Localized States in Engineered Carbon Nanoribbons

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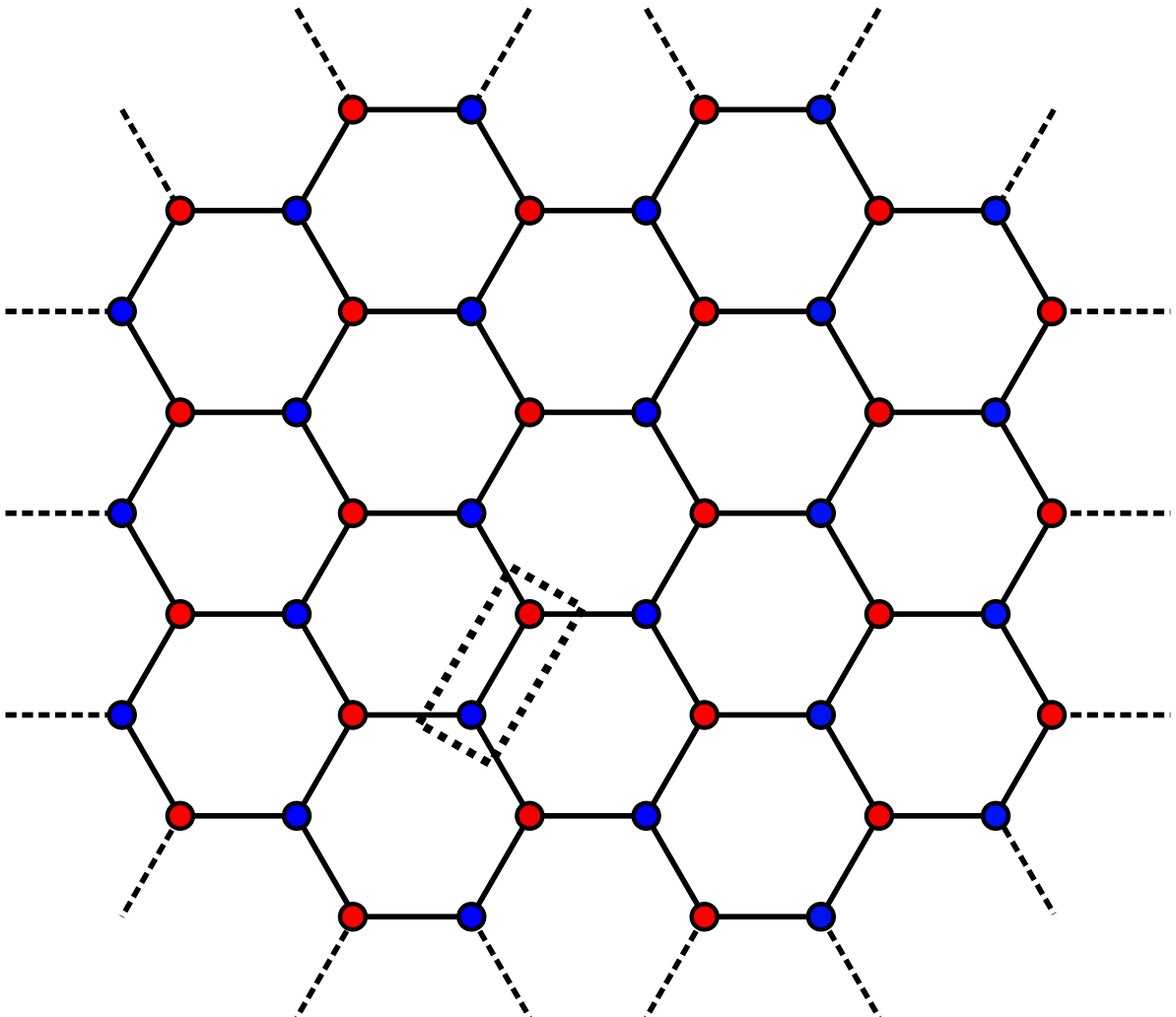
Introduction

