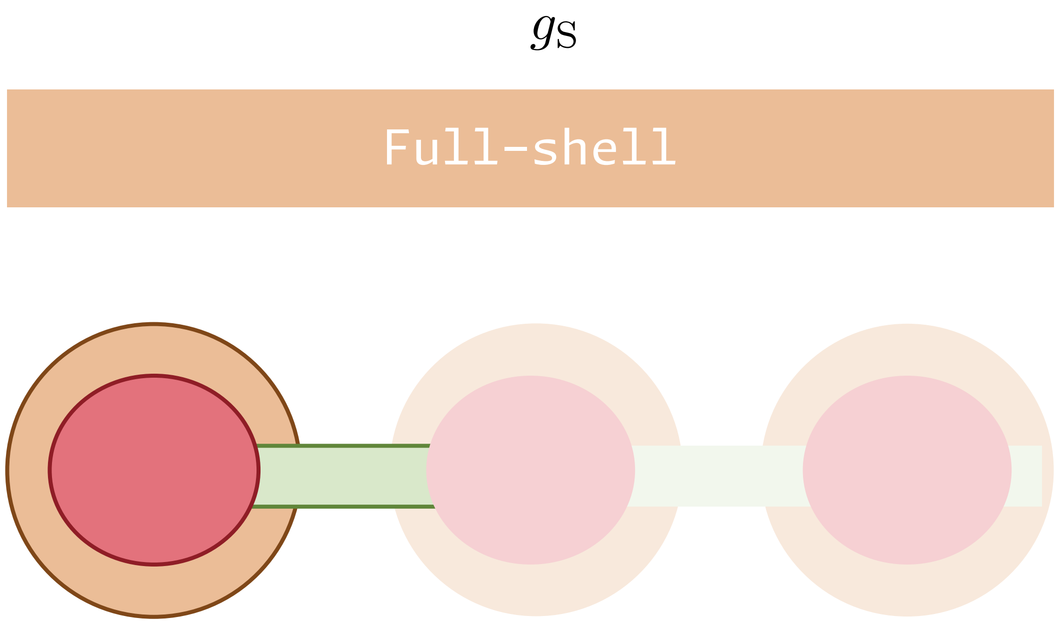
Quantica.jl

$$G = \frac{1}{\omega - H - \Sigma}$$

```
# Quantica modifier to apply self-energy to onsite terms
Σ! = @onsite!((o, r; ω = 0, B = 0, Γ = Δ) ->
        o + Γ * Σ(ω, Λ(B))
        )
hSC = hSM |> Σ!
```

Quantica.jl: our tight-binding toolkit





$$G = \frac{1}{\omega - H - \Sigma}$$

Quantica.jl

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# Quantica modifier to apply self-energy to onsite terms
Σ! = @onsite!((o, r; ω = 0, B = 0, Γ = Δ) ->
        o + Γ * Σ(ω, Λ(B))
        )
hSC = hSM |> Σ!
```

```
gS = hSC |> greenfunction(GreenSolvers.Schur(boundary = 0))
```

Quantica.jl: our tight-binding toolkit

Build Hamiltonian

Compute Green's functions

Calculate observables

g_S

Full-shell

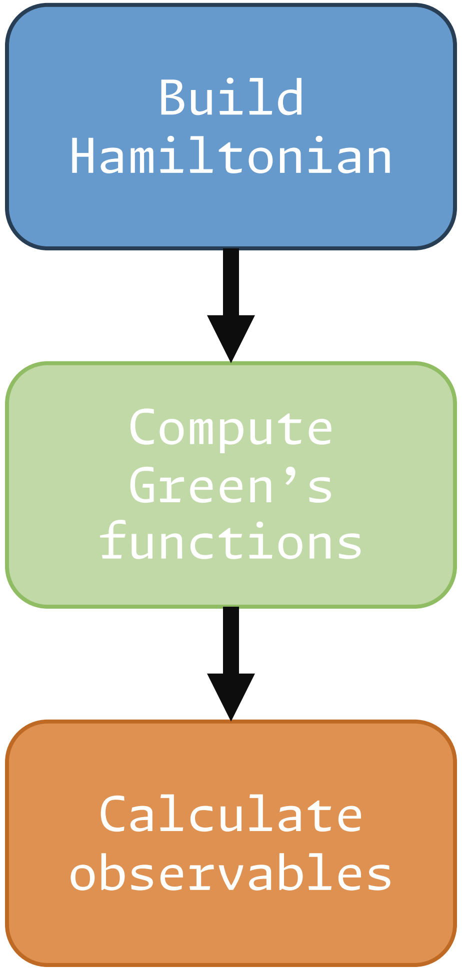
$$\mathrm{LDOS} = -\frac{1}{\pi}\mathrm{Im}\left\{\mathrm{Tr}\left[g_S\right]\right\}$$

Quantica.jl

```
julia> ρ = ldos(gS[cells = (1,)]; kernel = I)
LocalSpectralDensitySlice{Float64} : local density of states at a fixed
location and arbitrary energy
  kernel   : LinearAlgebra.UniformScaling{Bool}(true)

julia> ω = 0.1e-3
julia> ρ(ω; ω, B = 0.1)
1-element OrbitalSliceVector{Float64,Vector{Float64}}:
 0.001538907253553478
```

Quantica.jl: our tight-binding toolkit



Quantica.jl

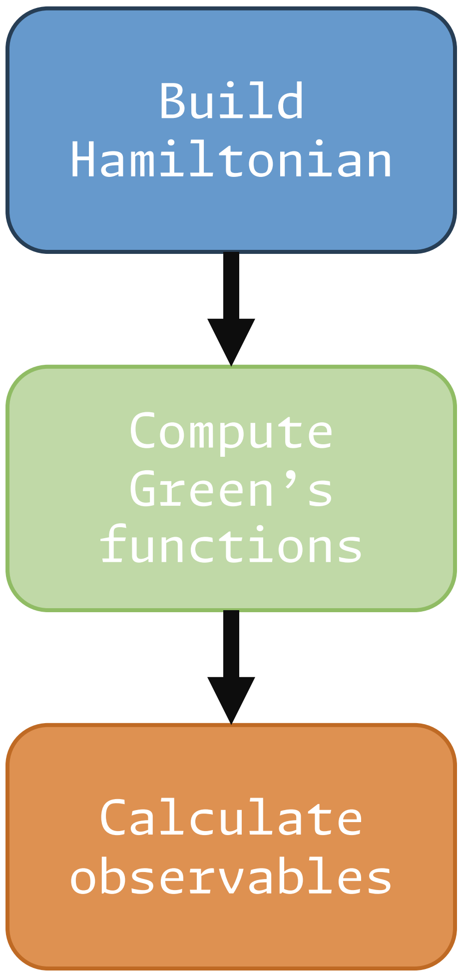
```julia
pts = Iterators.product(E_vals, B_vals, Z_vals)


LDOS = @showprogress pmap(pts) do (E, B, Z)
        return ρ(E; B = B, ω = E, Z = Z)[1]
end
```

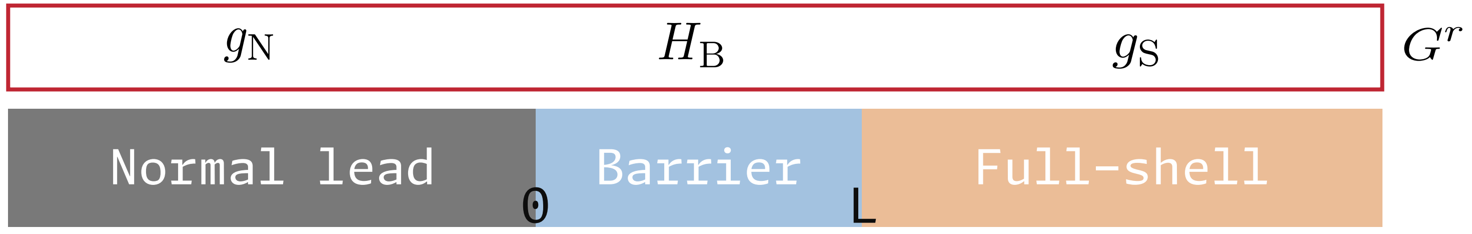
```
carlospaya@cap-mb Tutorial_QuanticaHybrids % julia --project main.jl
  Activating project at   CENSORED
======================================================================
RUNNING LDOS CALCULATION
======================================================================
Parameters:
  Energy points: 301
  Field points: 300
  Z sectors: 11 (from -5 to 5)
  Total evaluations: 993300

