Theory of Caroli-de Gennes-Matricon analogs in full-shell hybrid nanowires

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Phys. Rev. B. **107**, 155423 (2023)

Abstract.

Full-shell nanowires are hybrid nanostructures consisting of a semiconducting core encapsulated in an epitaxial superconducting shell. When subject to an external magnetic flux, they exhibit the Little-Parks (LP) phenomenon of flux-modulated superconductivity, an effect connected to the physics of Abrikosov vortex lines in type-II superconductors. We show theoretically that full-shell nanowires can host **subgap states** that are a variant of the **Caroli–de Gennes–Matricon (CdGM)** states in vortices. These CdGM analogs are shell-induced **Van Hove singularities** in propagating core subbands. We elucidate their structure, parameter dependence, and behavior in tunneling spectroscopy through a series of models of growing complexity. Using microscopic numerical simulations, we show that CdGM analogs exhibit a **characteristic skewness** towards higher flux values inside nonzero LP lobes resulting from the interplay of three ingredients. First, the orbital coupling to the field shifts the energy of the CdGM analogs proportionally to the flux and to their generalized angular momentum. Second, CdGM analogs coalesce into **degeneracy points** at flux values for which their corresponding radial wavefunctions are threaded by an integer multiple of the flux quantum. And third, the average radii of all CdGM-analog wavefunctions inside the core are approximately equal for realistic parameters and are controlled by the electrostatic band bending at the core/shell interface. As the average radius moves away from the interface, the **degeneracy points shift towards larger fluxes** from the center of the LP lobes, causing the skewness. This analysis provides a transparent interpretation of the nanowire spectrum that allows to **extract microscopic information** by measuring the number and skewness of CdGM analogs. Moreover, it allows to derive an **efficient Hamiltonian** of the full-shell nanowire in terms of a **modified hollow-core model at the average radius**.

Motivation: full-shell hybrid nanowire.

- Semiconducting nanowire encapsulated in a superconductor threaded by an axial magnetic field $\vec{B}$ (a,b) [1].
- Possible platform for Majorana Bound States.
- Interest beyond topology: rich subgap spectrum in transport measurements (c) [2].
- Superconductor shell has a doubly-connected geometry.
- Little-Parks (LP) effect [3]: quantized magnetic flux winding n, the "*fluxoid*".
  - Modulation of the superconducting gap: LP lobes.
  - Superconudcting order parameter: $\Delta(\vec{r}) = \Delta(r)e^{in\varphi}$ (Fig. 2(c,d)).

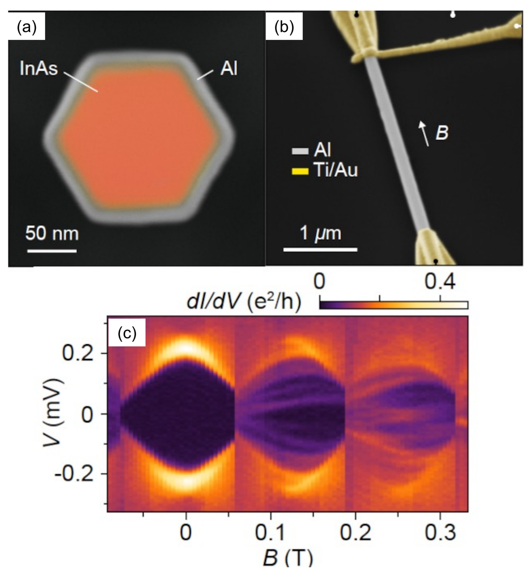

Figure 1. (a) Nanowire cross section. (b) Micrograph of the experimental setup. (c) Conductance vs. magnetic flux. Results by S. Vaitiekėnas. *et al.*

Caroli-de Gennes-Matricon analog states.

- Normal and Andreev reflections at the core/shell interface ⇒ subgap states.
- Analog to Caroli-de Gennes-Matricon (CdGM) in Abrikosov vortex lines of type-II superconductors (a).
- CdGM are subgap excitations.
- In vortices:
  - Bound to their center (b).
  - Total flux quantized.
- In nanowires:
  - Close to the interface due to the conduciton band bending $U(r)$ (d).
  - Only fluxoid n is quantized due to the superconductor thinness.