Graphene



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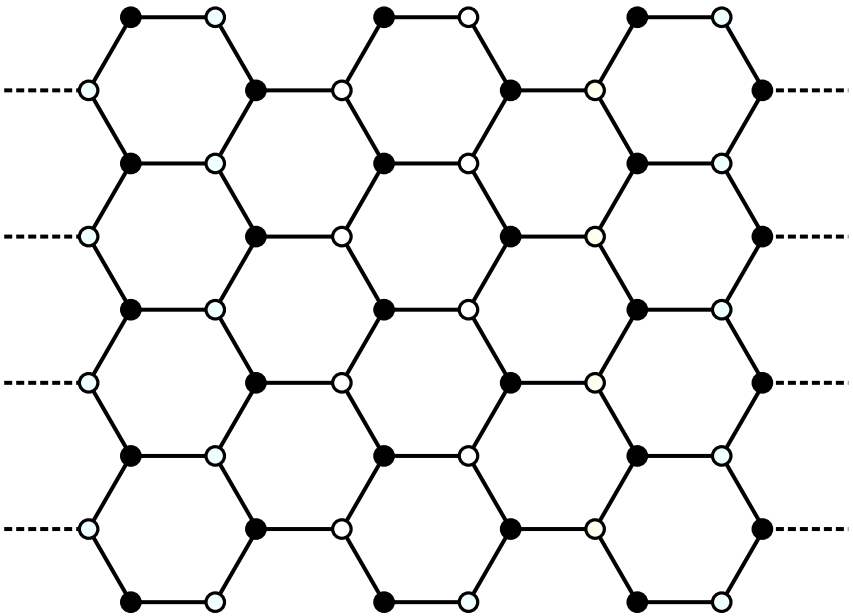

Figure: Armchair nanoribbon (ANR)

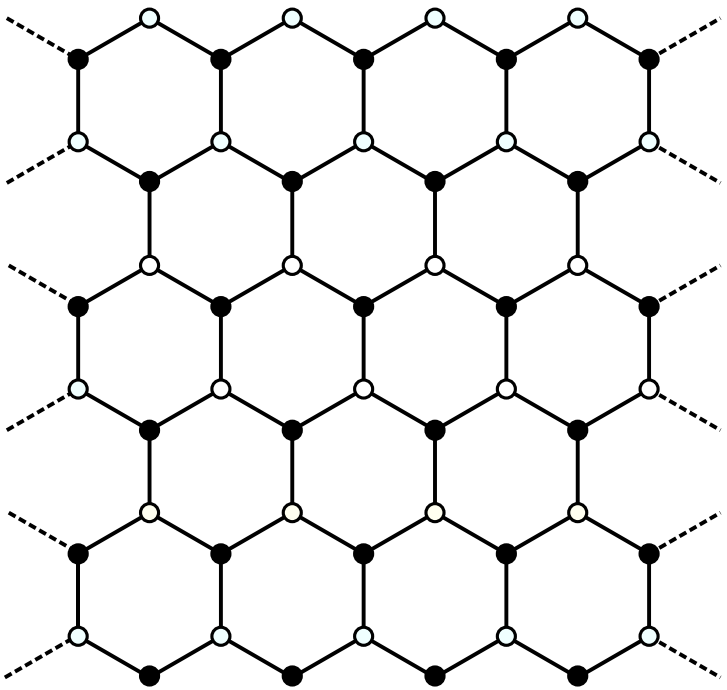

Figure: Zigzag nanoribbon (ZNR)

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Introduction

Dispersion Relations: Armchair[5]

