

# **Development of a QMC code to tackle interacting electronic systems in 2D with application to TMD nanoribbons**

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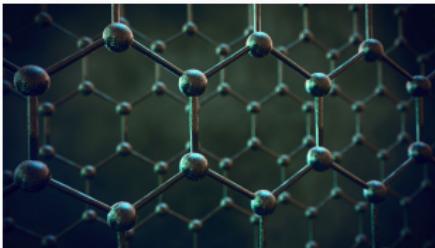
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# **Beyond graphene: TMD nanoribbons**

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# Graphene



**Figure 1:** Graphene's honeycomb lattice. ([graphene.manchester.ac.uk](http://graphene.manchester.ac.uk))

## Defying the Mermin Wagner Theorem

2D materials have been attracting interest since 2004, when graphene was isolated from a 3D graphite base (using scotch-tape), yielding a single layer of atoms.

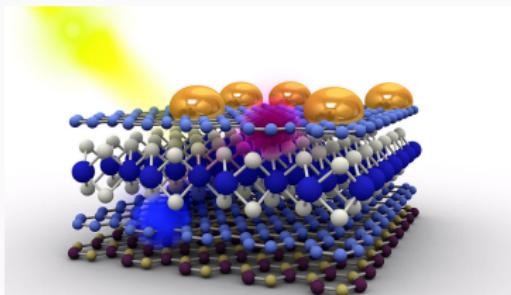
## New perspectives

Graphene and graphene-like materials have promising properties, with interesting as-yet-unseen phenomena occurring within them.

# Structure

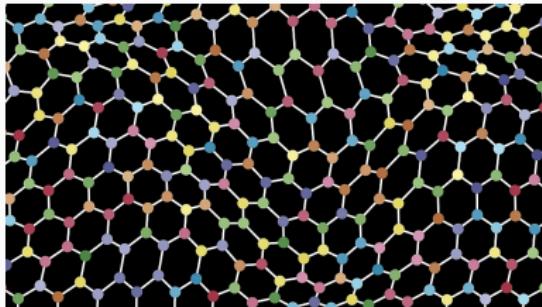


**Figure 2:** Dirac cones. (from *manchester*)



**Figure 3:** Heterostructure engineering. (from *manchester*)

## Interesting phenomena



**Figure 4:** Strain creates pseudo magnetic fields. (from *manchester*)



**Figure 5:** Hofstader's butterfly. (from *manchester*)

# Applications



**Figure 6:** Smart contact lenses and night vision. (from *manchester*)



**Figure 7:** Desalination and filtering of drinking water. (from *manchester*)

## 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

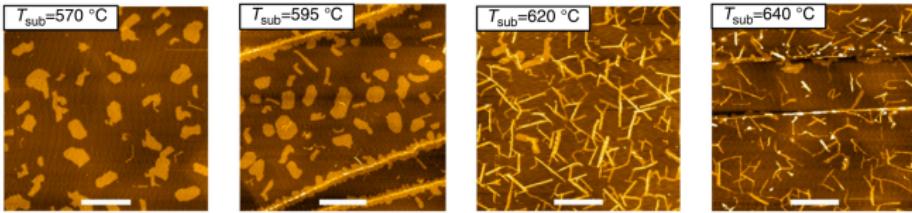
A nanoribbon consists of a 2D layer that is (nearly) infinitely long on one direction, but not on the other, so that edge states become relevant, and can be controlled to yield interesting properties.

## Intrinsic gap → better switching

Advantageous to design electronic components.

## Topological superconductivity

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

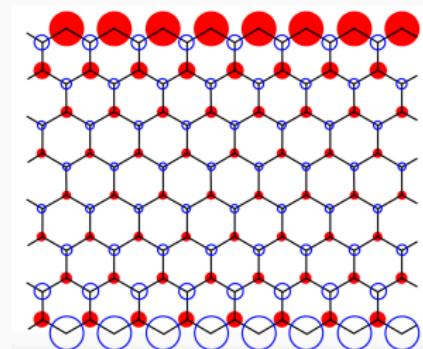
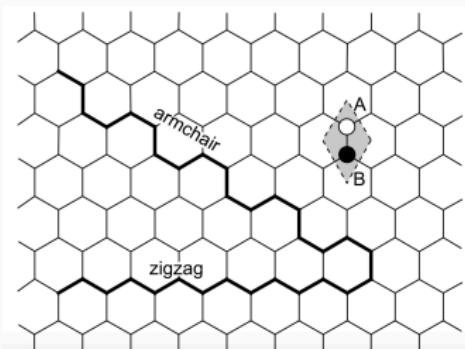