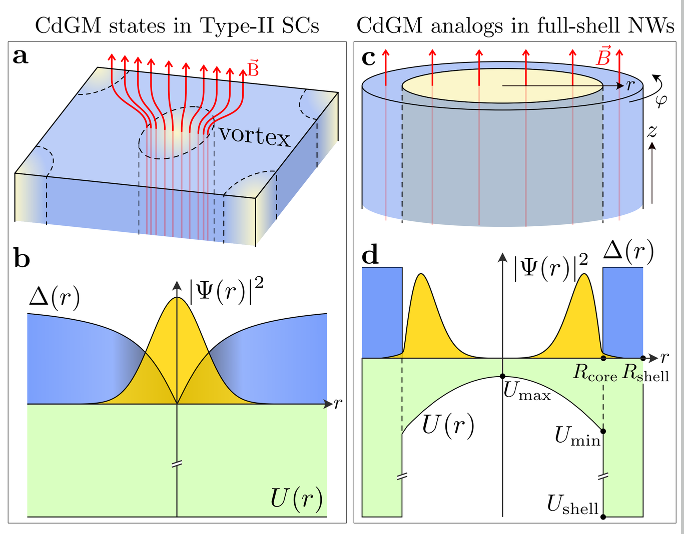

Figure 2. CdGM states sketch in a type-II SC vortex (a) and in a hybrid nanowire (c) and their energy sketches (b,d).

Hollow-core nanowire: charge localized at the core/shell interface.

The effective Hamiltonian of the system in the basis $\Psi = (\psi_\uparrow, \psi_\downarrow, \psi_\downarrow^\dagger, -\psi_\uparrow^\dagger)$,

$$H = \left[\frac{(p_\varphi + eA_\varphi\tau_z)^2 + p_z^2}{2m^*} - \mu\right]\tau_z + \Sigma_{\text{shell}}(\omega,\varphi), \tag{1}$$

with self-energy Σ_{shell} from the superconductor shell, satisfies $[L_z, H] = 0$, where $L_z = -i\partial_\varphi + \frac{1}{2}n\tau_z$ has eigenvalues

$$m_L = \begin{cases} \mathbb{Z} & n \text{ even} \\ \mathbb{Z}+\frac{1}{2} & n \text{ odd.} \end{cases} \tag{2}$$

Fig. 3 is the BdG band structure for different magnetic fluxes and fluxoids of an infinite hollow-core nanowire:

- Thin lines: decoupled from the superconducting shell.
- Thick lines: coupled to the shell. Superconductivity induced by proximity effect.
- Superconducting pairing turns electron-hole crossings with equal m_L into anticrossings.
  - Van Hove singularities arise at those gap edges (black dots).
  - For $\Phi/\Phi_0 = n$, Van Hove singularities are degenerate.

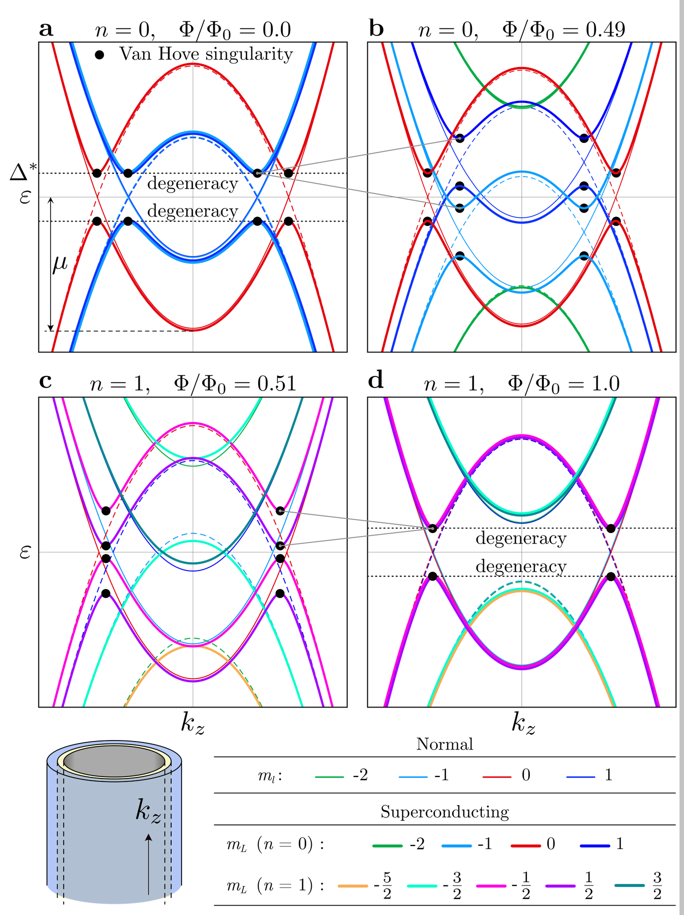

Figure 3. Nambu band structure inside the core. Solid lines → electrons, dashed → holes.