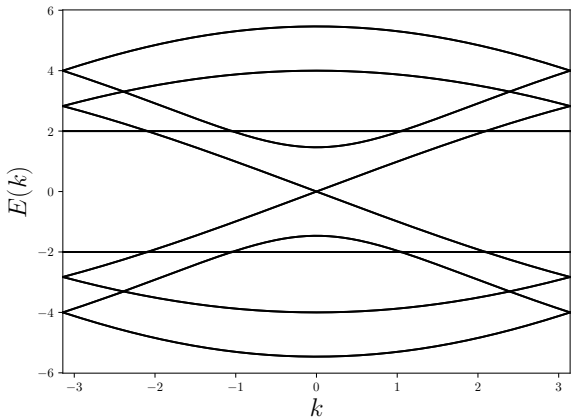

Figure: $W = 5$

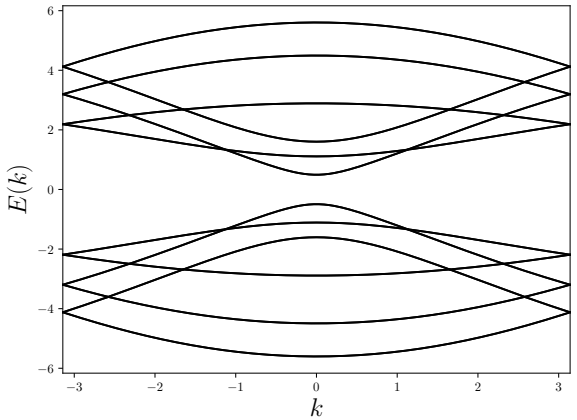

Figure: $W = 6$

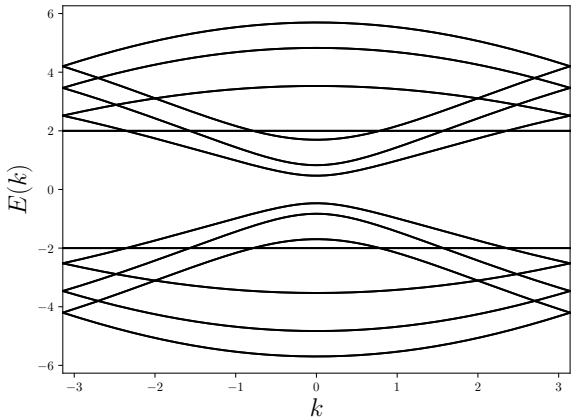

Figure: $W = 7$

- Dispersion depends on widths
- Zero crossing for $3m - 1$
- Gap $\sim 1/W$

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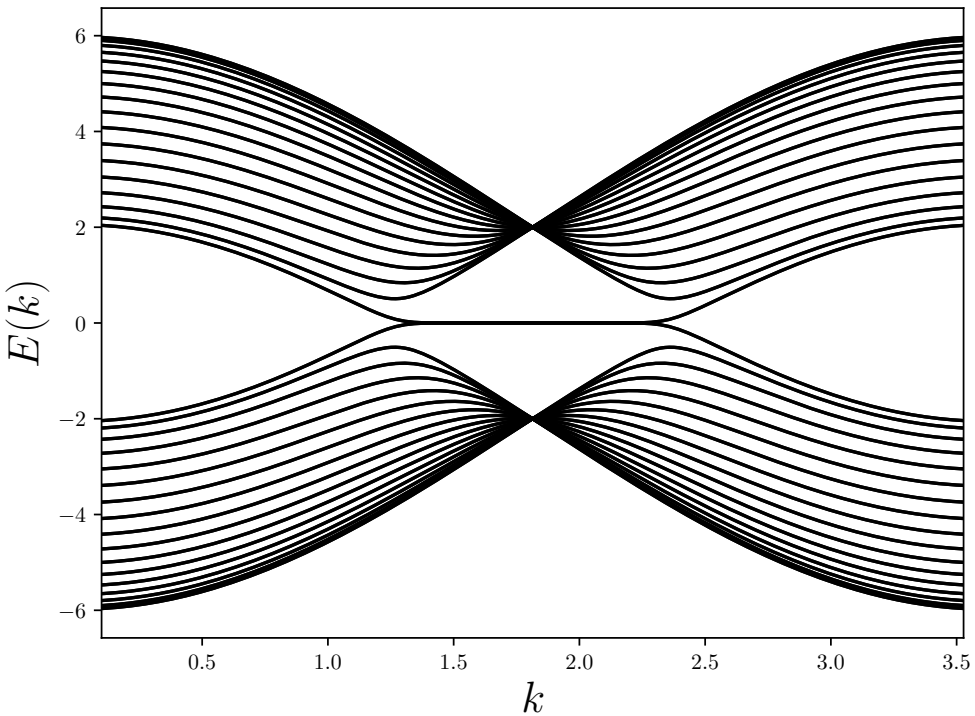
Introduction

