

# Phase Diagram and Crossover Phases of Topologically Ordered

## Graphene Zigzag Nanoribbons

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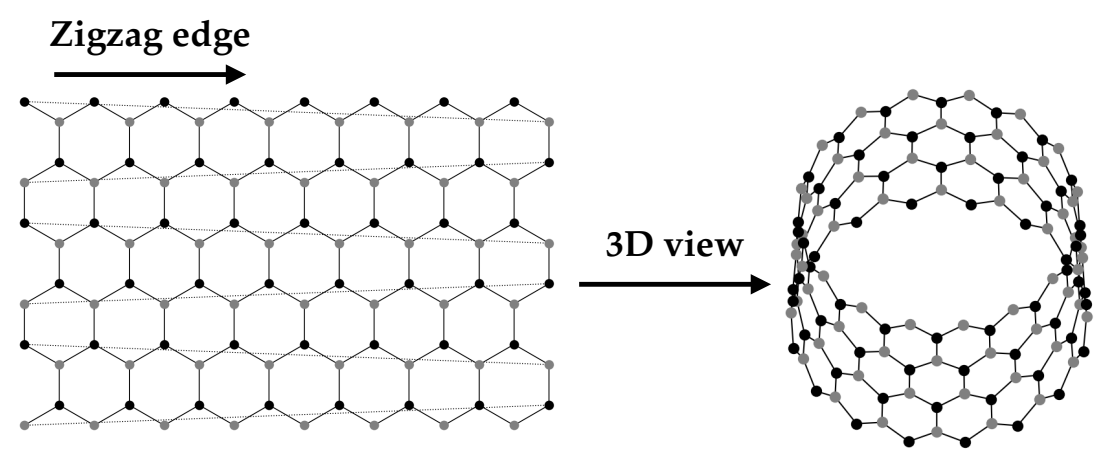
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### 1. Introduction

- **Topological order** is a new phase of matter beyond Landau theory [1].
- **Zigzag graphene nanoribbon (ZGNRs)** [2] displays topological order due to interplay between on-site repulsion and disorder [3].



- A phase diagram of ZGNRs is computed as a function of on-site repulsion, doping concentration and disorder strength.