======================================================================
Running parameter sweep...
Progress:
100%|████████████████████████████████████████████████████████████████
████████████████████████████████████████████| Time: 0:02:26
151.871329 seconds (195.82 M allocations: 15.532 GiB, 1.41% gc time, 506 lock
conflicts, 4.65% compilation time)
```

Quantica.jl: our tight-binding toolkit



For Conductance: attach a barrier and a lead

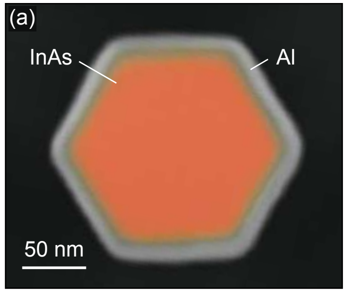


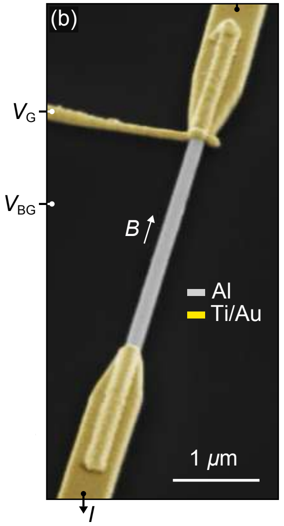
Quantica.jl

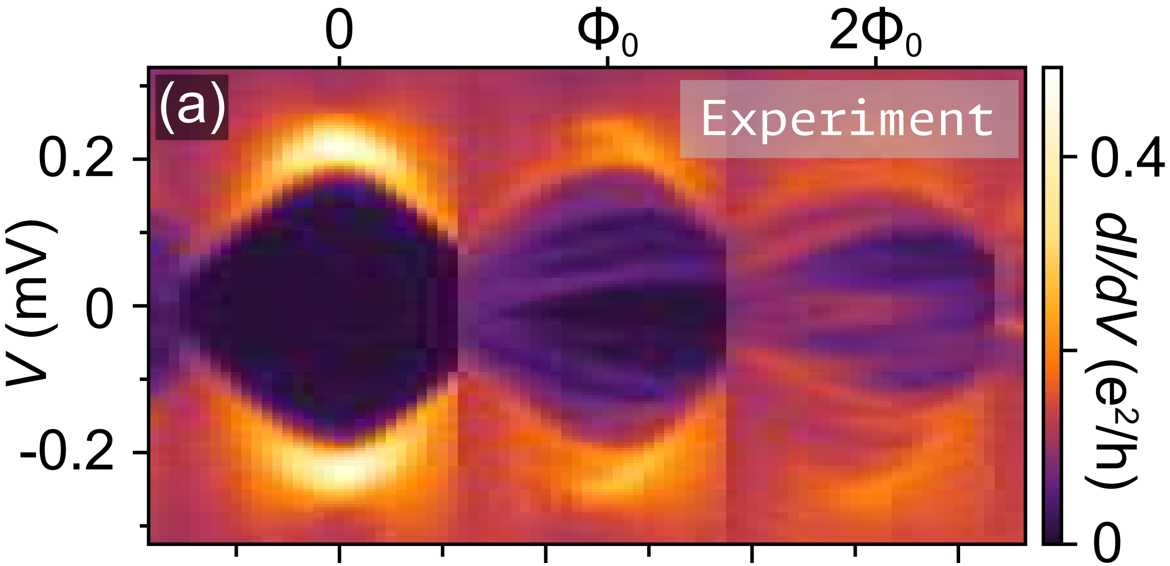
```
Gr = hB |> attach(gN; region = r -> r[1] == 0) |> attach(gS; region = r ->
r[1] == L) |> greenfunction()