Dispersion Relations: Zigzag[5]



- No width dependence
- Flatband in the middle third of the BZ
- Exponentially localized edge states

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Hybrid Armchair Nanoribbon

Reasoning

- Less covered in literature (arXiv search results: armchair/zigzag $\approx 1/2$)
- Can be synthesized from ground up [2]
- Has been shown to have topological properties

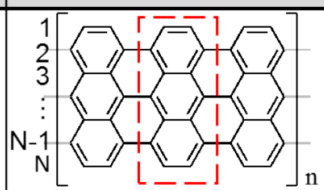
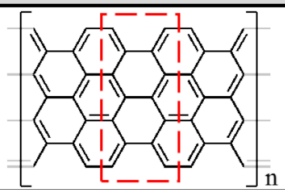
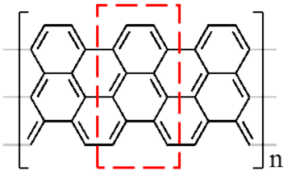
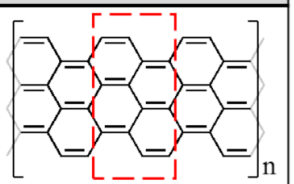
Termination type	Zigzag (N = Odd)	Zigzag' (N = Odd)	Zigzag (N = Even)	Bearded (N = Even)
Unit cell shape				
Bulk Symmetry	Inversion/mirror	Inversion/mirror	Mirror	Inversion
Z_2	$\frac{1+(-1)^{\lfloor \frac{N}{3} \rfloor + \lfloor \frac{N+1}{2} \rfloor}}{2}$	$\frac{1-(-1)^{\lfloor \frac{N}{3} \rfloor + \lfloor \frac{N+1}{2} \rfloor}}{2}$		$\frac{1-(-1)^{\lfloor \frac{N}{3} \rfloor}}{2}$

Figure: Z2 invariant of an armchair nanoribbon [1]

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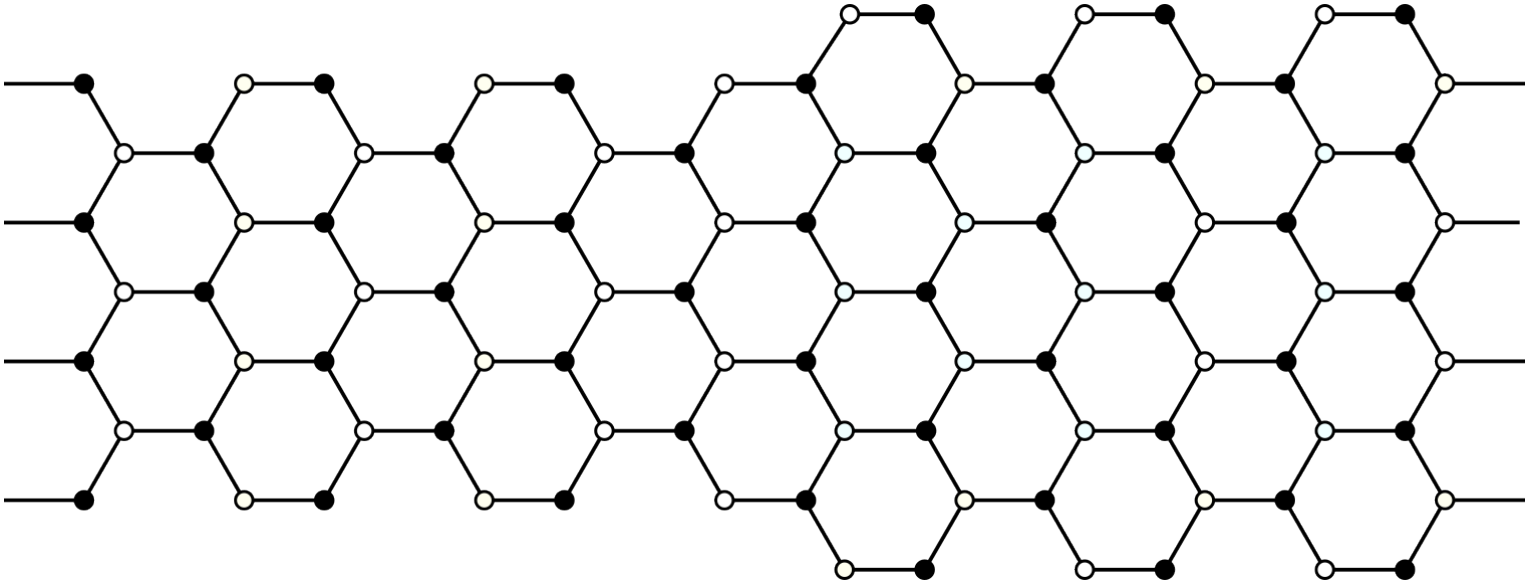

