USE OF A QUANTUM ANNEALER IN OPTIMIZATION PROBLEMS

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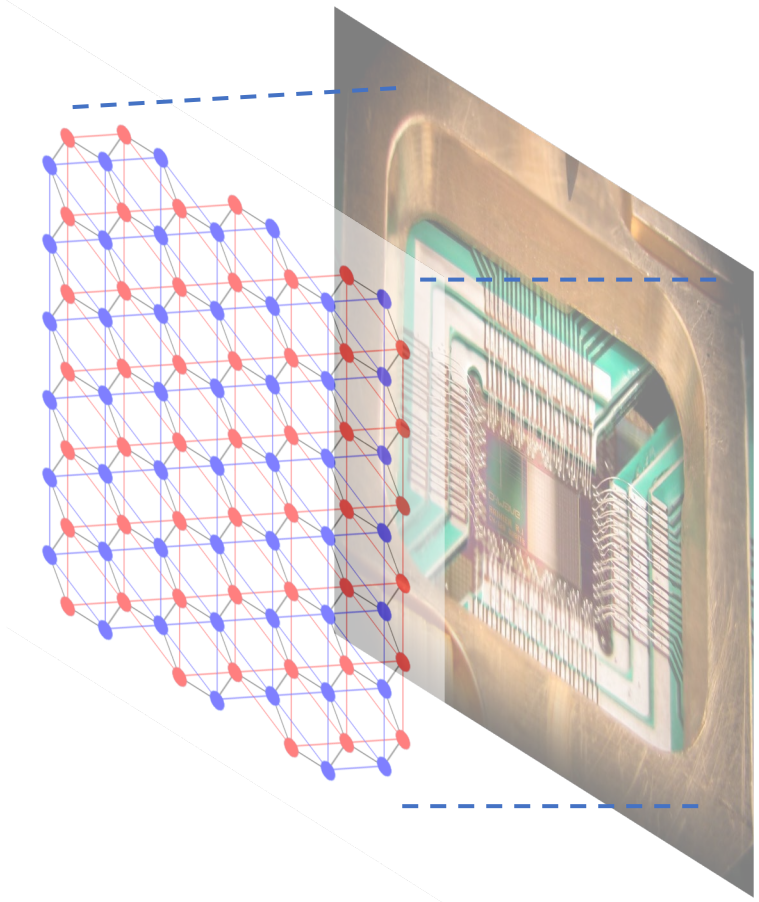
1. Motivation
2. Frustrated Ising model on D-Wave: phase transitions
3. Topological transitions in graphene: Kane-Mele-Hubbard model on D-Wave?
4. Lessons learned
5. Outlook



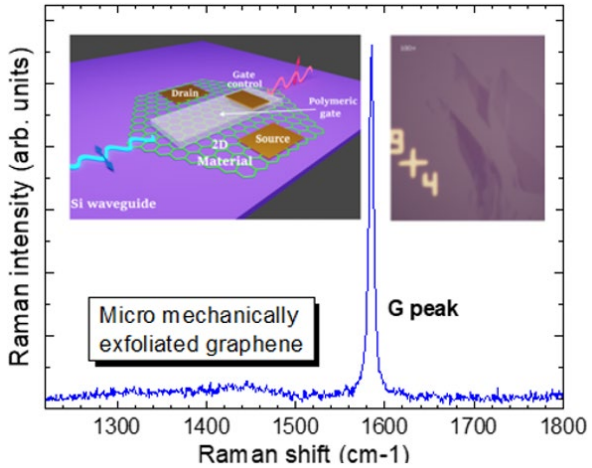
Quantum Computing @ INFN
Bologna, 15/11/2022

1 MOTIVATION

- Our interest in computing with D-Wave stems from the activities of our group within the **INFN QUANTEP** (**QUAN**tum**T**echnologies **E**xperimental **P**latform) project (CSN5)

Goals of QUANTEP:

1. study and development of silicon photonics integrated circuits for Quantum Computing applications (C-NOT gate)
2. Integration on chip of single photon sources and detectors
3. Polarization control with innovative 2D materials (nanowires and **graphene**)



- **Q@TN grant** for Projects on the **CINECA** Quantum Computing facility - Call 2021
  1. to model excitonic and e-e many body interactions in 2D materials to support the interpretation of our recent experimental data
  2. to explore the use of a Quantum Annealer as a **computing opportunity** for the study of topological transitions in graphene and other 2D materials
  3. to learn Quantum Computing techniques

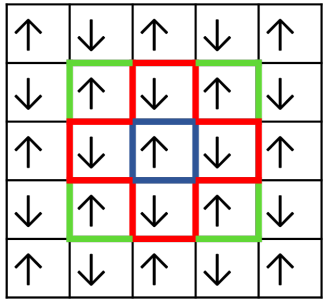
- **Challenges**: no previous work on D-Wave and activity done in the last 8 months

2 FRUSTRATED ISING MODEL ON D-WAVE

Hamiltonian and Phase Transitions

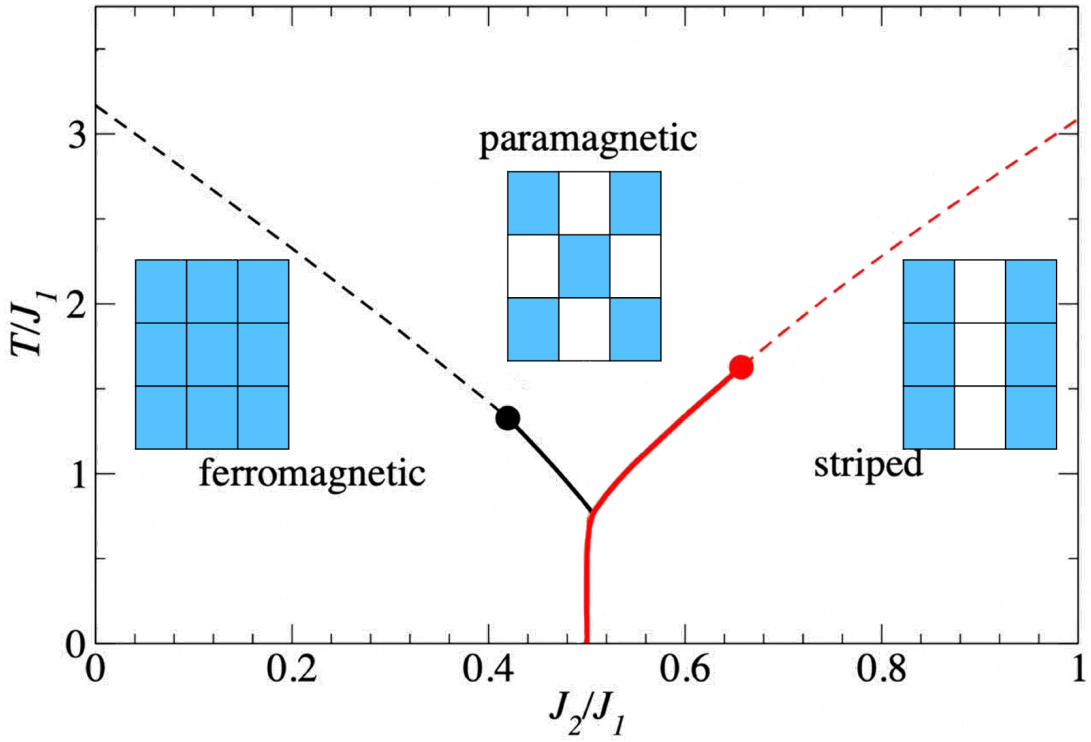
$$H = J_1 \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z + J_2 \sum_{\langle\langle i,j \rangle\rangle} \sigma_i^z \sigma_j^z + \mu_0 B \sum_i \sigma_i^z$$