**Figure 8:** Fabrication of TMD nanoribbons. (from Chen et al. 2017)

## 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.

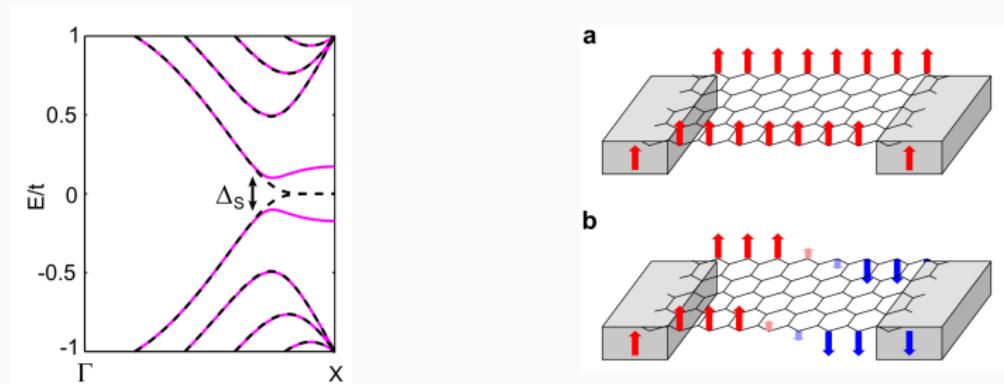
**MF Hubbard** → magnetic moments localized at the edges.



**Figure 9:** Left: 2 possible edges of a nanoribbon in a honeycomb lattice. Right: Accumulation of  $e^-$  edge states, corresponding to an AF ground state (opposite edges with opposite spins). (from Yazyev 2010)

## Magnetic ordering of zigzag edges

While the zigzag graphene nanoribbon antiferromagnetic ground state is semiconducting, a state with interedge ferromagnetic orientation is a metal. An example of an application based on the switching between the two states is a magnetoresistive sensor.

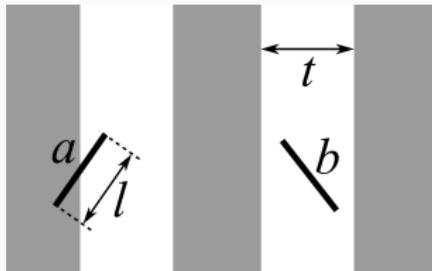


**Figure 10:** Left: Opening of a gap  $\Delta_S$  due to electron interactions, for  $U/t = 1.2$ . Right: Switching between low (a) and high-resistance (b) configurations, corresponding, respectively, to parallel, and antiparallel configurations of the ferromagnetic leads. (from Yazyev 2010)

# Monte Carlo

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# Exploiting randomness



**Figure 11:** Buffon's experiment.

## Buffon (1777)

Estimate  $\pi$  by repeatedly throwing a needle onto a sheet of paper with evenly spaced lines.  $\pi = \lim_{N \rightarrow \infty} \frac{2NI}{Mt}$

## Metropolis (1949)

More generally, we may produce accurate estimates of deterministic integrals by using randomness.

# Classical Monte Carlo

- Integral as **expectation** of a random variable.
- Draw independent samples: a good **approximation** of the integral is the **sample mean**.
- To do this, design an *ergodic* **Markov Chain** with a stationary distribution coinciding with the desired one.
- After the *warm up* steps, the algorithm generates samples from the target distribution.
- Perform **independent measurements** of physical quantities (introducing decorrelation steps between them).

## Detailed balance

Let  $\mu$  and  $\nu$  be two possible states of the system. On average, transitions between  $\mu$  and  $\nu$  are just as frequent as those from  $\nu$  to  $\mu$ . This corresponds to time-reversal symmetry, related to the concept of reversibility in thermodynamics.

## Importance sampling

Drastically improves convergence speed. This is done by variance reduction. An acceptance-rejection scheme is implemented to ensure that we focus on the most representative part of the state space.