Figure: 7/9 Junction Armchair Nanoribbon

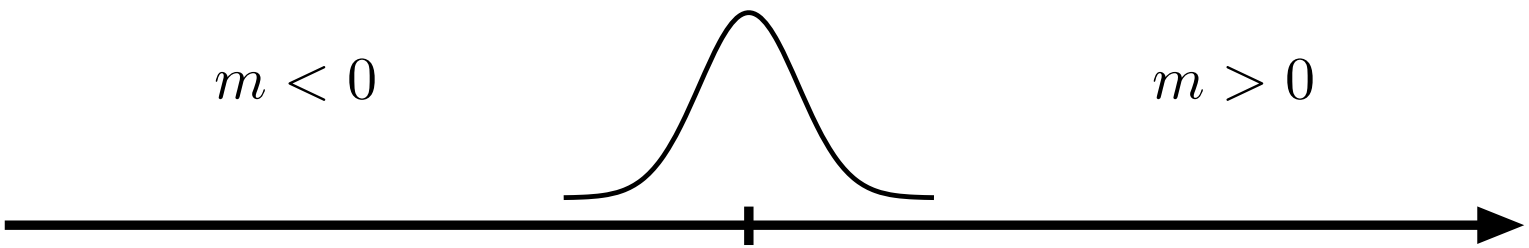

Figure: Jackiw-Rebbi Zero Mode[4]