G = conductance(Gr[1, 1]; nambu = true)
```

CdGM: experiment vs calculation







Number of CdGMs -> Chemical potential: $\mu_{m_L} = \frac{1}{2m^*}\left(\frac{m_L^2}{R_{\mathrm{av}}^2} + \frac{1}{4R_{\mathrm{av}}^2} + \frac{1}{4}\frac{R_{\mathrm{av}}^2}{R_{\mathrm{LP}}^4} - \frac{1}{2R_{\mathrm{LP}}^2}\right)$

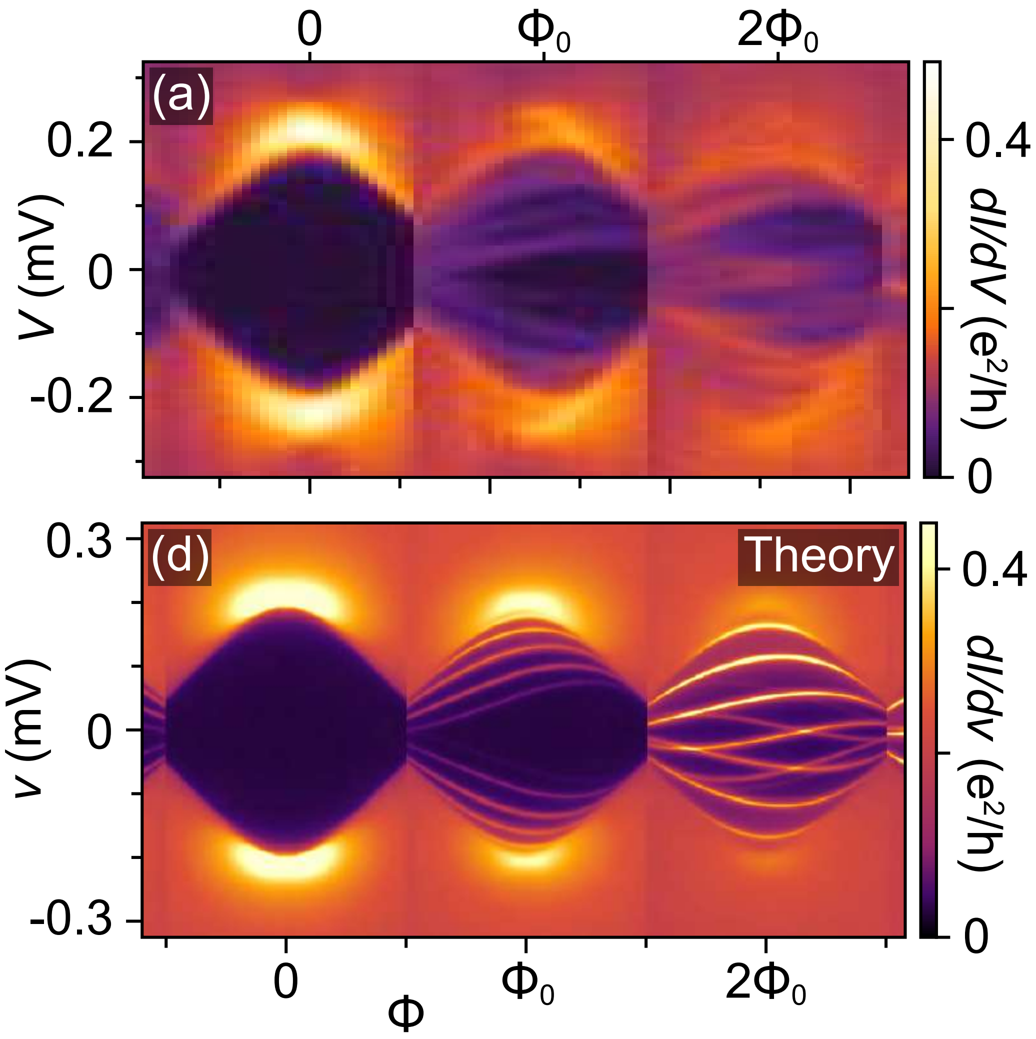
Effective gap -> Coupling to superconductor: $\Gamma = \Delta_0^* \sqrt{\frac{\Delta_0 + \Delta_0^*}{\Delta_0 - \Delta_0^*}}$

$$\omega_d = \epsilon_0(m_L) - \epsilon_0(m_L - 1) = \frac{1}{2m^*}\left(\frac{1}{R_{\mathrm{av}}^2} - \frac{1}{R_{\mathrm{LP}}^2}\right)$$

