

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

Francisco Monteiro de Oliveira Brito

January 31, 2018



Beyond graphene: TMD nanoribbons

Graphene

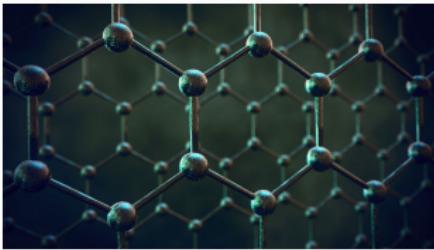


Figure 1: Graphene's honeycomb lattice. (graphene.manchester.ac.uk)

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*)

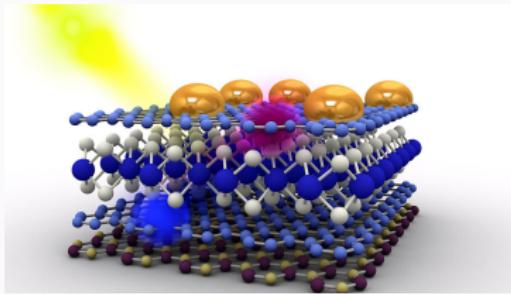


Figure 3: Heterostructure engineering. (from *manchester*)

Interesting phenomena

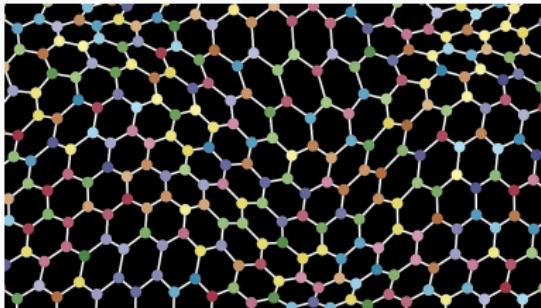


Figure 4: Strain creates pseudo magnetic fields. (from *manchester*)



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.

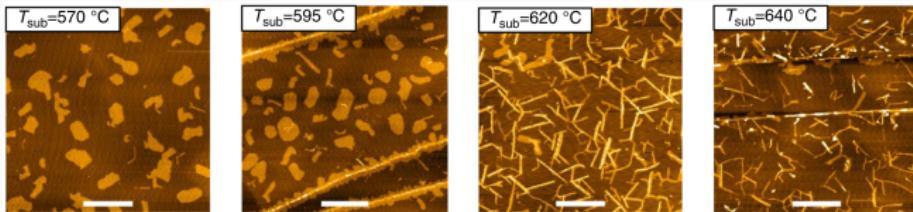


Figure 8: Fabrication of TMD nanoribbons. (from Chen et al. 2017)

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.

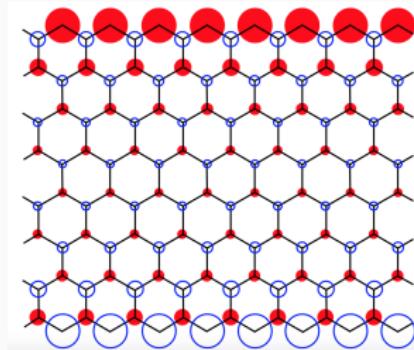
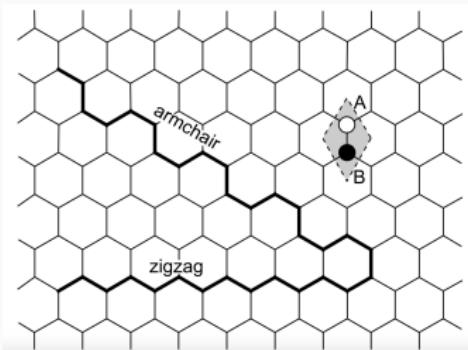


Figure 9: Left: 2 possible edges of a nanoribbon in a honeycomb lattice. Right: Accumulation of e^- edge states, corresponding to an AF ground state (opposite edges with opposite spins). (from Yazyev 2010)

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.

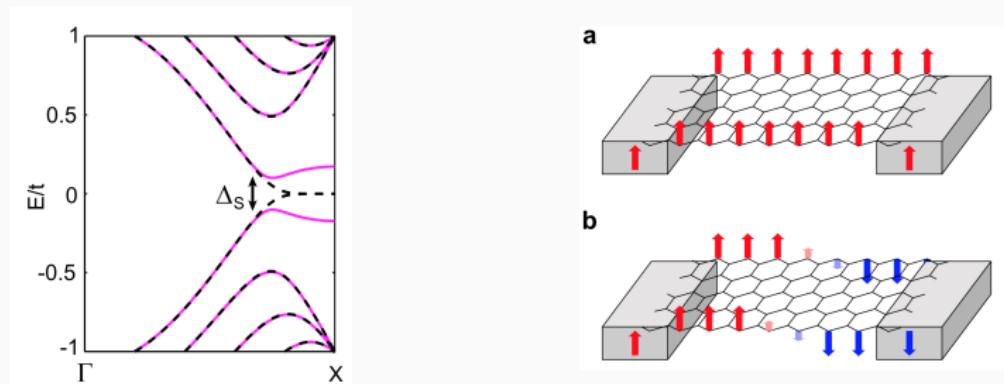


Figure 10: Left: Opening of a gap Δ_S due to electron interactions, for $U/t = 1.2$. Right: Switching between low (a) and high-resistance (b) configurations, corresponding, respectively, to parallel, and antiparallel configurations of the ferromagnetic leads. (from Yazyev 2010)

Monte Carlo

Exploiting randomness

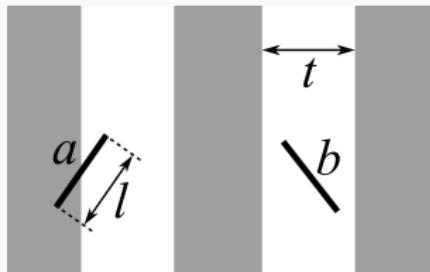


Figure 11: Buffon's experiment.

Buffon (1777)

Estimate π 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 μ and ν be two possible states of the system. On average, transitions between μ and ν are just as frequent as those from ν to μ . 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_{μ} .

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

Variational principle

Give your best guess

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

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

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

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

$$d \rightarrow d + 1$$

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

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

I would like to thank João Lopes and Eduardo Castro for supervising and advising me in this project, as well as Paulo Martins for filming the video.