## Classical Monte Carlo

Suppose you want to measure the average of a given *classical* quantity  $Q$ .

$$\langle Q \rangle = \frac{\sum_{\mu} Q_{\mu} e^{-\beta E_{\mu}}}{\sum_{\mu} e^{-\beta E_{\mu}}}$$

Very expensive because it requires the computation of the energies of all possible configurations.

Solution: **Choose only a subset of states** at random with probability (distribution)  $p_{\mu}$ .

## Classical Monte Carlo

The estimator of the expectation becomes

$$Q_{MC} = \frac{\sum_{i=1}^M Q_{\mu_i} p_{\mu_i}^{-1} e^{-\beta E_{\mu_i}}}{\sum_{j=1}^M p_{\mu_j}^{-1} e^{-\beta E_{\mu_j}}}$$

# Classical Monte Carlo

Approximate by drawing  $M$  samples, and taking the sample mean.

**Naïve estimator** ( $p_\mu \sim$  Uniform distribution)

$$Q_U = \frac{\sum_{i=1}^M Q_{\mu_i} e^{-\beta E_{\mu_i}}}{\sum_{j=1}^M e^{-\beta E_{\mu_j}}}$$

**Importance sampling** ( $p_\mu \sim$  Boltzmann distribution)

$$Q_B = \frac{1}{M} \sum_{i=1}^M Q_{\mu_i}$$

# So what?

## Quantum Monte Carlo

Instead of simulating thermal fluctuations, we use analogous techniques to simulate *quantum* fluctuations.

## Variational Monte Carlo

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# Variational principle

## Give your best guess

We introduce a trial wave function  $\phi(\mathbf{r})$  with adjustable parameters  $\alpha$ .

## Optimize it

The expectation we wish to approximate may be written as an integral, i.e. we optimize according to equation (1).

$$E(\{\alpha_i\}) = \frac{\langle \phi | \mathcal{H} | \phi \rangle}{\langle \phi | \phi \rangle} = \frac{\int \phi^*(\mathbf{r}) \mathcal{H} \phi(\mathbf{r}) d\mathbf{r}}{\int |\phi(\mathbf{r}')|^2 d\mathbf{r}'} \geq E_0 \quad (1)$$

# Diffusion Monte Carlo

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## Schrödinger equation in imaginary time $\tau = -it$

### What if we cannot come up with a good guess?

A reliable trial wave function may be difficult to construct. The many-body system can be simulated with less *a priori* knowledge of its properties.

A Wick rotation turns the Schrödinger equation into the diffusion equation. Additionally, shifting the energy scale,

$$\partial_\tau \psi = -\frac{1}{2m} \partial_x^2 \psi - [V(x) - E_T] \psi$$

# Ground state as the last man standing

## Transient family

The mapping  $\tau = -it$  allows us to recast the eigenfunctions of the hamiltonian as a family of transients  $e^{-E_n\tau}$ .

## The last survivor

In the new time, the longest lasting transient corresponds to the ground state.

Thus, for any  $\psi(x, \tau)$  with which we start the algorithm:

$$\lim_{\tau \rightarrow \infty} \psi(x, \tau) \propto \phi_0(x)$$

# **The sign problem for many-fermion systems**

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# Fixed-Node approximation

## Many-fermion systems are tricky to simulate

The *antisymmetric* many-fermion wave function causes a numerical instability, associated with its **nodes**.

## Circumventing the problem

Force convergence to the fermionic wave function by **fixing the nodes of the trial wave function** as the same as those of the fermionic ground state.

## In a nutshell

Diffusion method applied to  $\mathcal{H}_{FN}$ , which is simply the model hamiltonian with infinite potential barriers at the nodes of  $\psi(\mathbf{r})$

# **Determinantal / Auxiliary Field QMC**

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$$d \rightarrow d + 1$$

## Back to classical Monte Carlo

The Hubbard Stratonovich transformation maps the *quantum  $d$ -dimensional problem to a classical  $d + 1$ -dimensional problem*, at the expense of introducing an *auxiliary field  $\mathbf{h}$* .

## 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*, leading to a random walk representation of the imaginary time evolution.

## **Why QMC? Emergence from strong electron correlations**

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## 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**.

## Acknowledgements

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