Low-energy CdGM spacing -> Radial distribution: $\omega_{m_L} \simeq \Delta_0 \left(\frac{\Gamma^2 - (m_L\omega_d)^2}{\Gamma^2 + (m_L\omega_d)^2}\right)$

 M. T. Deng, **CP**, *et al.* Phys. Rev. Lett. 134, 206302 (2025)

CdGM: experiment vs calculation



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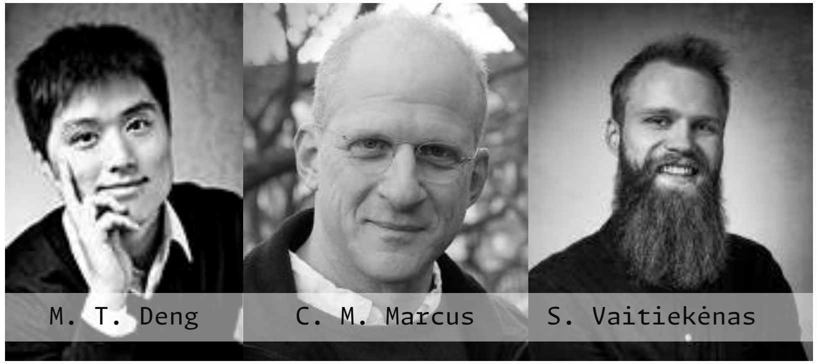

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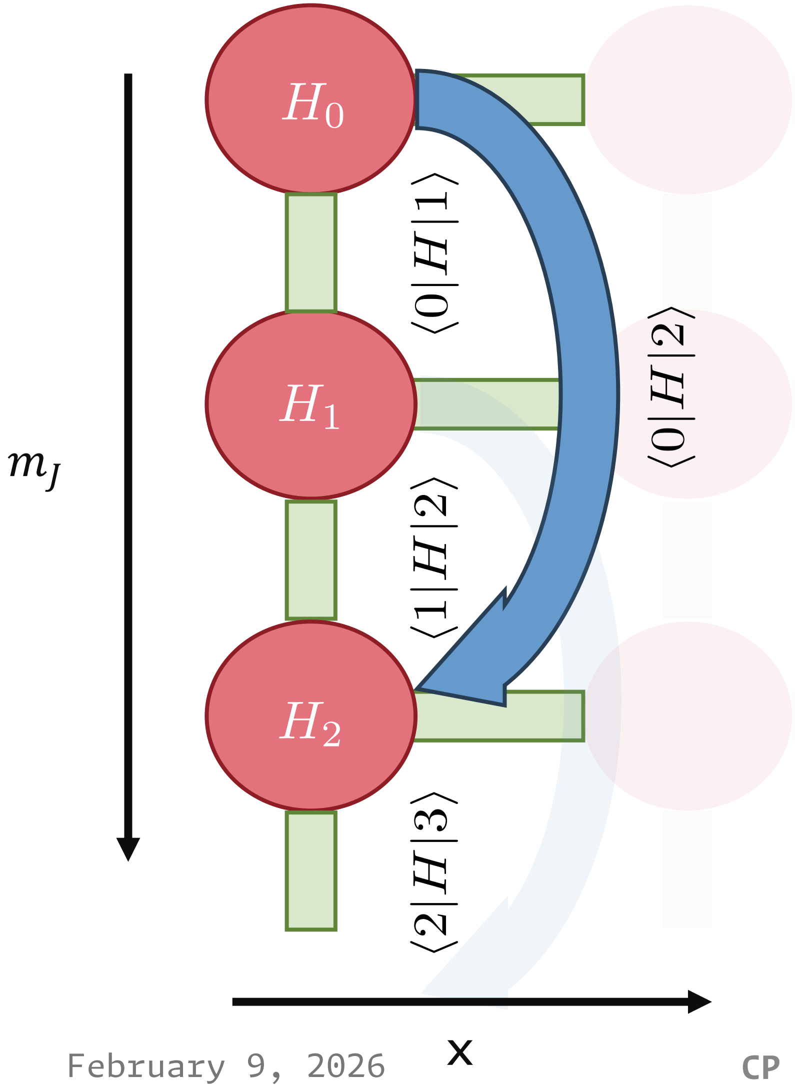
Expanding the model: multi-mode



$$H = \sum_{m_J} H_{m_J} = \mathrm{Tr}\left[H_{m_J} \otimes I_{m_J}\right]$$

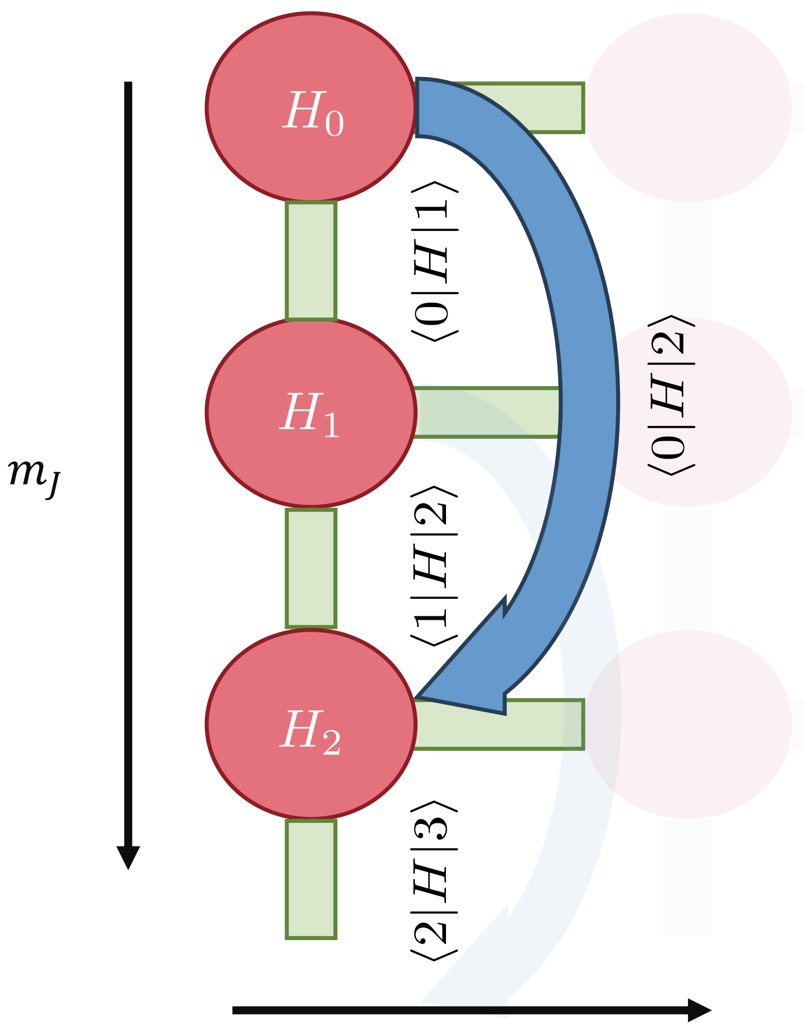
$$H = H_{m_J} \otimes I_{m_J} + \sum_{\ell} \langle m_J|H|m_J + \ell\rangle$$

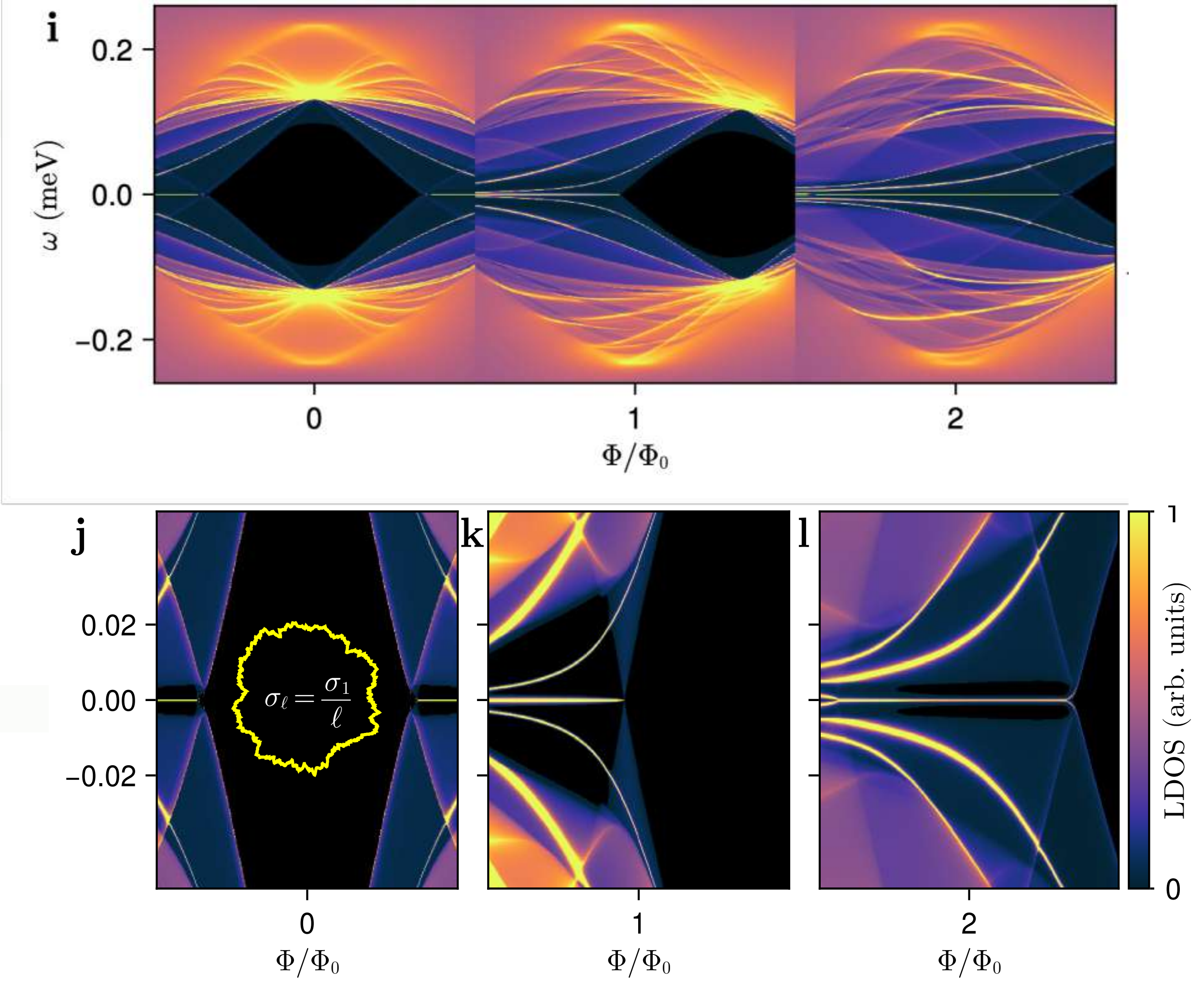
Quantica.jl