### 2. Model and method

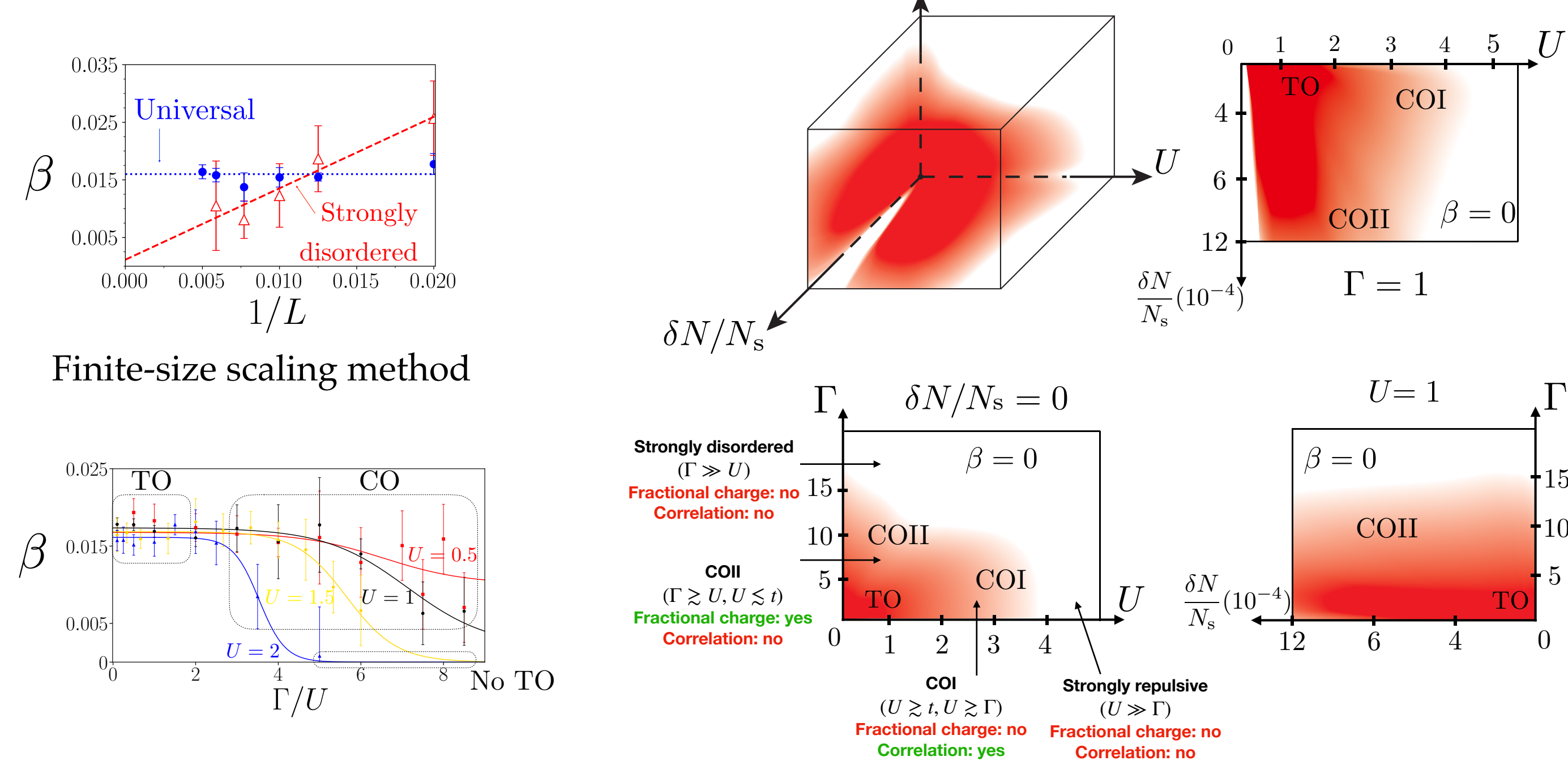
- Mott-Anderson Hamiltonian with periodic boundary condition is employed

$$H = -t \sum_{\langle ij \rangle, \sigma} (c_{i, \sigma}^\dagger c_{j, \sigma} + c_{j, \sigma}^\dagger c_{i, \sigma}) + U \sum_i n_{i, \uparrow} n_{i, \downarrow} + \sum_i V_i n_{i, \sigma}$$

hopping term                      on-site repulsion                      disorder

