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Use of a quantum annealer in optimization problems

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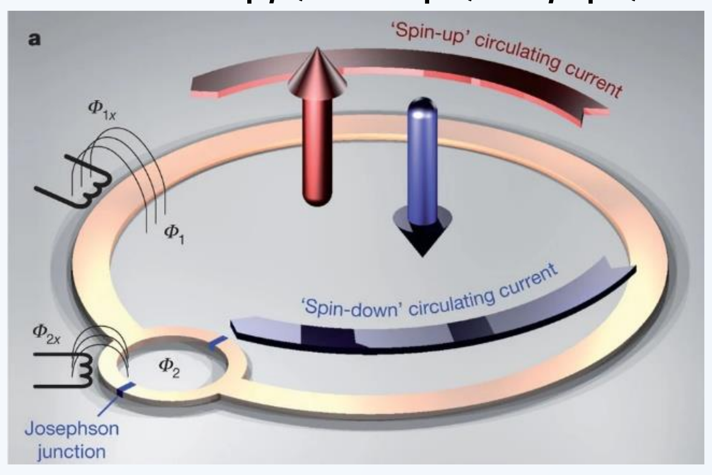
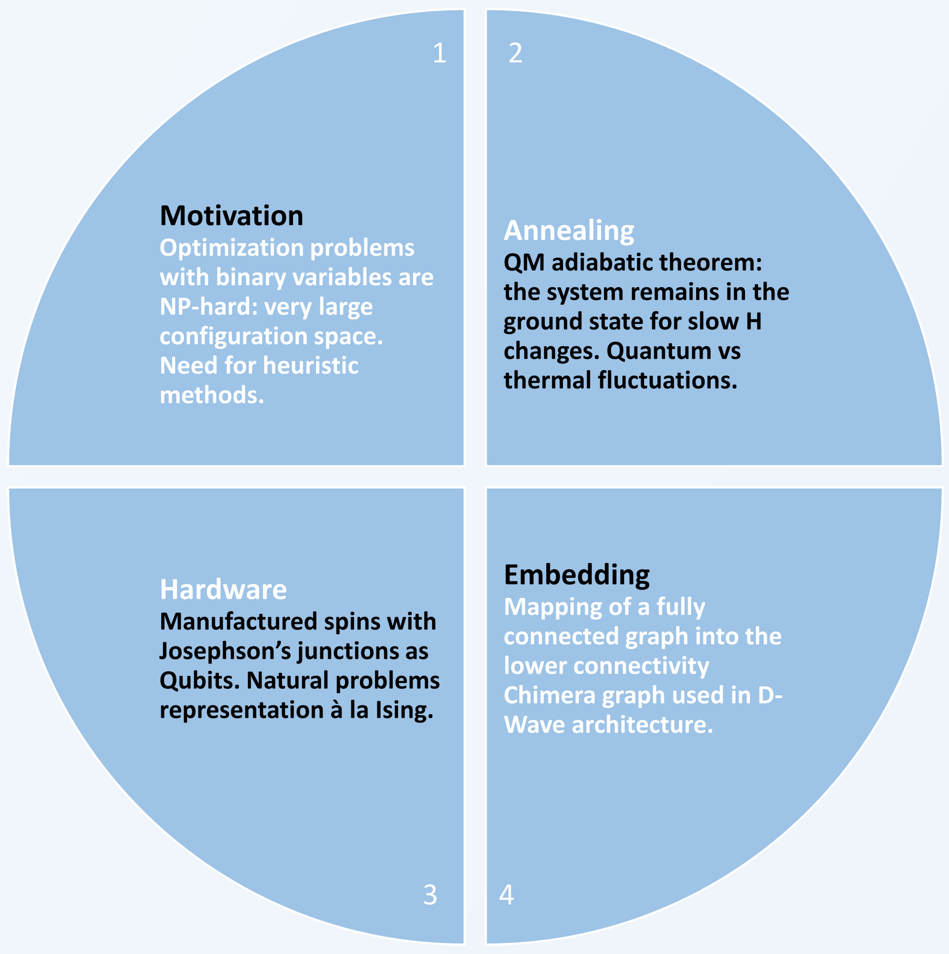
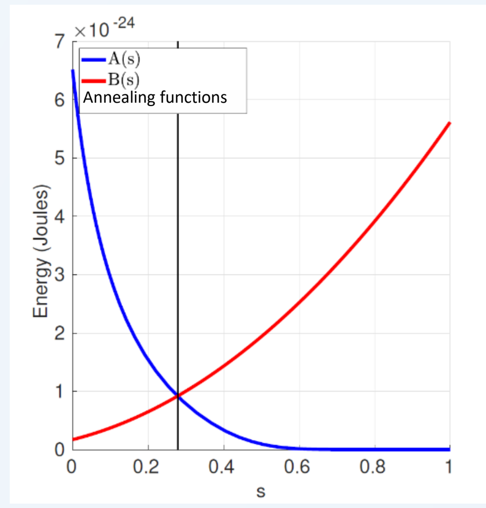
We apply quantum annealing techniques to solve with D-Wave two relevant problems in the study of phase transitions: 1- the known **frustrated Ising model**; 2- the more challenging **Kane-Mele-Hubbard**