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Tubular nanowire: charge localized at a finite-thickness region inside the core.

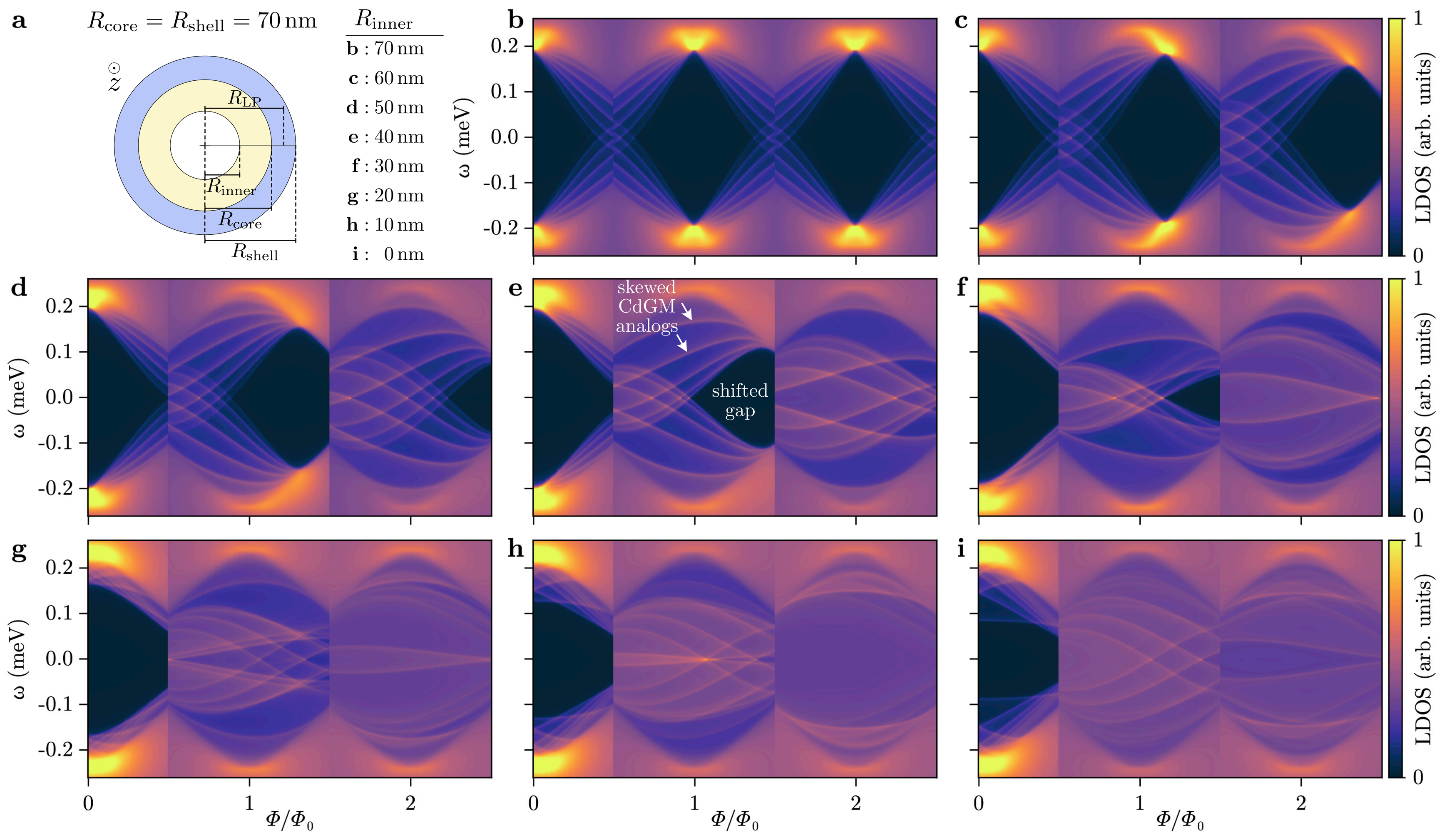

Figure 4. LDOS at the edge of a semi-infinite nanowire vs. magnetic flux for different core thicknesses.