$\sigma_i^z = \pm 1$, B variable external field



$J_i < 0$ ↑↑ spins favoured => ferromagnetic configuration
$J_i > 0$ ↑↓ spins favoured => paramagnetic configuration

Frustration introduces new fundamental states



Park & Lee, *Phase transition of Frustrated Ising model via D-wave Quantum Annealing Machine*, arXiv:2110.05124v1 (2021)
S. Jin et al., *Phase transitions in the frustrated Ising model on the square lattice*, arXiv 1212.5339v1

D-WAVE SETUP AND EMBEDDING

Loading the problem (BQM)

```
bqm = dimod.BinaryQuadraticModel.empty(dimod.SPIN)
bqm.add_variable(v=node_name, bias=h)
bqm.add_interaction(f"{x}-{y}", f"{x+1}-{y+1}", J2)
bqm.add_interaction(f"{x + 1}-{y}", f"{x}-{y + 1}", J2)
bqm.add_interaction(node1, node2, J1)
```

Selecting the Solver

```
from dwave.system import DWaveSampler, EmbeddingComposite
qpu = DWaveSampler(profile='CINECA')
```

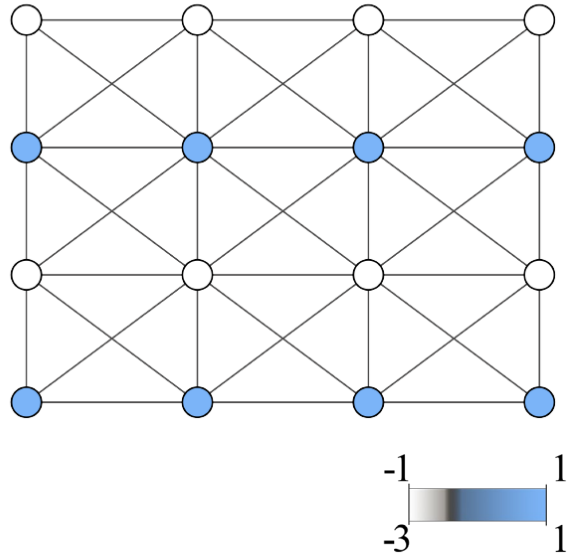
Embedding on Chimera graph

```
sampler = EmbeddingComposite(qpu)
```

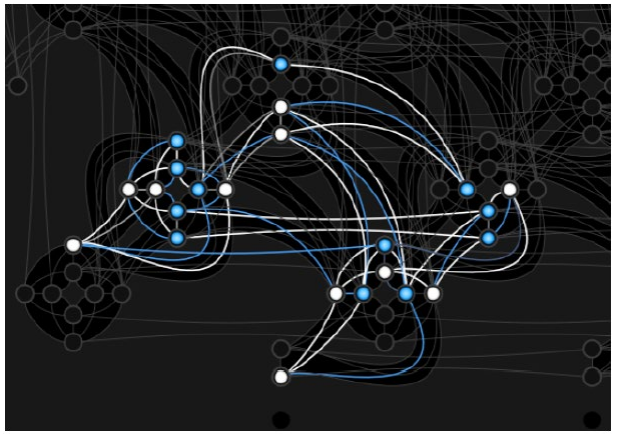
Setting annealing parameters

```
sampleset = sampler.sample(bqm, num_reads=num_reads,
annealing_time=at, chain_strength=cs, label=f'Ising
Frustrated {i}/{ratios.size}')
```