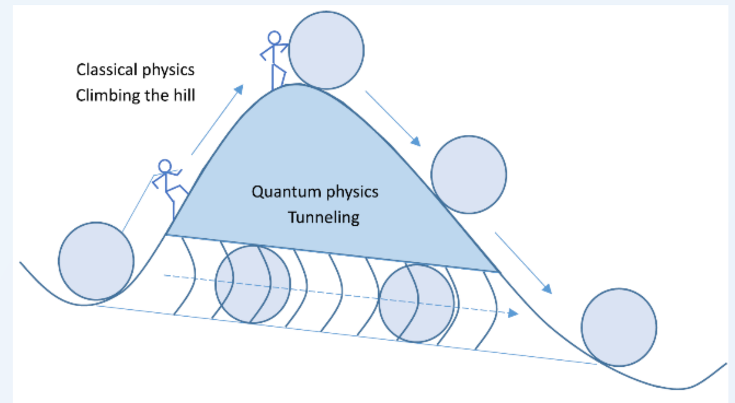
D-WAVE in short

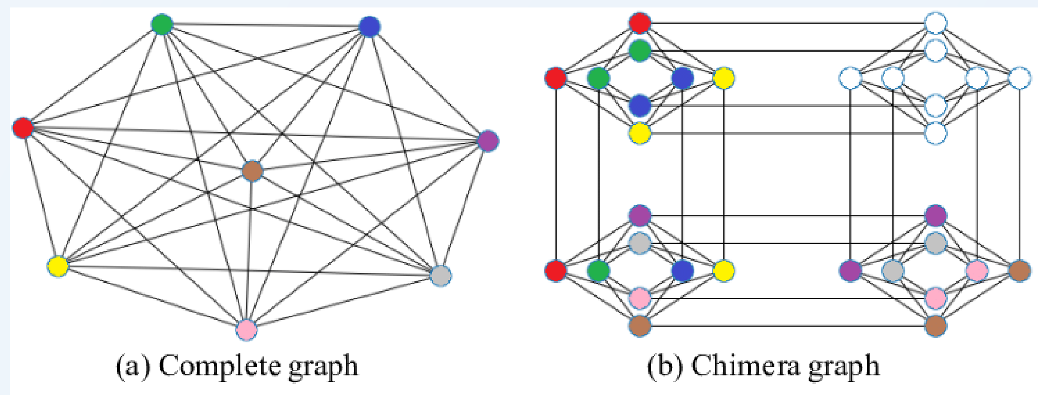
Qubit: $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$