```
lat = LP.square(; a0) |> supercell((1,0), region = r ->
abs(r[2]/a0) <= num_mJ)
```

`abs(r[2]/a0)` is m_J

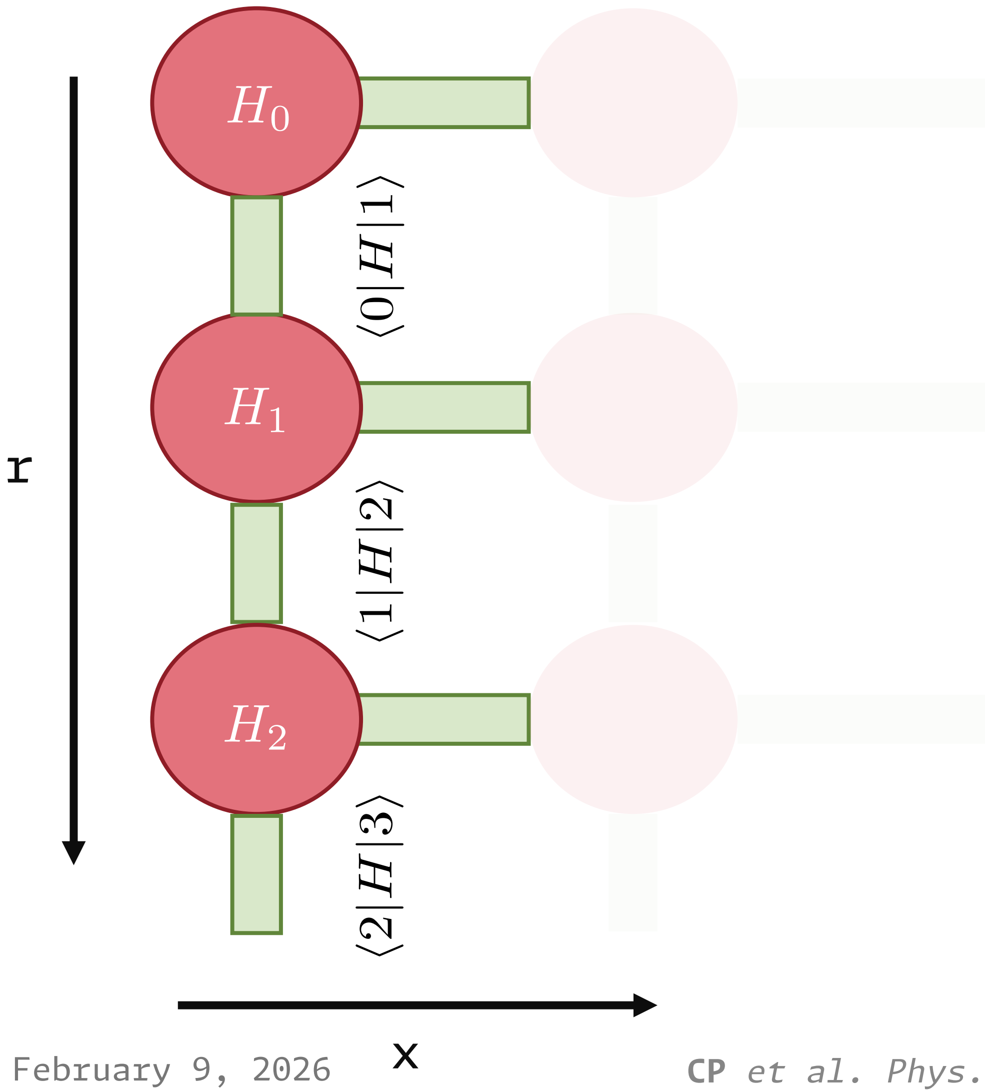
Expanding the model: multi-mode

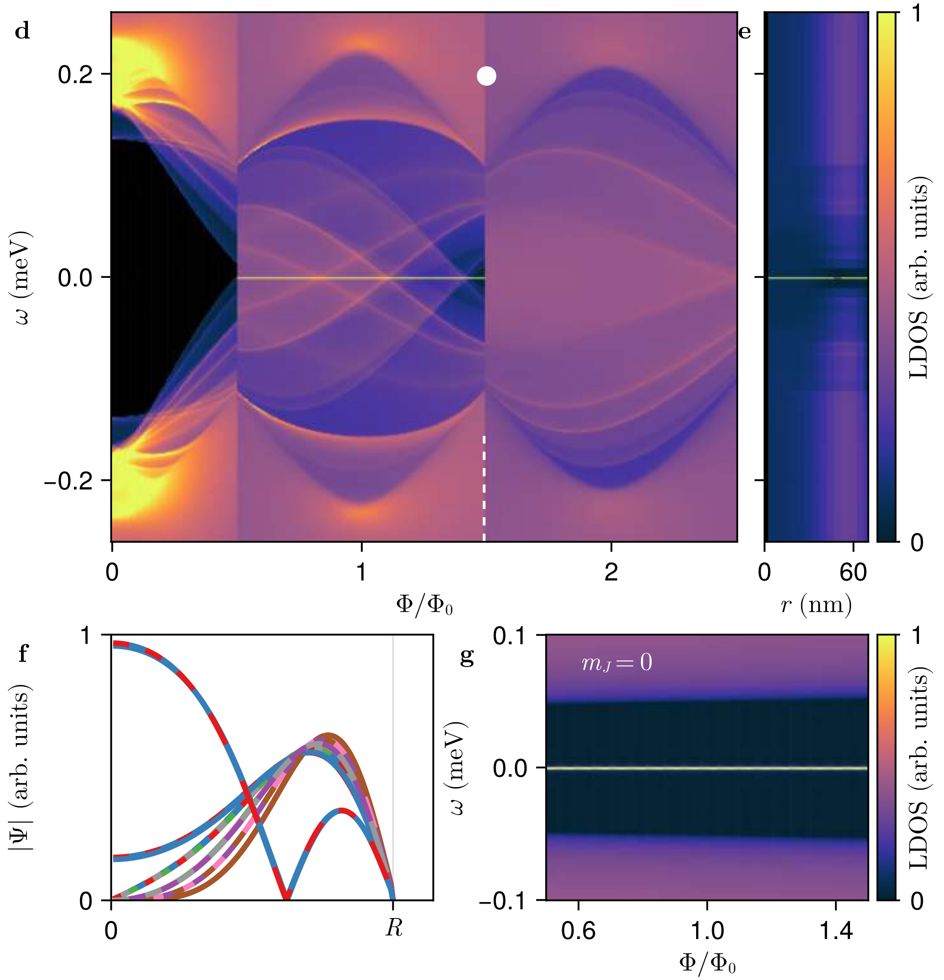




CP *et al. Phys. Rev. B* 109, 115428 (2024)

Expanding the model: multi-mode





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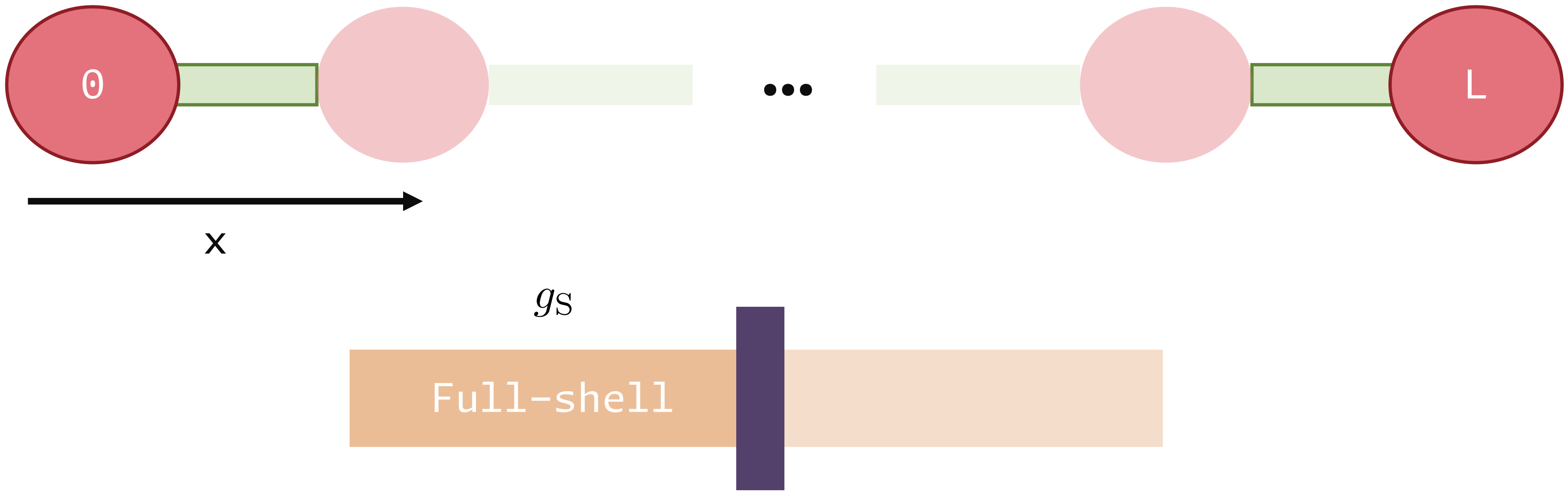
Expanding the model: finite length



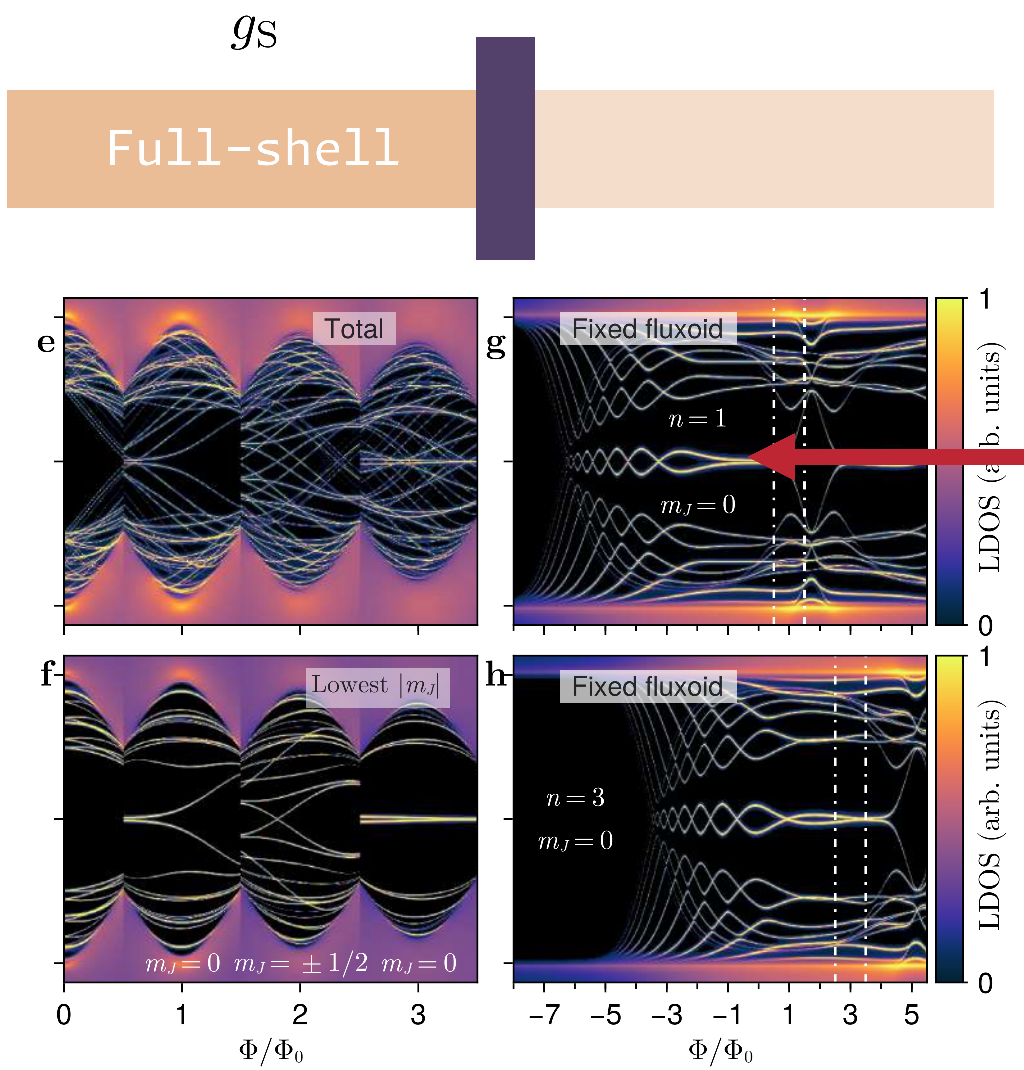
Impurity $\rightarrow$ $\Sigma = \infty \sigma_0 \tau_z$

Quantica.jl