Model Lattice



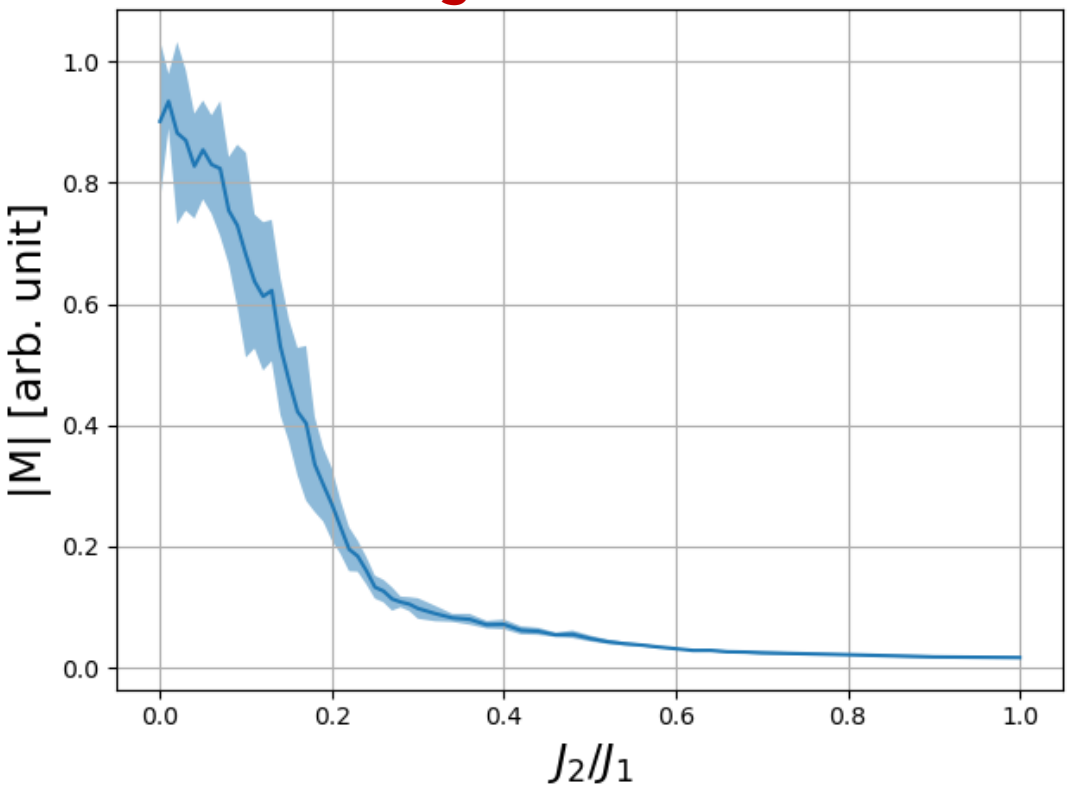
Model Embedding



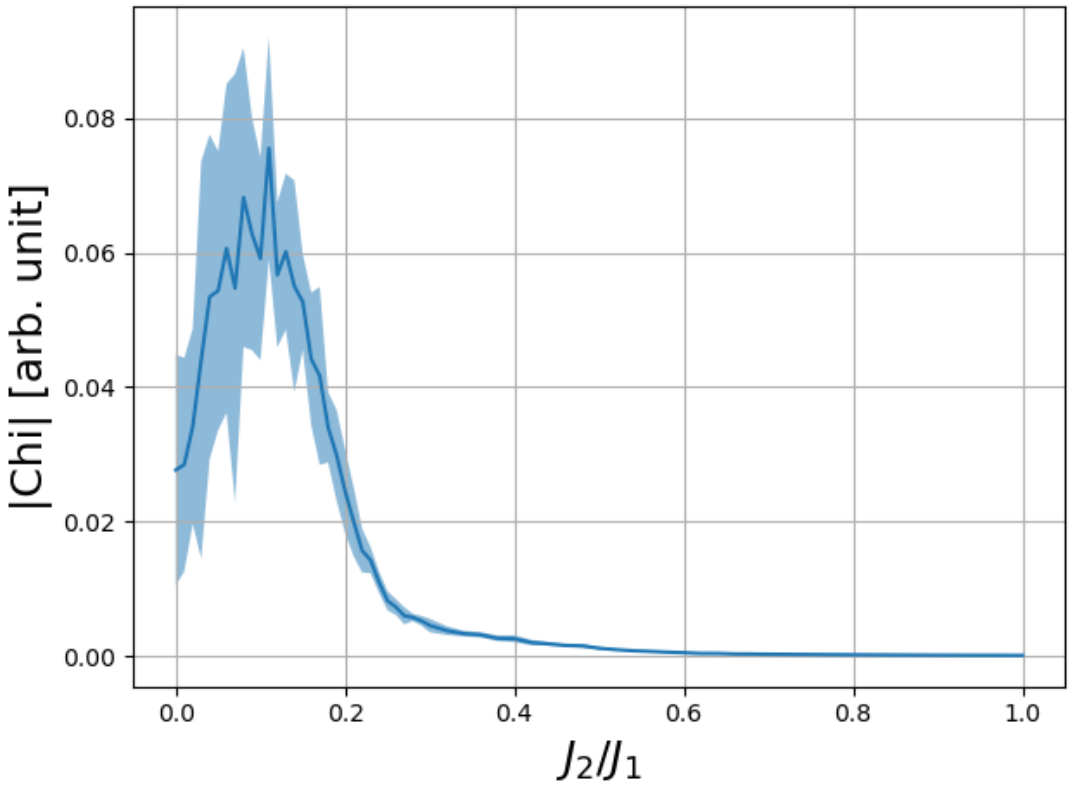
RESULTS WITH B=0

Lattice size 20 x 20

Magnetization



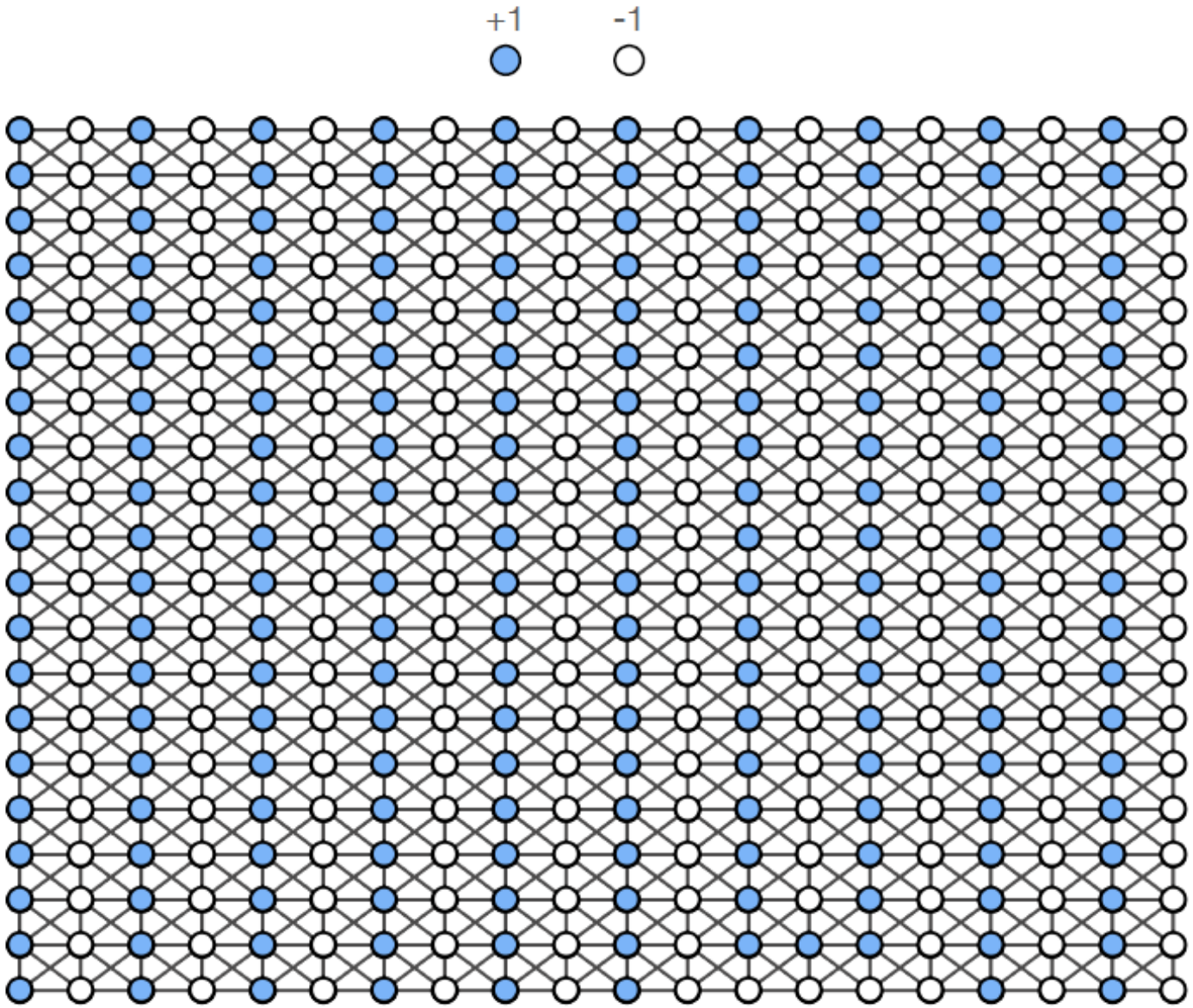
Susceptibility