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Non-interacting Dispersion

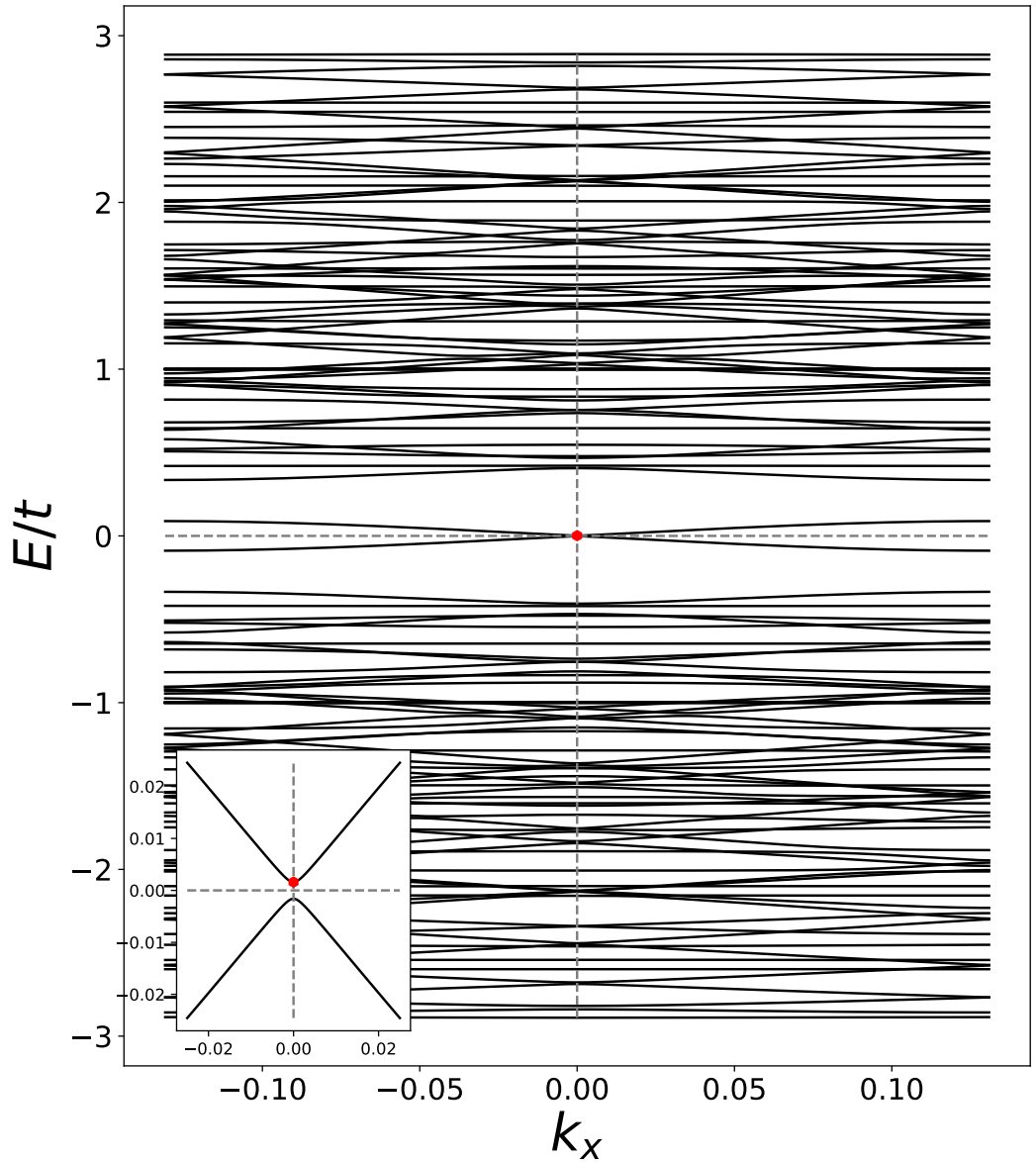

Figure: Low Lying $k_x = 0$ state is highlighted in red

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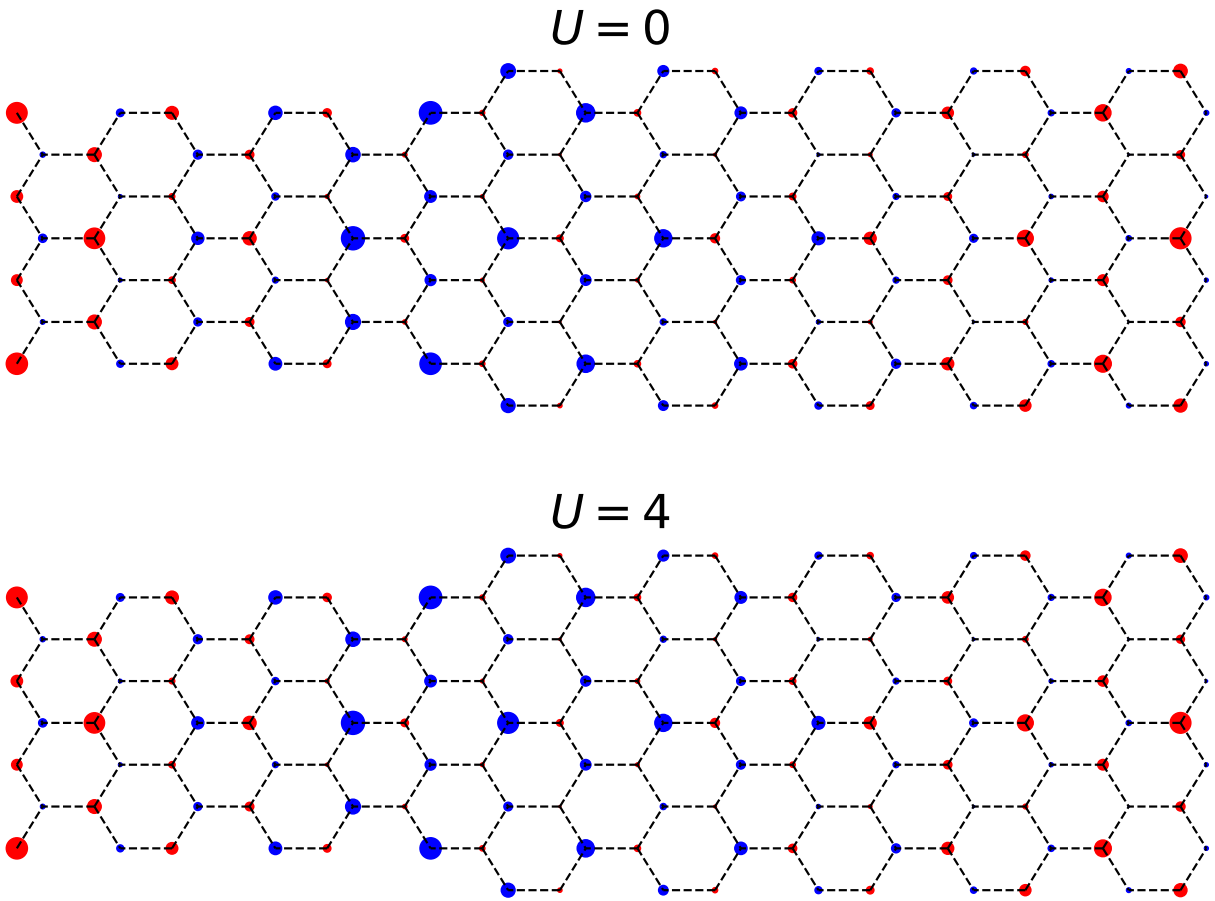

Figure: GS densities are effectively independent of U

BCS-Hubbard Hamiltonian[3]

$$H = -\sum_{\langle i,j\rangle\sigma} (tc^{\dagger}_{i\sigma}c_{j\sigma} + \Delta c_{i\sigma}c_{j\sigma} + h.c.) + U\sum_{k}\left(n_{k\uparrow} - \frac{1}{2}\right)\left(n_{k\downarrow} - \frac{1}{2}\right)$$

Symmetric lines condition ($t = \Delta$)

- For any bipartite lattice is exactly solvable
- Investigate behaviour for arbitrary U
- 2^N disjoint sectors
  - Ferromagnetic & Antiferromagnetic