- CdGM analogs are Van Hove singularities + tails till the parent gap.
- Hollow core case (b):
  - Slope with flux proportional to m_L.
  - Repelled by gap edge as given by self-energy Σ_{shell}.
  - Degeneracy of Van Hove singularities visible as degeneracy points (DPs) at integer fluxes.
- Tubular nanowire (c-i):
  - Wavefunctions spread ⇒ experienced flux decreases ⇒ DPs shift to higher fluxes.

Solid Core: potential well close to the core/shell interface. Transport simulations.

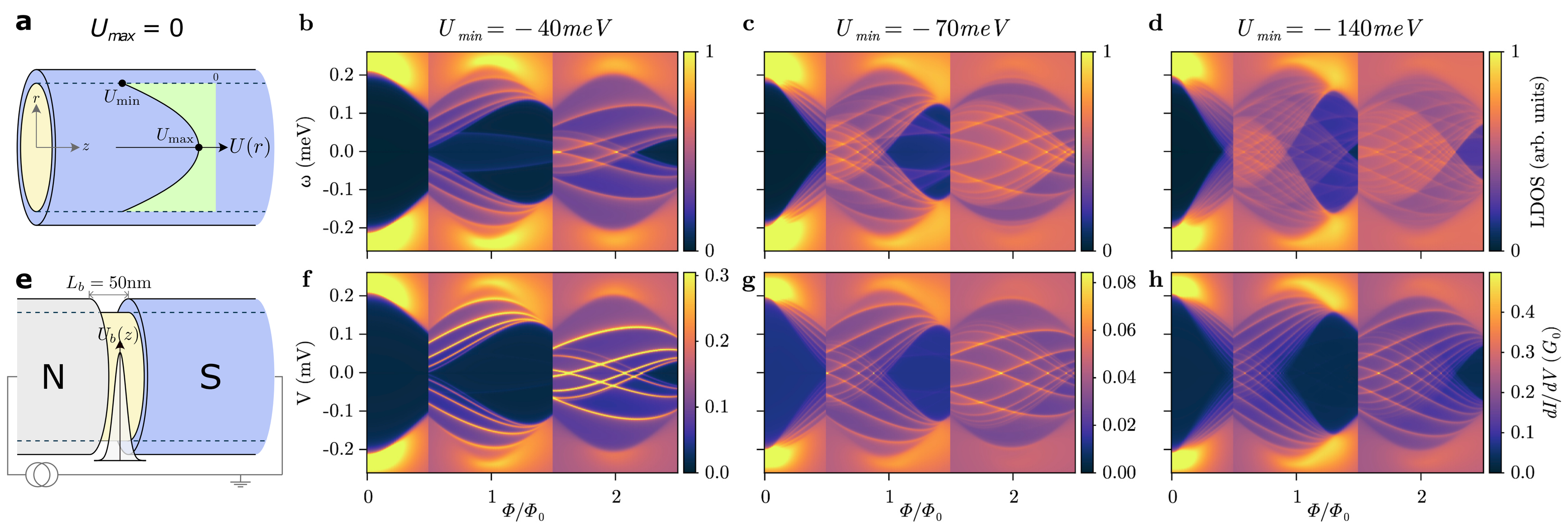

Figure 5. (a) Hybrid nanowire sketch with the semiconductor electrostatic potential superimposed. (b-d) LDOS vs. magnetic flux for different band bendings. (f-h) Transport simulations through the barrier in (e).

- Core/shell interface ⇒ work function difference ⇒ nonhomogeneous electrostatic potential.
- We model it with a conduction band bending in the semiconductor:

$$U(r) = U_{\text{min}} + (U_{\text{max}} - U_{\text{min}})\left(\frac{r}{R_{\text{core}}}\right)^\nu. \tag{3}$$

- Potential well close to the core/shell interface ⇒ LDOS similar to the tubular model (compare (b-d) to Fig. 4).
- Tunneling spectroscopy through dI/dV. For high, short barriers it matches the LDOS (f-h) with three differences:
  - Sharper Van Hove singularities.
  - Particle-hole asymmetry.
  - More sensitive to small $|m_L|$ ⇒ large ones (close to zero energy) loose visibility.