Default annealing parameters: chain strength=1 and annealing time=20 μs

D-Wave systematic errors: fluctuations

PHASE TRANSITION



We have obtained the **striped phase**

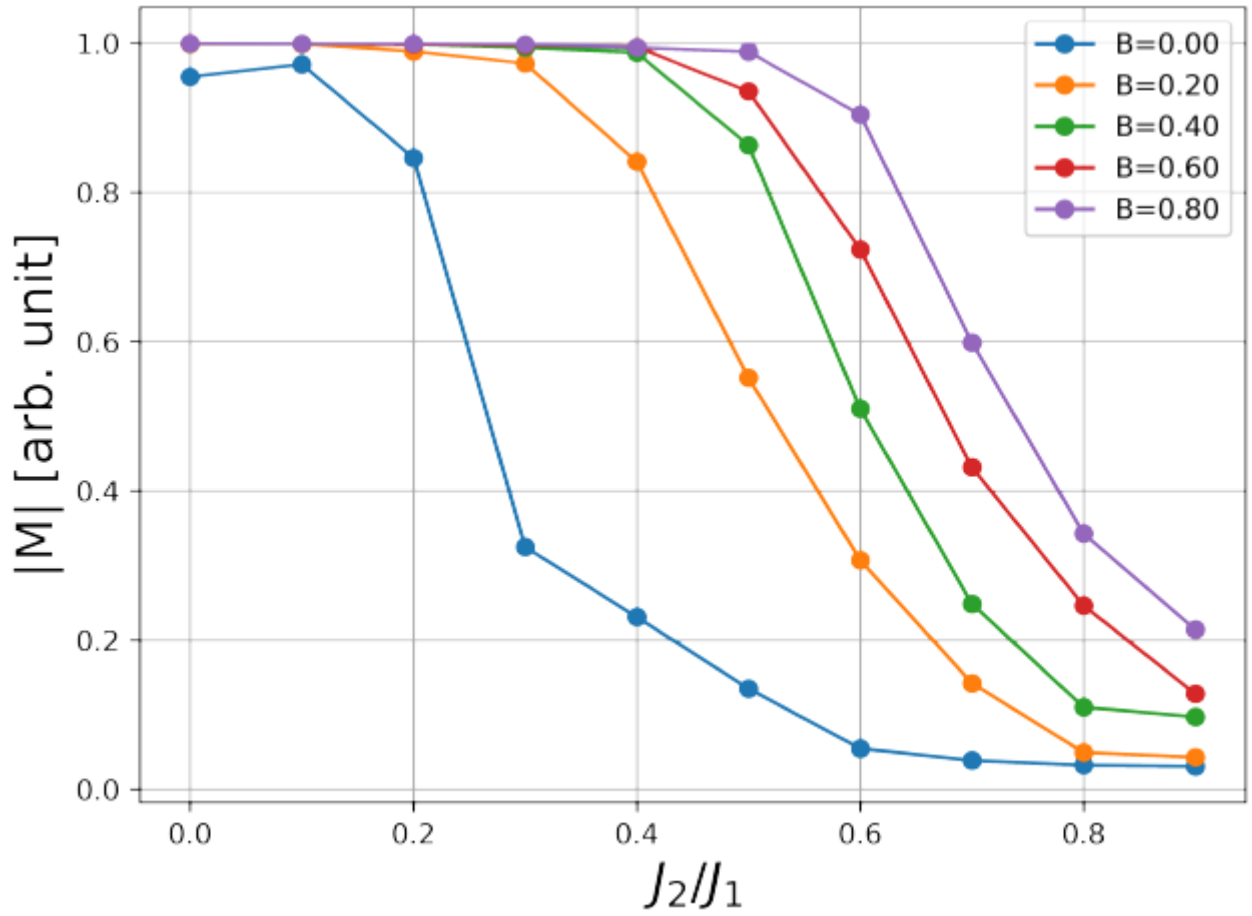
Parameters:

J_2/J_1: 1.0

Mean Magnetisation per site $\simeq 0$

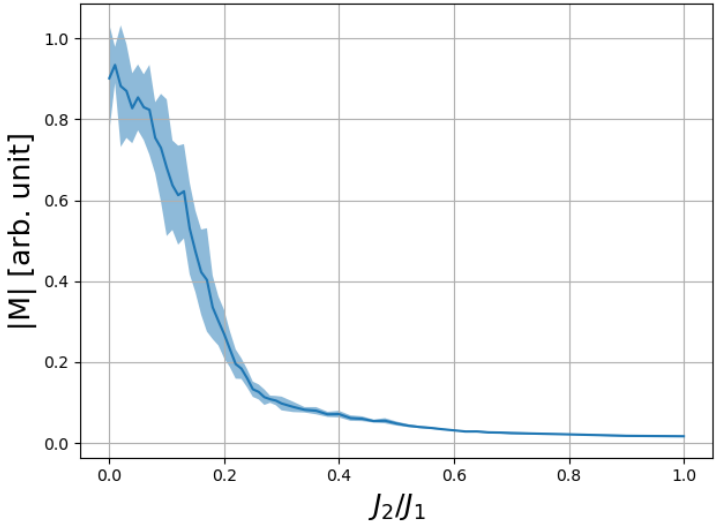
EFFECT OF AN EXTERNAL FIELD

Magnetization

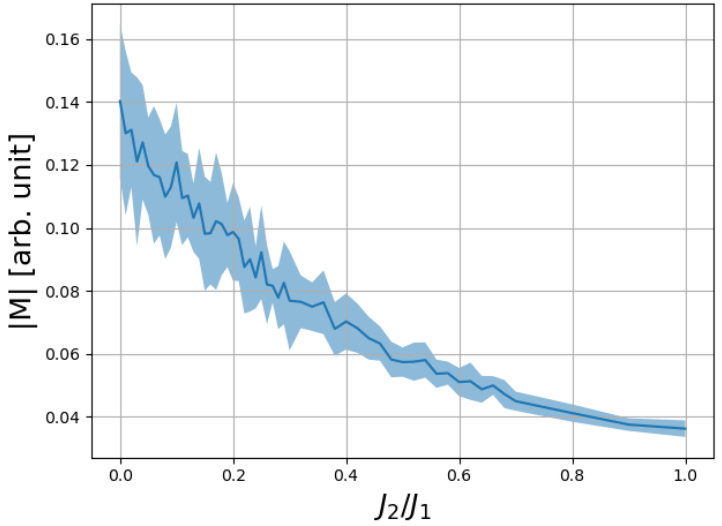


DEPENDENCE ON ANNEALING PARAMETERS

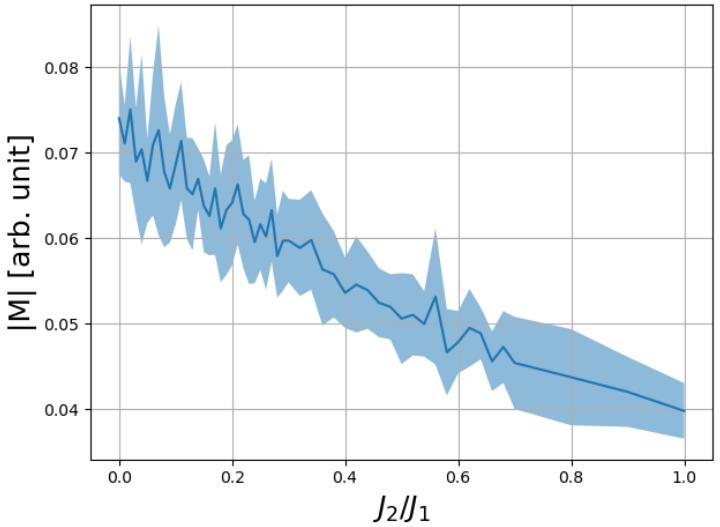
Magnetization for different **chain strengths**