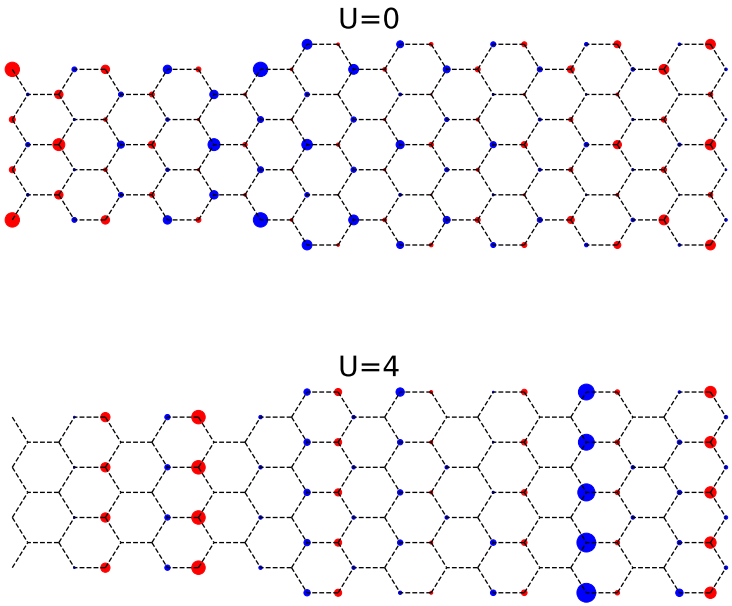

Figure: Ferromagnetic

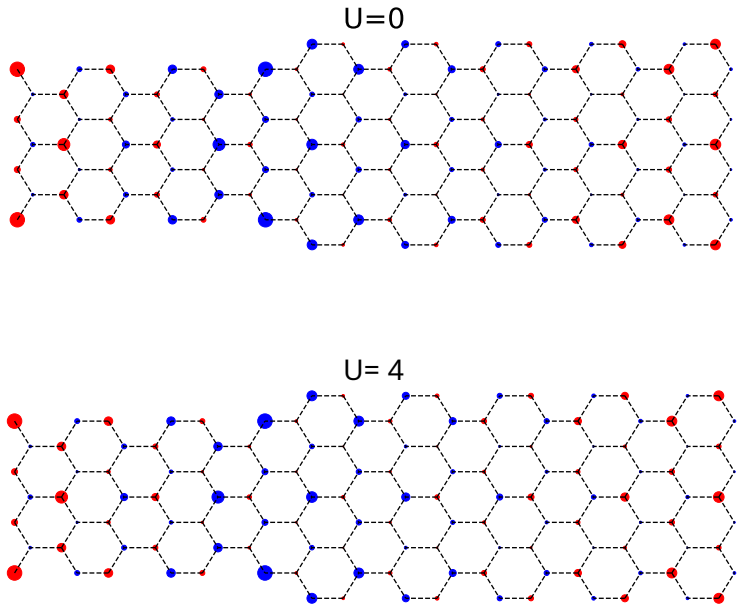

Figure: Antiferromagnetic

Summary

Hybrid ANR's

- Low-lying energy state
- Exponentially localized
- Resilient against Hubbard interaction
- Locality persists even with SC pairs

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Summary

Hybrid ANR's

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Localization of Electronic States in Hybrid Nano-Ribbons in the Non-Perturbative Regime

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Abstract

We investigate the localization of low-energy single quasi-particle states in the 7/9- and 13/15-hybrid nanoribbon systems in the presence of strong interactions and within a finite volume. We consider two scenarios, the first being the Hubbard model at half-filling and perform quantum Monte Carlo simulations for a range U that includes the strongly correlated regime. In the second case we add a nearest-neighbor superconducting pairing Δ and take the symmetric line limit, where Δ is equal in magnitude to the hopping parameter t. In this limit the quasi-particle spectrum and wavefunctions can be directly solved for general onsite interaction U. In both cases we extract the site-dependent quasi-particle wavefunction densities and demonstrate that localization persists in these non-perturbative regimes under particular scenarios. Our findings suggest that such localization under the presence of interactions and within a finite volume is a generic feature of hybrid nanoribbons composed of topologically distinct regions.

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Figure: arXiv:2204.02742v2

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Thank You

Thank You

Thank You

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[4] R. Jackiw and C. Rebbi. Solitons with fermion number ½. *Phys. Rev. D*, 13:3398–3409, Jun 1976.

[5] Katsunori Wakabayashi, Ken ichi Sasaki, Takeshi Nakanishi, and Toshiaki Enoki. Electronic states of graphene nanoribbons and analytical solutions. *Science and Technology of Advanced Materials*, 11(5):054504, Oct 2010.

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