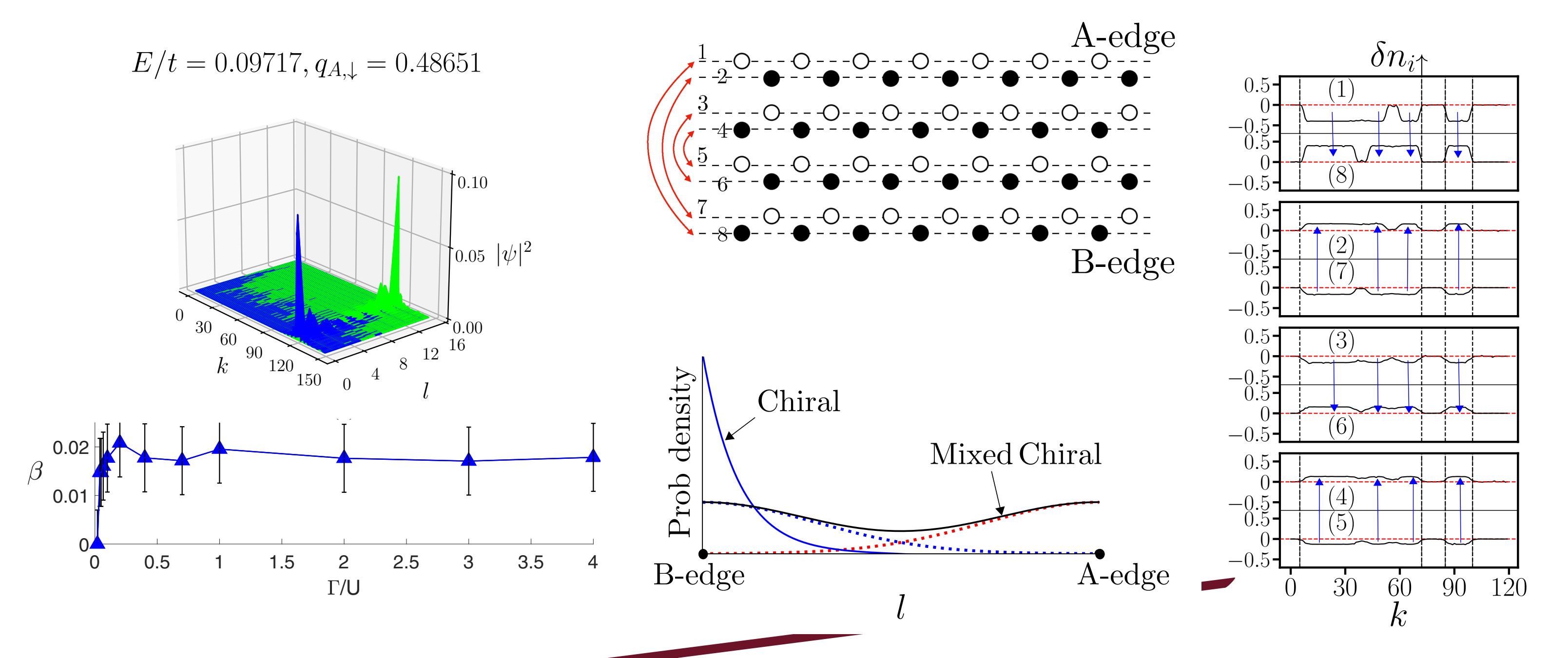
- The Hamiltonian is solved within **Hartree-Fock approximation**. The solutions are consistent with DFT and DMRG.
- Construct phase diagram via analyzing (1) **topological entanglement entropy  $\beta$  (TEE)** [4], (2) **edge charge correlations** and (3) **existence of fractional charges**.