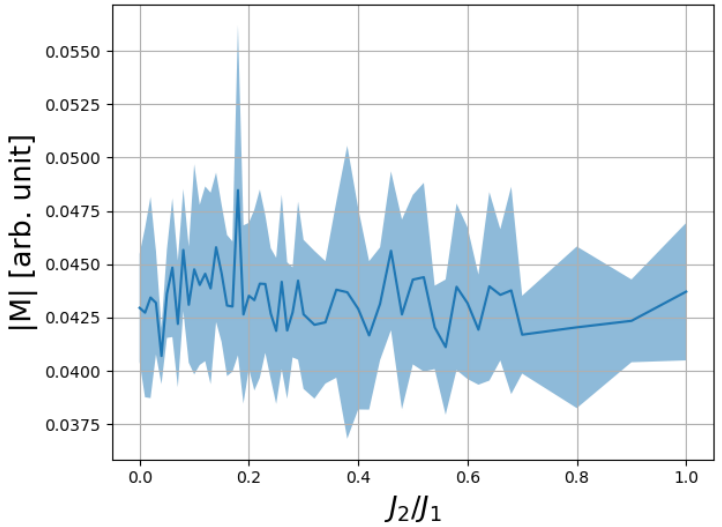
CS 1
default



CS 10



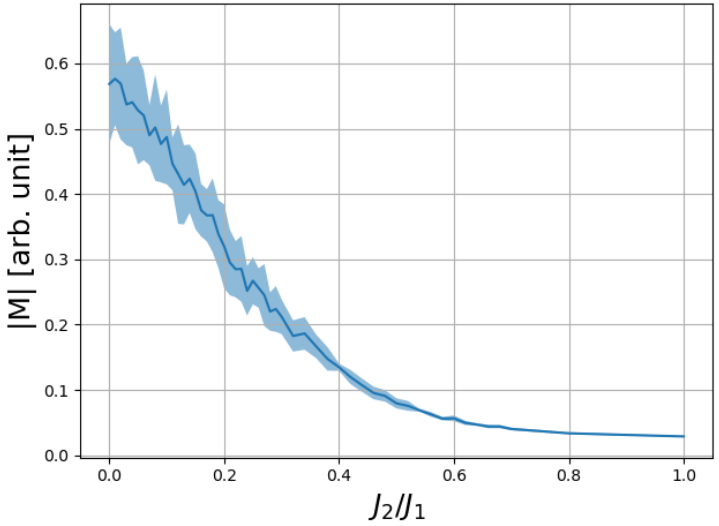
CS 100



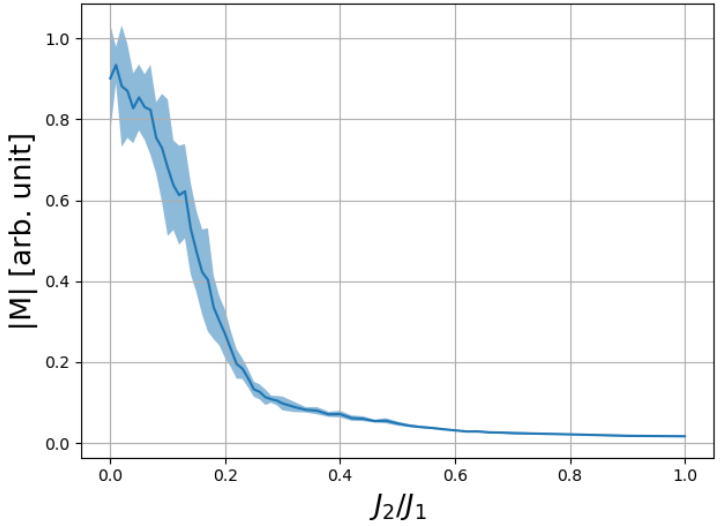
CS 1000

DEPENDENCE ON ANNEALING PARAMETERS

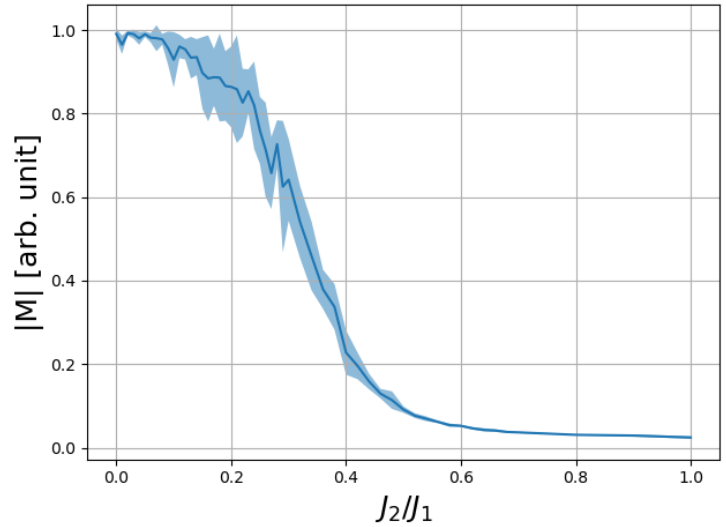
Magnetization for different **annealing times**



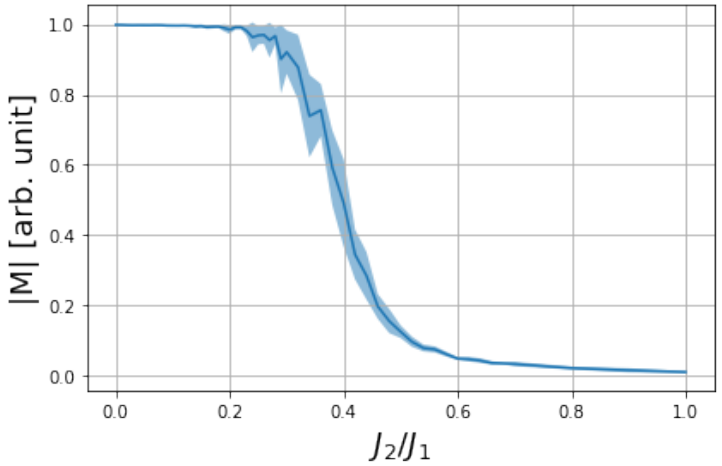
AT 1 μs



AT 20 μs
default



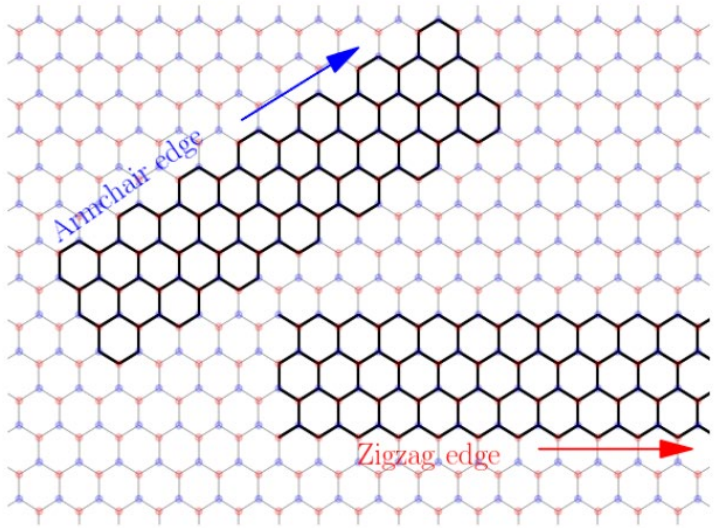
AT 100 μs



AT 900 μs

3 MAGNETISM IN GRAPHENE

- Graphene exhibits **nontrivial magnetic properties**
- Different **phase transitions** are under investigation with and without magnetic fields
- Importance of edge intrinsic magnetism: **armchair** or **zigzag** edges
- Nanoscale magnetism stems from imbalances in the two sublattices (e.g. induced by vacancies, doping, defects or strain): ***ribbons*** vs **flakes**



- **Hubbard model**: reference in the study of electron-electron interaction in solids. Two terms: kinetic energy describing nearest-neighbor hopping and repulsive electron-electron Coulombian on the same site

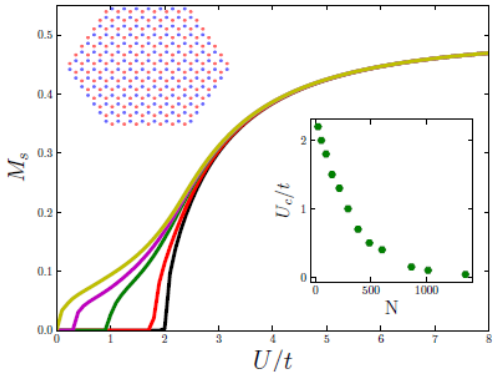
$$H = -t \sum_{<i,j>\sigma} \left(c_{i\sigma}^{+} c_{j\sigma} + h.c.\right) + U \sum_{i} \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right)$$

$c_{i\sigma}^{+}/c_{i\sigma}$	creation/annihilation operators for electron with spin σ at site i
t	hopping amplitude t~ 2.8 eV
U	repulsive Coulomb energy

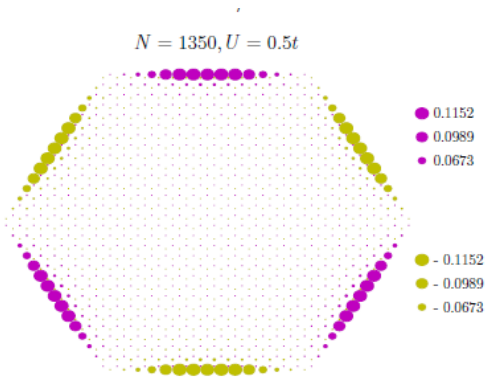
3 EXAMPLES

Microscopic scale magnetism (from literature)

- **Magnetism** in graphene **nanoflakes**: transition from paramagnetic to antiferromagnetic phase



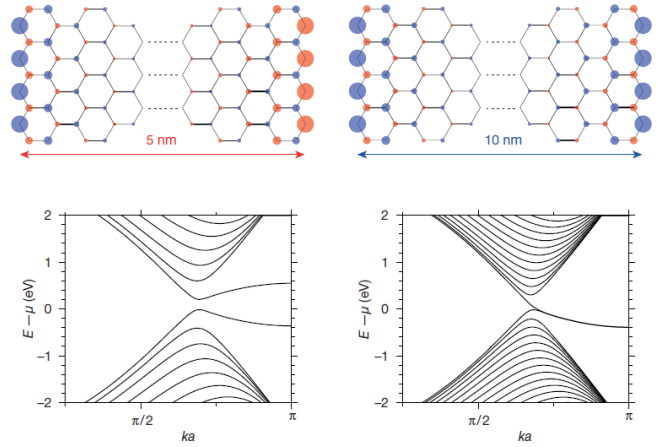
Staggered magnetization on the edges of an hexagonal graphene nanoflake



