# Quantum Monte Carlo Simulations of the Hubbard Model

## Application to an interacting electronic systems in 2D: the TMD nanoribbon

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# Beyond graphene: TMD nanoribbons

# Graphene's drawbacks

**Single layer graphene is gapless**

...while bilayer graphene has only a limited gap. A tunable gap is desirable in electronics applications.

**Superconductivity?**

A superconducting phase has been predicted for graphene. However, it is hard to achieve. It remains challenging to use it for applications.

# TMD nanoribbons: a possible solution

A nanoribbon consists of a 2D layer that is (nearly) infinitely long on one direction, but not on the other, so that edge states become relevant, and can be controlled to yield interesting properties.

**Intrinsic gap $\rightarrow$ better switching**

Advantageous to design electronic components.

**Topological superconductivity**

*Electron interactions* could be responsible for the appearance of a promising superconducting phase.

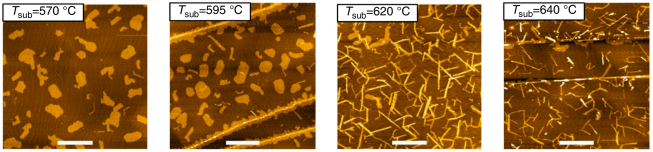


**Figure 1:** Fabrication of TMD nanoribbons. (from *Chen et al. 2017*)

# $e^- - e^-$ interactions and magnetism of metallic zigzag edges

## Origin of magnetism

A high density of low-energy electronic states is localized at the zigzag edges, decaying quickly in the bulk, which suggests the possibility of magnetic ordering.

**MF Hubbard** $\rightarrow$ magnetic moments localized at the edges.

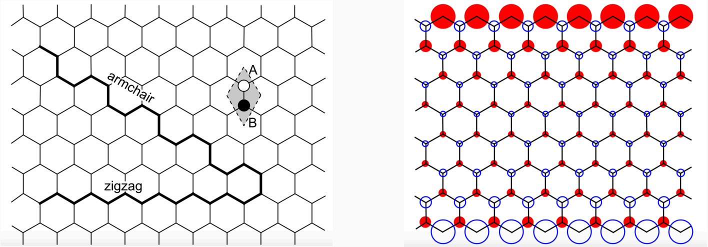


**Figure 2:** Left: 2 possible edges of a nanoribbon in a honeycomb lattice. Right: Accumulation of $e^-$ edge states, leading to magnetism. (from *Yazyev 2010*)

# Determinantal / Auxiliary Field QMC

# $d \to d+1$

### Back to classical Monte Carlo

Map the *quantum d-dimensional problem to a classical* $d+1$*-dimensional* problem, at the expense of introducing an *auxiliary field* $\boldsymbol{h}$.

### Decoupling the fermions

Establish a *formal correspondence* between a system of *interacting fermions* and an ensemble of *non interacting fermion systems coupled to fluctuating external potentials*.

# Computational complexity and the sign problem

# $NP = P$?

- **Fermion sign problem** $\rightarrow$ exponential increase of the computing time with the number of particles. Solving the sign problem would imply $NP = P$ (million dollar question).
- Which models allow a **partial solution of the sign problem**? Does the **2D fermionic Hubbard model** belong to this class?
- **Ultracold atoms** in an optical lattice? $\rightarrow$ quantum simulator to study the phase diagrams of correlated quantum systems.

# Why QMC? Emergence from strong electron correlations

## Closing remarks

- QMC accurately captures the **effects of correlations** in *many-fermion* systems.
- Some properties, like *superconductivity*, arise precisely due to such effects.
- This state-of-the-art method allows us to study the **phases arising within 2D nanostructures**, which have numerous applications, namely in **healthcare and electronics**.

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