### 3. Phase diagram



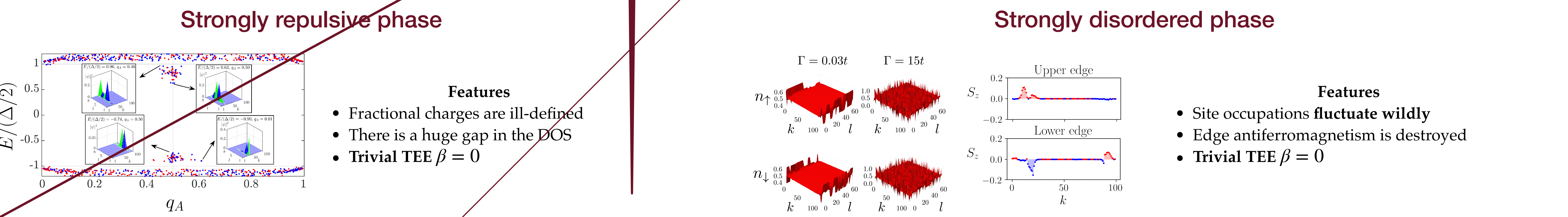
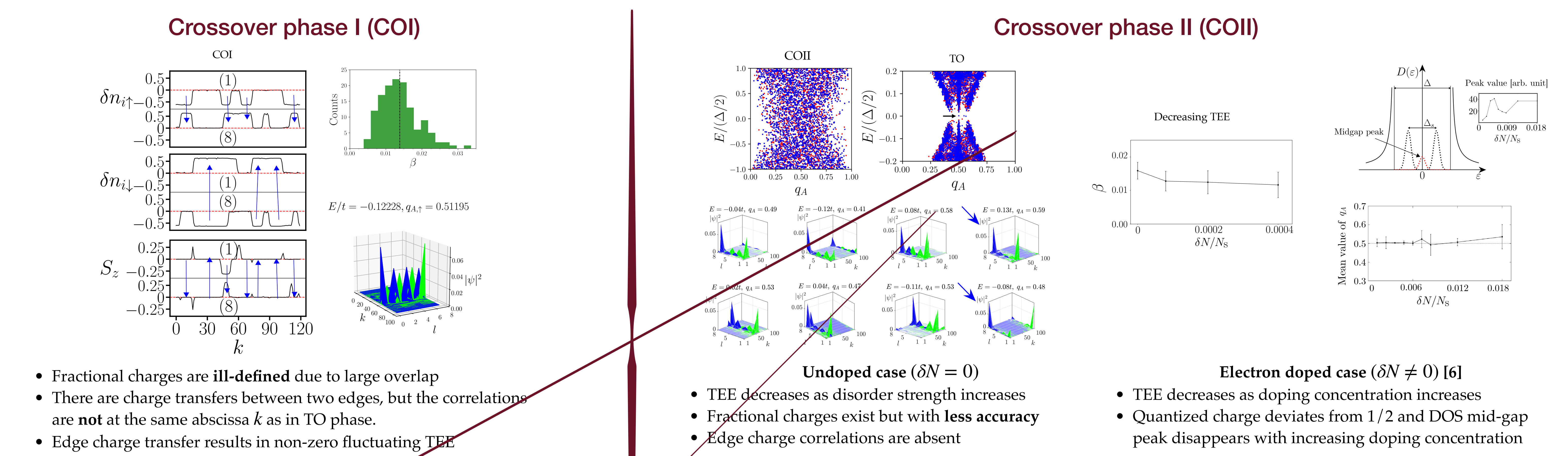
- Characteristics of TEE**
- $\beta \approx 0.016$ , **small variance**
  - $0 < \beta < 0.016$ , **large variance**
  - $\beta = 0$  (No TO)
- Phase diagram**
- Red: topological order
  - Blurred red: crossover phases (COI and COII)
  - White: non-topological order

### 4. Topologically ordered phase



- Fractional charges exists
  - Universal TEE  $\beta = 0.016 \pm 0.003$  [5]
  - Spin-charge separation [2]
- Charge correlation**
- Increase/decrease in occupation numbers are **correlated at nearly same abscissa  $k$**  (blue arrows).
  - Such correlations also exhibit **inside ribbon**
  - Mixed chiral gap states contribute to this correlation

### 5. Crossover phases and non-topological phases



### 6. Conclusion

- We have constructed a phase diagram of ZGNRs in the parameter space.
- The phase diagram constructed based on computation of TEE is similar to one obtained by analyzing edge charge correlations and existence of fractional charges.
- There exists crossover phases with different properties.
- Physical properties of these crossover phases as well as two non-topological phases, strongly disordered and strongly repulsive phases, are delineated.

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### References

- [1] X.-G. Wen, Rev. Mod. Phys. **89**, 041004 (2017).
- [2] M. Kolmer et al., Science **369**, 571 (2020).
- [3] S.-R. Eric Yang, Topologically Ordered Zigzag Nanoribbon (World Scientific, 2023).
- [4] A. Kitaev and J. Preskill, Phys. Rev. Lett. **96**, 110404 (2006).
- [5] Y. H. Kim et al., Phys. Rev. B **103**, 115151 (2021).
- [6] Y. H. Kim et al., Scientific Reports **12**, 14551 (2022).