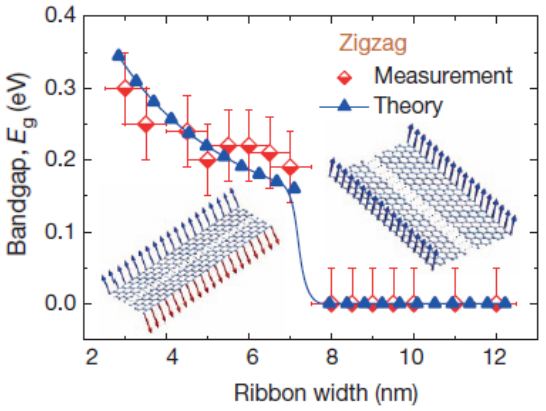
Local magnetic moments: magnitude of spin-up (pink circles) and spin-down (yellow) densities

T.T. Phung, *Numerical studies of magnetism and transport properties in graphene nano-devices*, PhD. Thesis 2019
M. Raczkowski et al., Phys. Rev. B 101, 125103

- **Edge magnetism** in zigzag graphene **ribbons**: antiferromagnetic to ferromagnetic transition



- narrow zigzag ribbons: antiferromagnetic semiconductors
- wider (>8 nm) zigzag ribbons display a ferromagnetic inter-edge coupling and no bandgap.



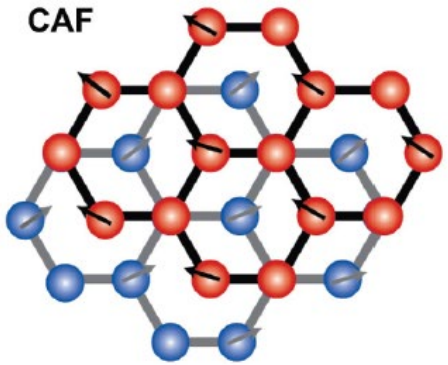
- In zigzag ribbons a sharp semiconductor (antiferromagnetic) to metal (ferromagnetic) transition is detected

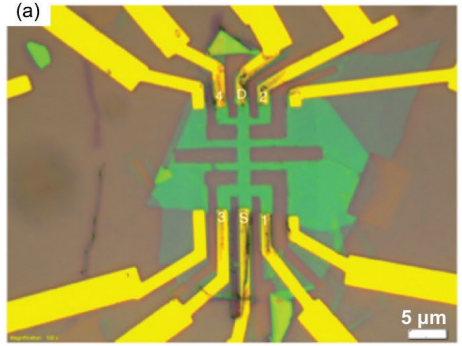
G.Z. Magda et al., Nature 514 (2014) 608

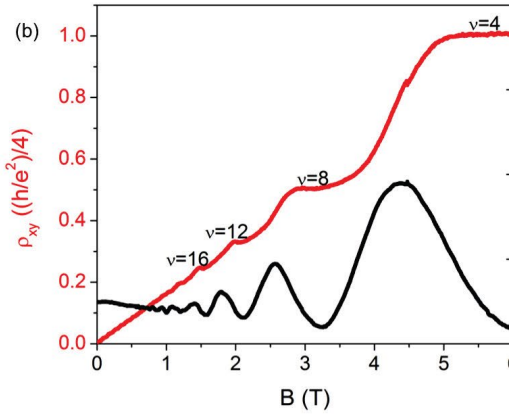
EXAMPLES

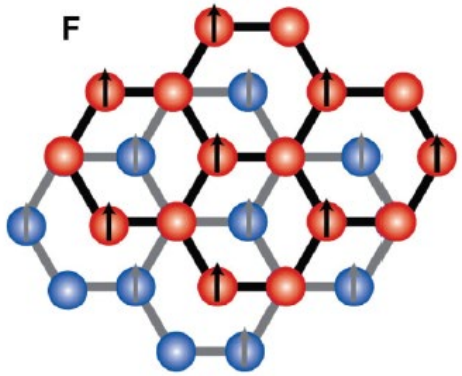
Macroscopic scale magnetism (from our measurements)

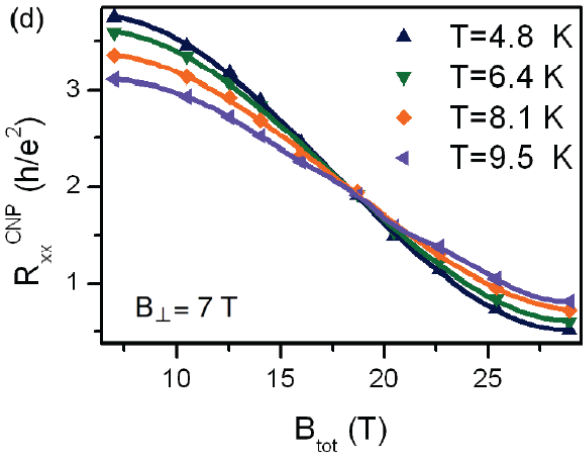
Magnetism in **bilayer** graphene enclosed in h-BN flakes: transition from a canted antiferromagnetic (CAF) to a ferromagnetic (F) spin ordered phase











S. Pezzini, C. Cobaleda, B.A. Piot, V. Bellani & E. Diez. *Critical point for the canted antiferromagnetic to ferromagnetic phase transition at charge neutrality in bilayer graphene*, Phys. Rev. B 90, 121404 (2014).