Modified hollow core: charge localized at R_{av}.

- Radially resolved LDOS (b) shows that subgap states localize around a R_{av}.
- We derive a simplified model: a hollow-core but fixing the radial coordinate at R_{av} instead of R_{core}:
  - Its L_z rotated Hamiltonian is:

$$\tilde{H} = \left[\frac{\left(m_L - \frac{1}{2}n\tau_z + \frac{1}{2}\frac{\Phi}{\Phi_0}\frac{R_{\text{av}}^2}{R_{\text{LP}}^2}\tau_z\right)^2}{2m^*R_{\text{av}}^2} + \frac{k_z^2}{2m^*} - \mu\right]\tau_z + \Sigma_{\text{shell}}(\omega, 0). \tag{4}$$

  - $R_{LP} = \frac{1}{2}(R_{\text{core}} + R_{\text{shell}})$
  - DP shift:

$$\frac{\Phi_{\text{dp}}}{\Phi_0} = \frac{R_{\text{av}}^2}{R_{\text{LP}}^2} \tag{5}$$

  - $\Phi_0 = 2e/h$.
  - Similar phenomenology (compare a and c) and numerically almost trivial.
  - Valid while degeneracy points are well-defined ⇒ all m_L have the same R_{av}.
  - m_L of each CdGM analog in white in (c).

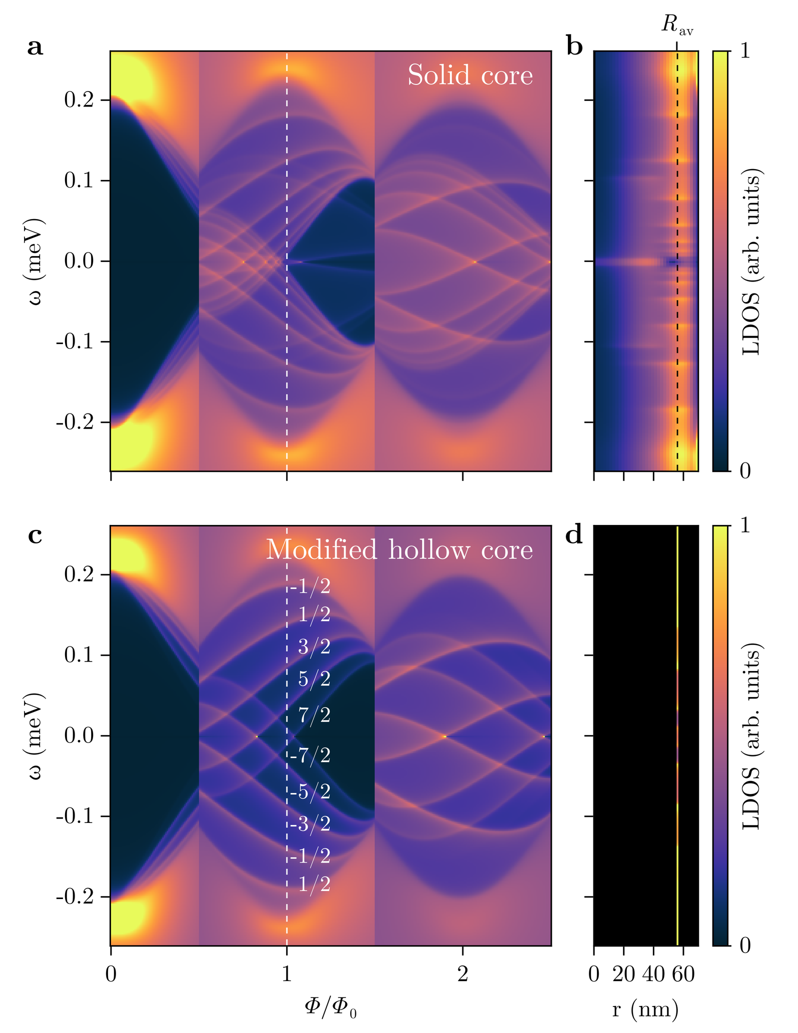

Figure 6. (a,b) Solid-core LDOS. (c,d) Modified hollow-core equivalent system. $R_{\text{av}} = 56$nm.

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