```
g = hSC |> attach(onsite(1e9 * σ0τz,), cells = (L,)) |> greenfunction(GS.Schur(boundary = 0))
```


CP *et al. Phys. Rev. B* 110, 115417 (2024)

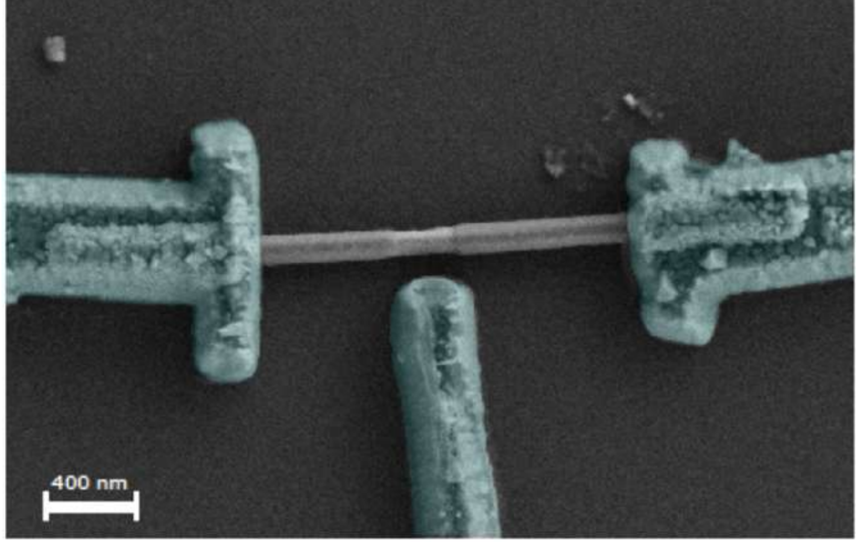
Expanding the model: finite length



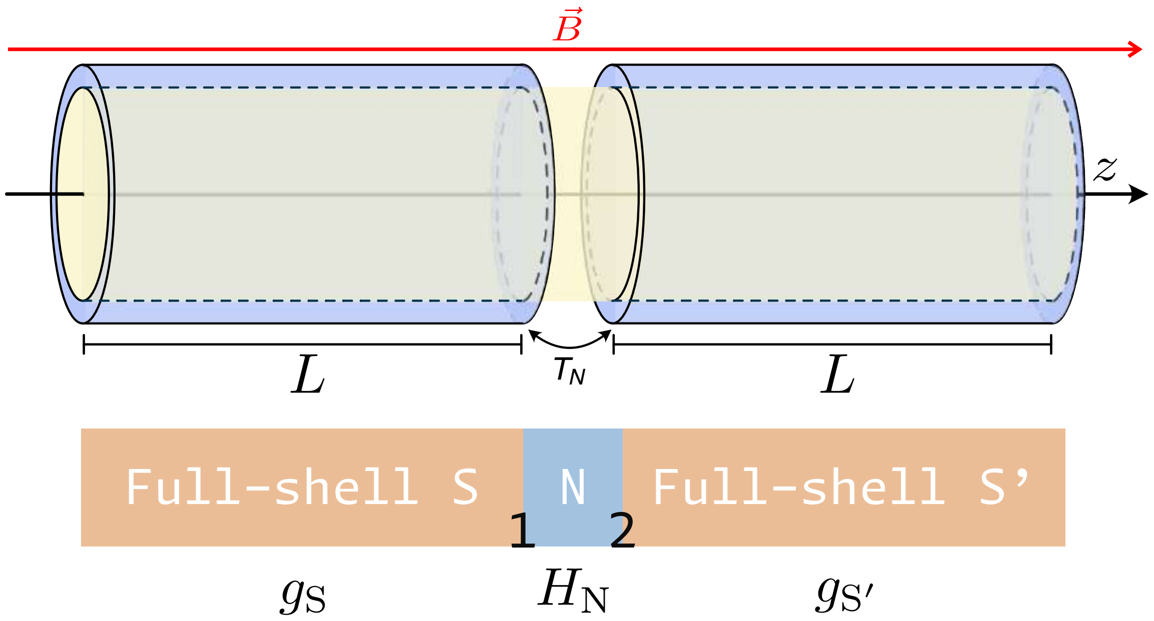
Majorana oscillations are larger than a Little-Parks lobe

Building other setups: Josephson Junction

Motivation

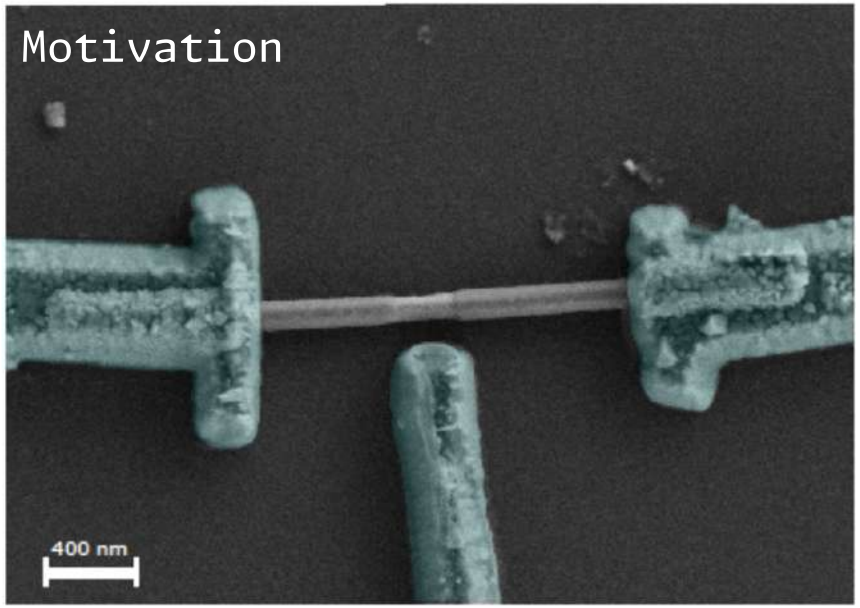


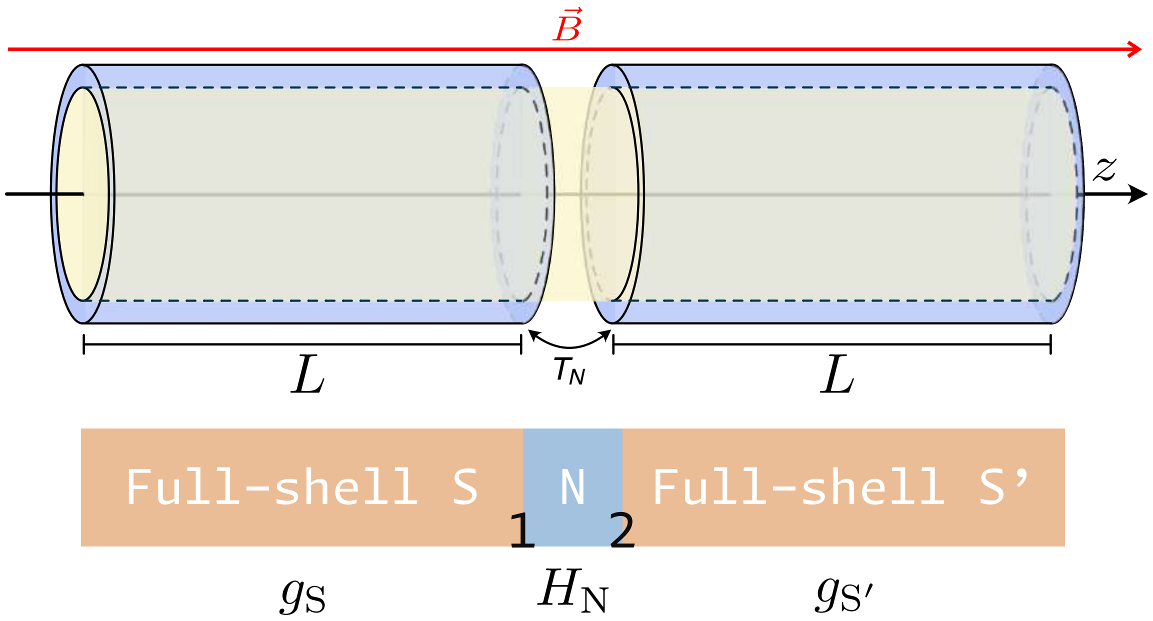
IFIMAC
CONDENSED MATTER PHYSICS CENTER



CP *et al. Phys. Rev. B* 111, 235420 (2025)
Ángel Ibabe, **CP**, *et al. in preparation*

Building other setups: Josephson Junction





Quantica.jl