KANE-MELE-HUBBARD MODEL

- **Kane-Mele-Hubbard model** adds **spin-orbit coupling** to explain the Quantum Spin Hall Effect and other properties of **graphene** as **topological insulator**:

$$H_{KMH} = -t \sum_{<i,j>\sigma} \left(a^{+}_{i\sigma} b_{j\sigma} + b^{+}_{j\sigma} a_{i\sigma}\right) + i\lambda \sum_{\ll i,j \gg} \sum_{<i,j>\sigma\sigma'} \left(a^{+}_{i\sigma} a_{j\sigma'} + b^{+}_{i\sigma} b_{j\sigma'}\right)$$
$$+ U \sum_{i} \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right)$$

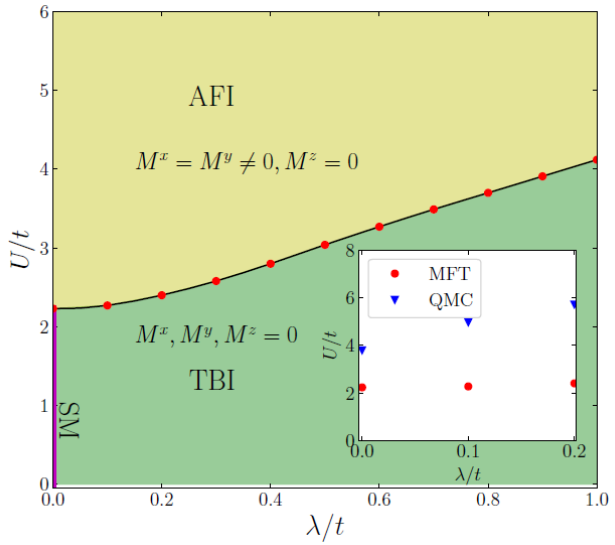
$a^{+}_{i\sigma}/b_{i\sigma}$

creation/annihilation operators of A/B sublattices for spin σ at site i

λ

amplitude of spin-orbit coupling

- **Phase diagram** using KMH model at Mean Field Theory level:



Three phases depending on U and λ:

- Gapless semimetal (SM)
- Topological band insulator (TBI)
- Antiferromagnetic insulator (AFI)

Other techniques available (Hartree-Fock, QMC…)

Is it possible to solve it on D-Wave?

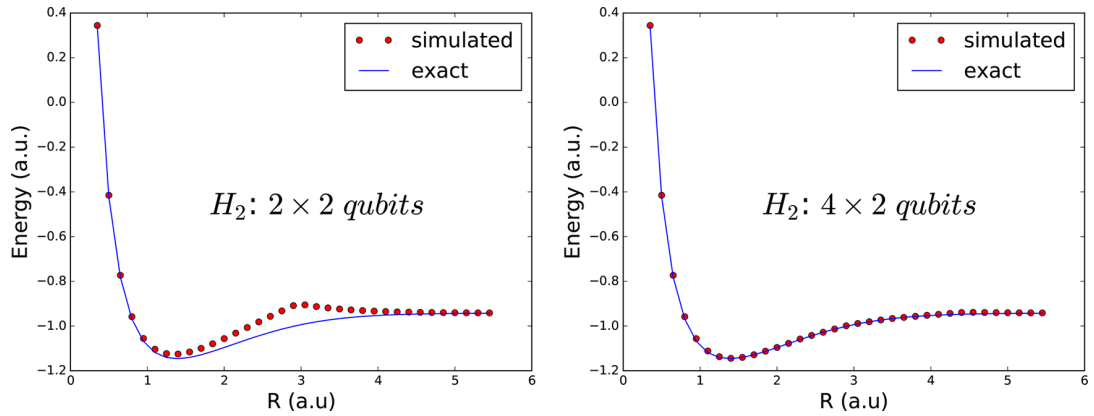
KANE-MELE-HUBBARD MODEL ON D-WAVE?

How to find a representation of this Hamiltonan in the form of a classical spin glass system by the Ising Hamiltonian?

- A **possible method** proposed by Xia et al.. Calculation in **four steps**:

  1. to write the Hamiltonian in terms of creation/annihilation fermionic operators
  2. to use the Jordan-Wigner transformation to move from fermionic operators to spin operators
  3. to reduce the spin Hamiltonian to a 2-local (two-body interactions) Hamiltonian
  4. to map this Hamiltonian to an Ising-type Hamiltonian

- Good results for H_2,He_2, HeH^+ and LiH for different (low) numbers of qubits



Details in:

R. Xia et al., *Electronic structure calculations and the Ising hamiltonian*. The Journal of Physical Chemistry B 122 (2017) 3384

SOME IDEAS FROM LITERATURE

- We start with a simple **two spin ½ electrons** (two sites lattice with **4 qubits**):

$$H = -\frac{J}{2}(1+\gamma)\sigma_1^x \otimes \sigma_2^x - \frac{J}{2}(1-\gamma)\sigma_1^y \otimes \sigma_2^y - B\sigma_1^z \otimes I_2 - BI_1 \otimes \sigma_2^z$$

$\gamma = 1$: Ising model

$\gamma = 0$: XY model

- Complex mapping procedure to reduce the Hamiltonian to a **2-local Ising type** form:

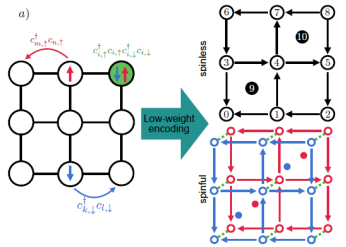
$$H' = \sum_i g_1\sigma_{i_1}^z + g_2\sigma_{i_2}^z + g_3\sigma_{i_1}^z\sigma_{i_2}^z + f(\sigma_z)$$

- This Hamiltonian depends only on σ_z

- Embedding on D-wave?

- **How many** qubits for useful results?

- Recent study for an implementation of Hubbard model on a dedicated hardware for up to a **6x6 square lattice:** R. Levy et al., *Towards solving the Fermi-Hubbard model via tailored quantum annealers*, arXiv:2207.14374v1



1. to introduce r ancillary qubits for all n qubits in the original Hamiltonian
2. to map each Pauli operator to new Pauli operators in the larger (rxn)-qubit Hilbert space
3. by increasing r, it is possible to increase the precision of the results

Following the **QT4HEP conference @ CERN** we started considering the quantum gate approach

4 LESSONS LEARNED

- The knowledge of these techniques is **fundamental** for a modern physicist!
- The mapping of a complex Hamiltonian to an Ising form is a new, emerging and **not trivial** activity: is there (yet) a **general procedure**?
- It involves the development of both algorithms and hardware *("The D-Wave hardware is the algorithm", M. Rogers - LANL*)
- Recent results in literature with **few qubits:** microscopic magnetism with few d.o.f
- **What lattice size** to achieve a computing advantage and high precision results in **real Physics** use cases?

5 OUTLOOK

- We are interested in continuing this work to explore the use of **D-Wave** and **gate-based** QC as a **computing opportunity** for modeling topological transitions in **2D materials**

- We still have a lot to learn in this field and we are **open** to suggestions and new collaborations!

- This work is subject of the **thesis** of C. Marin (University of Rome Tor Vergata)

- Results presented by C. Marin at 2nd **EMFL Summer School 2022** (21-25/9/2022) and at **QT4HEP conference @ CERN** (1-4/11/2022)

Thank you