```
g = hN |> attach(gS[cells = (-1)], coupling1;) |> attach(gS´[cells = (1)], coupling2) |>
greenfunction()
```

```
J = josephson(g[1], ipath)
```

```
J(kBT; params…)
```


CP *et al. Phys. Rev. B* 111, 235420 (2025)
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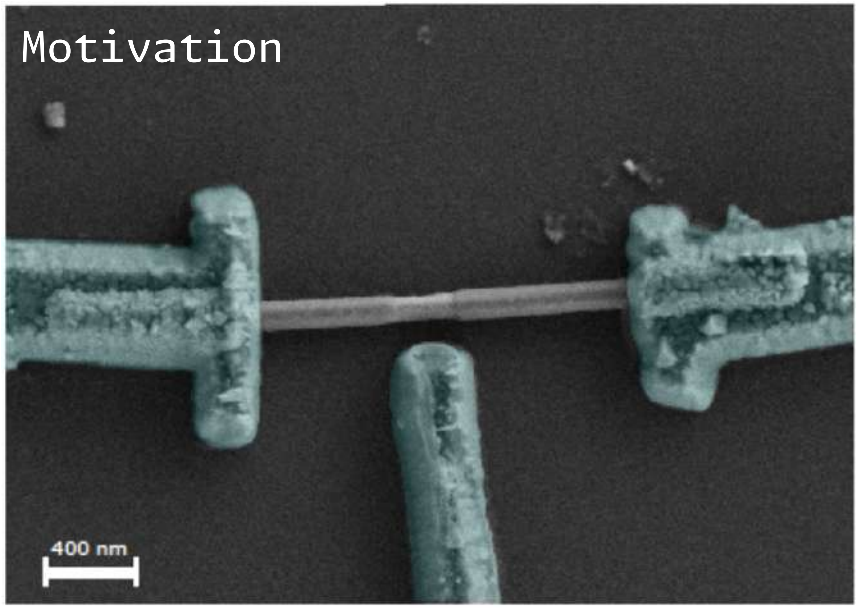

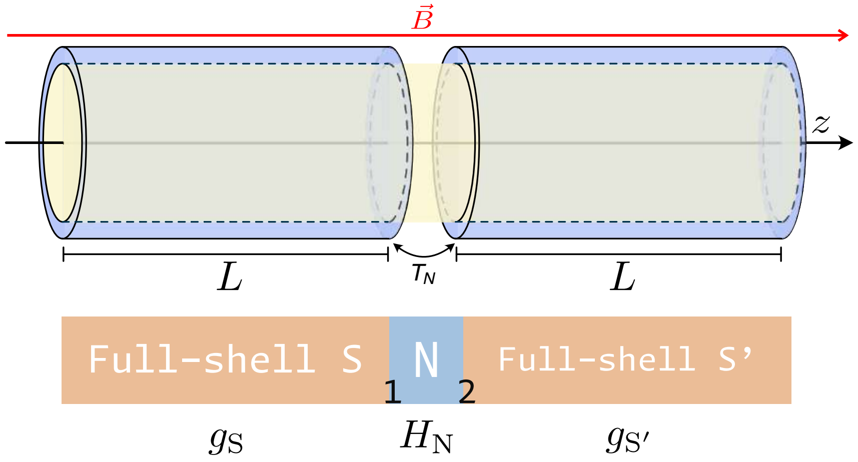

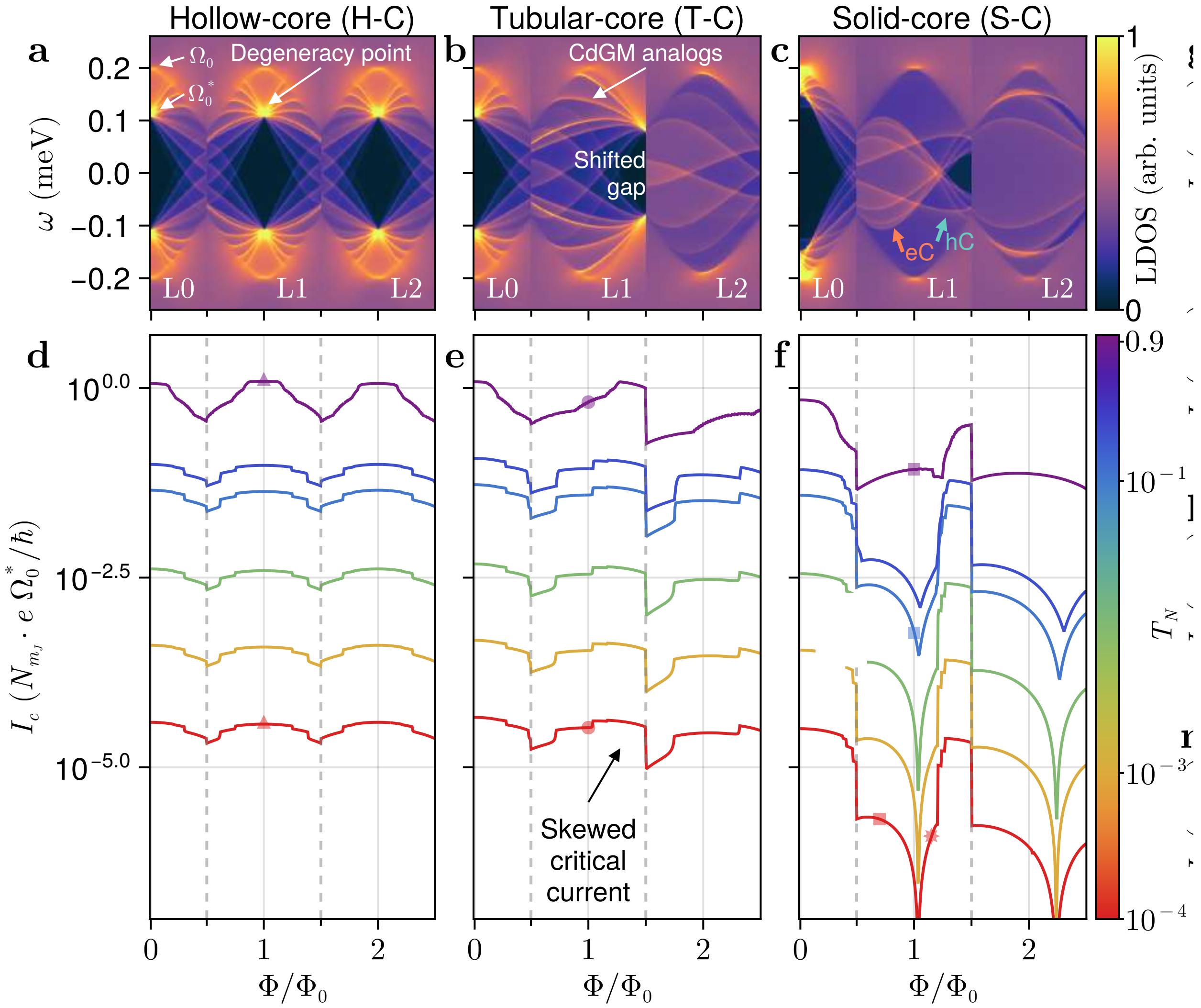

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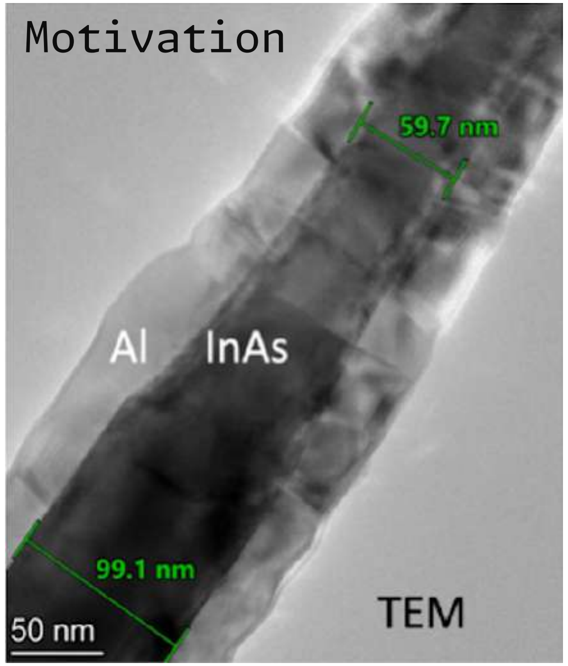
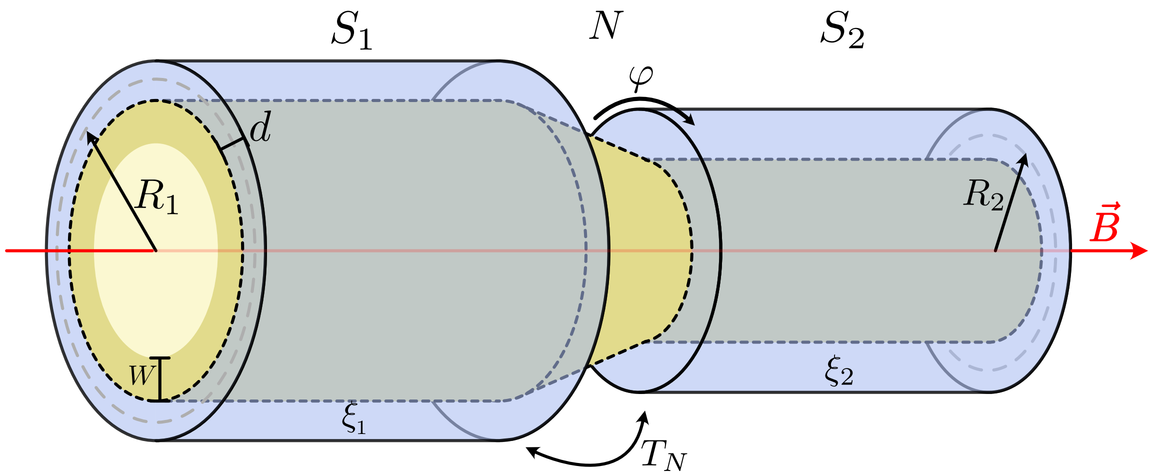
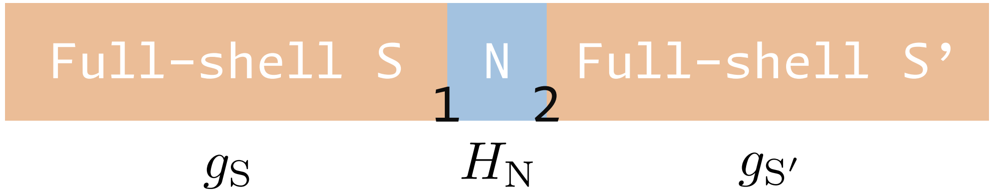
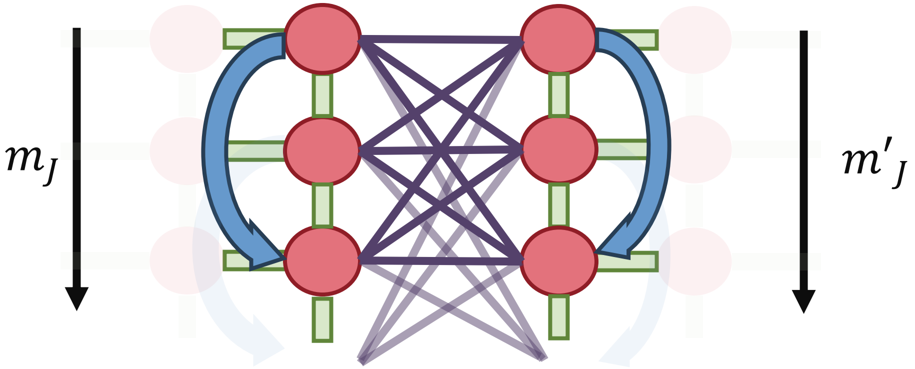
Building other setups: Fluxoid Valve









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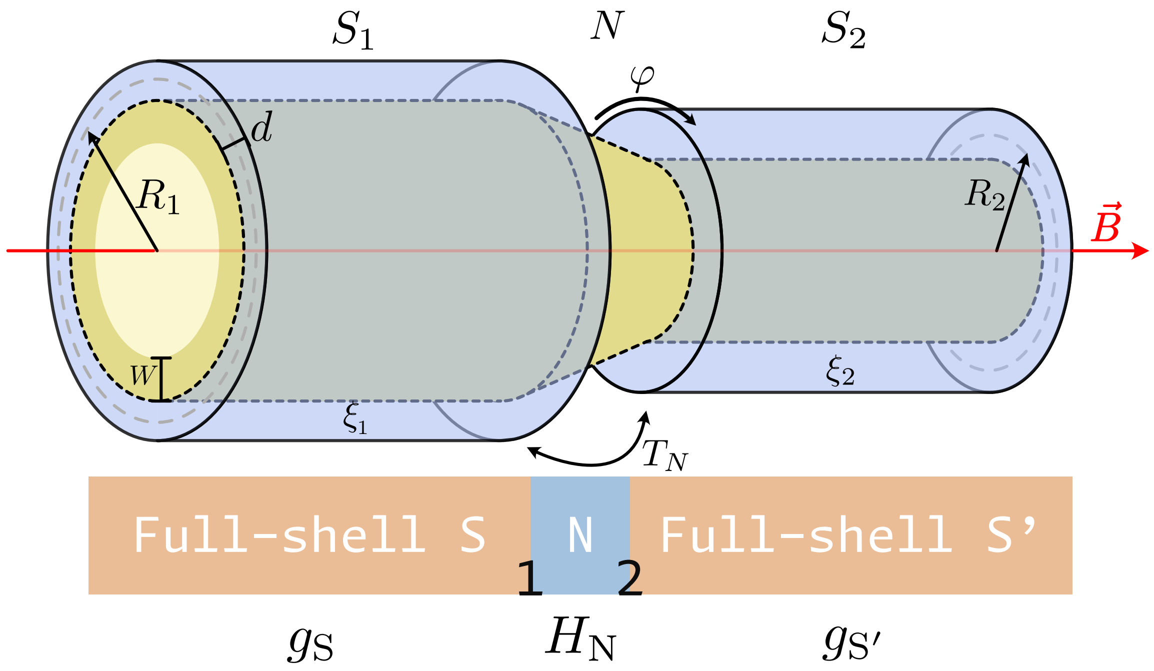
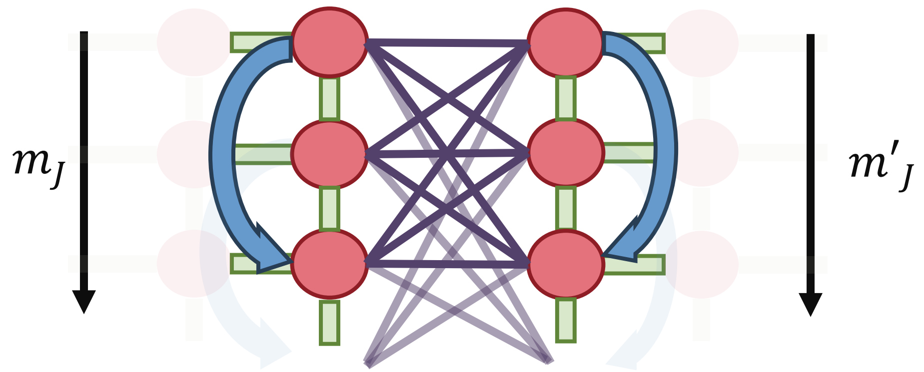
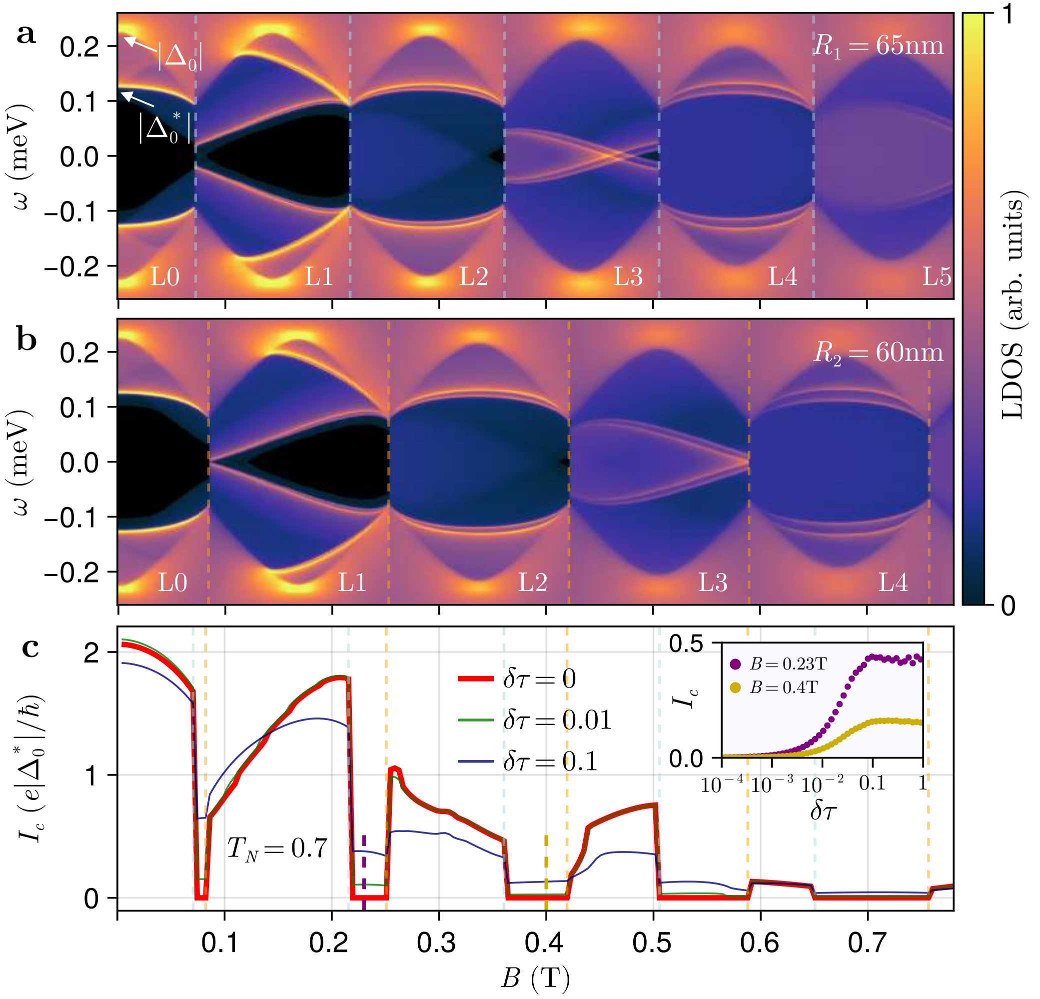
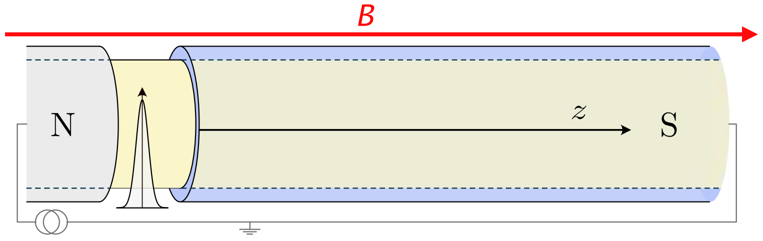
Building other setups: Fluxoid Valve



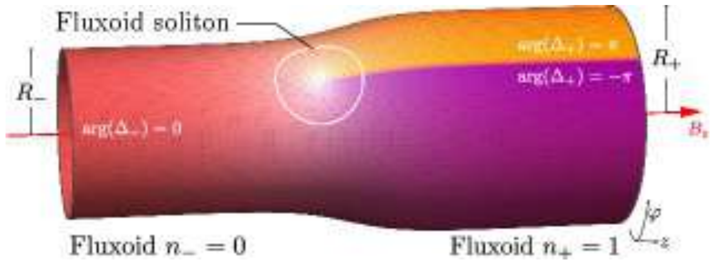




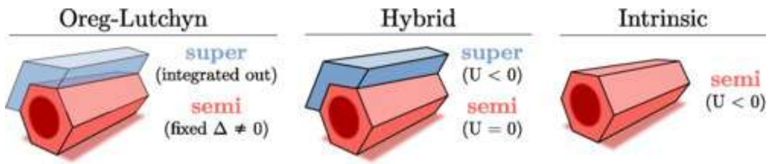
Quantica: simple and versatile



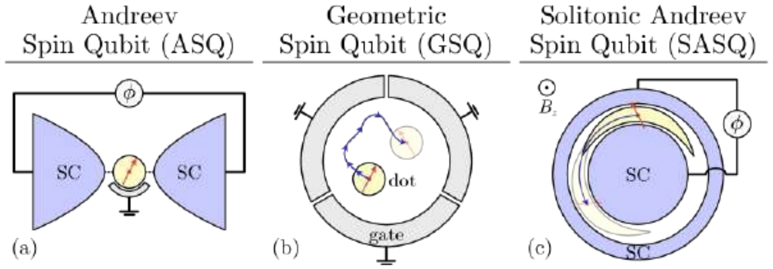
Full-Shell Project: **CP** thesis



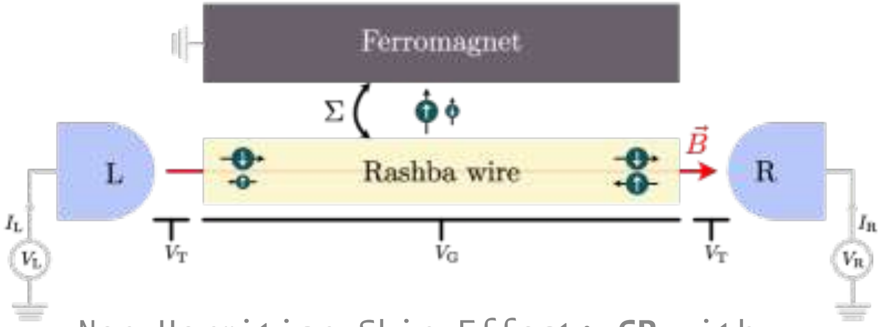
Tapered SC wires: T. Kokkeler *et al.*



Intrinsic Majorana wires: F. Lobo *et al*



Solitonic Andreev Spin Qubit: P. San-Jose and E. Prada



Non-Hermitian Skin Effect: **CP** with K. Flensberg (*et al*)

…

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Code for this tutorial

Realistic Modeling of 1D Hybrid Superconductors

Carlos Payá

International Workshop on Super-Semi Hybrids
Villard-de-Lans, France - 5 February 2026

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