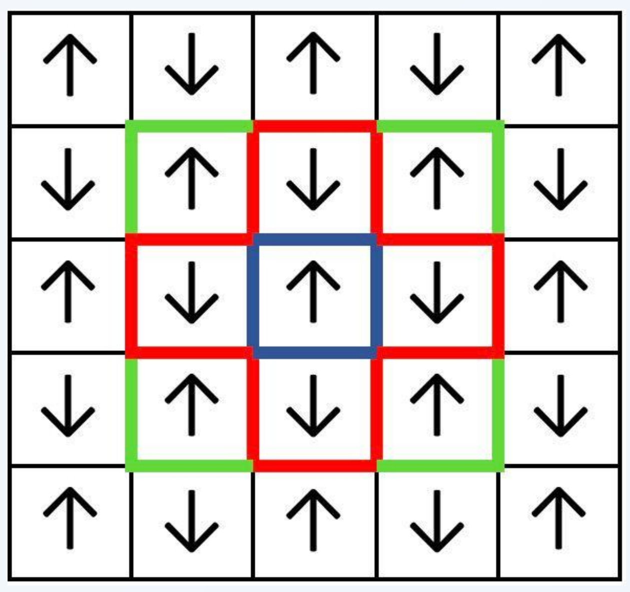


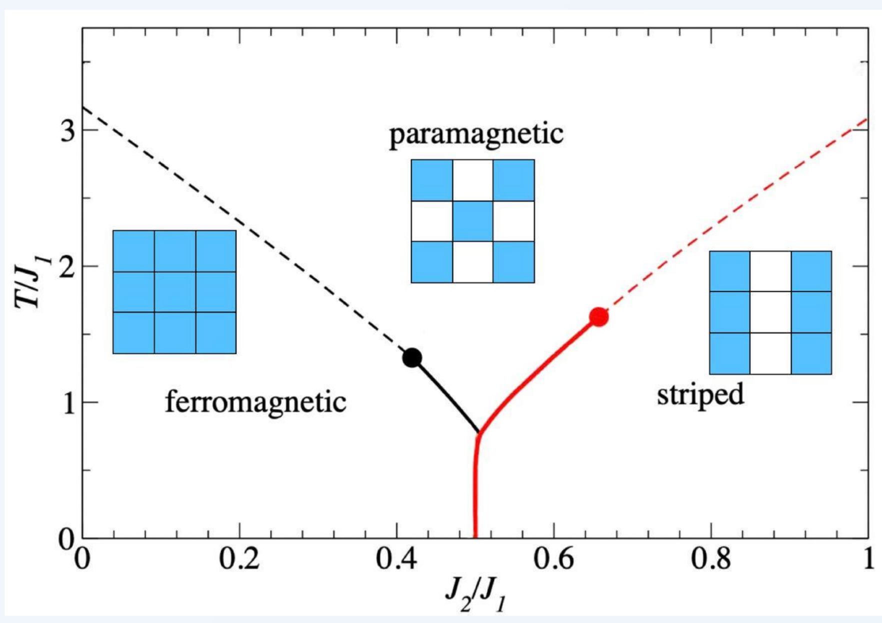




Frustrated Ising Model

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

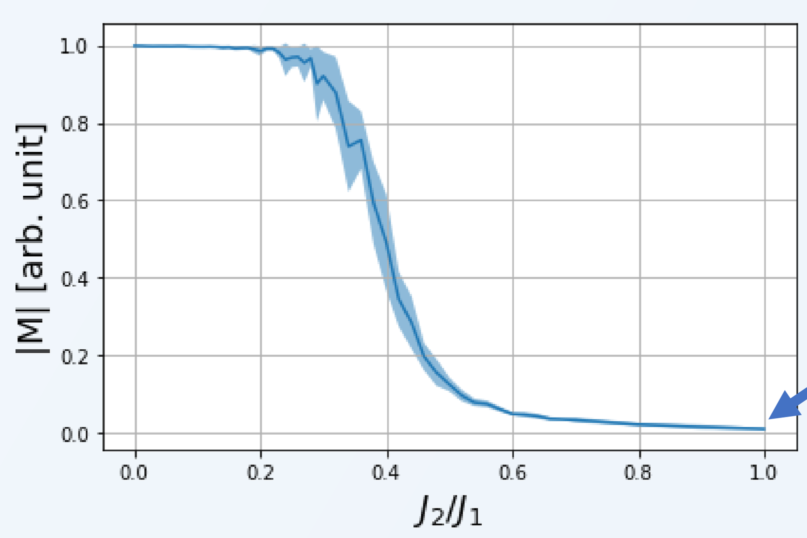


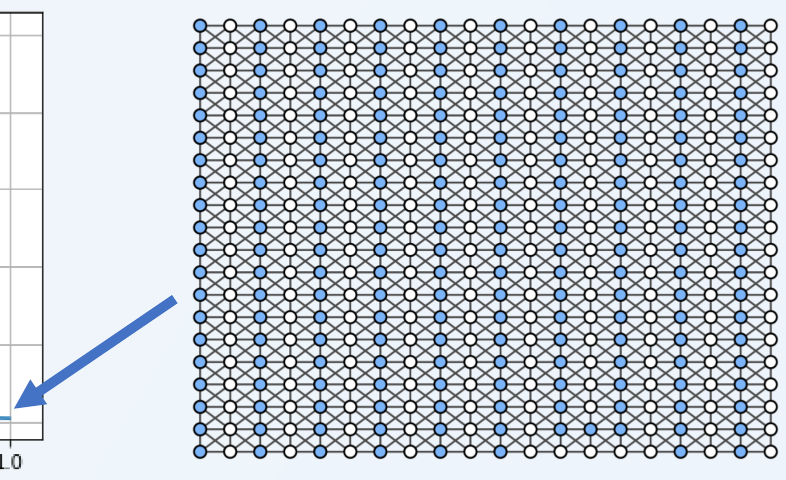


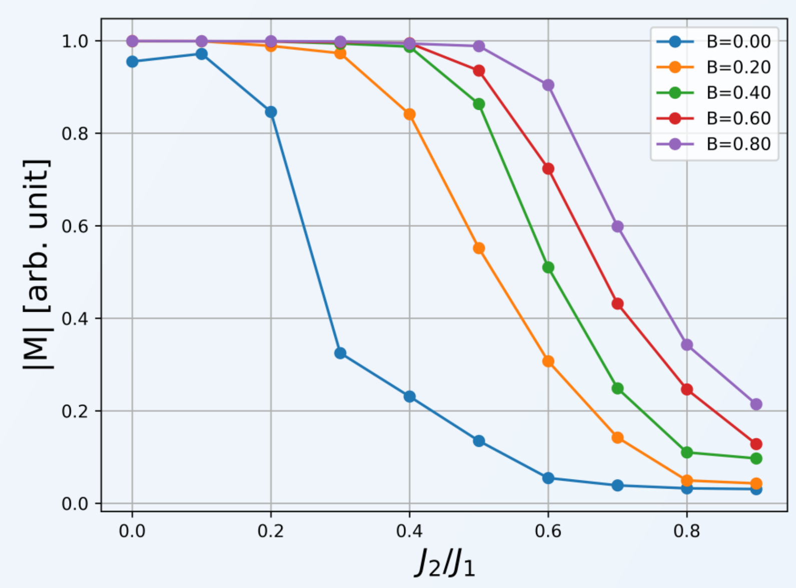
The model exhibits different ground states [1]:

- The ferromagnetic: all the spins are aligned in the same direction
- The paramagnetic: all the spins are misaligned
- The striped: the spins aligns in linear groups

Results



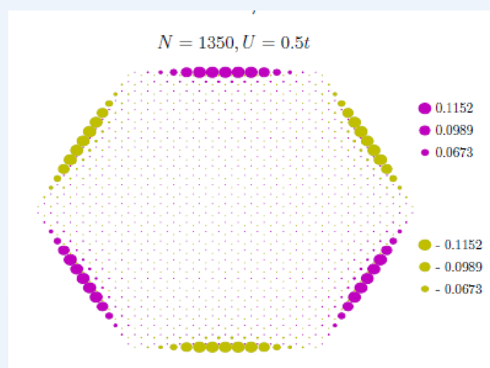


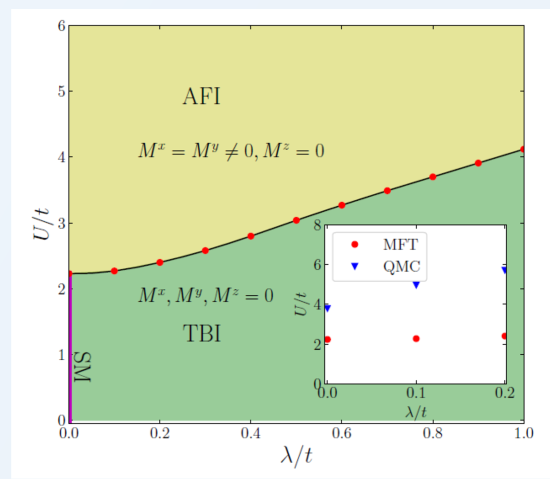


- Phase transition simulated!
- Striped phase simulated! (J_2/J_1=1)
- The transition point depends on the external magnetic field!

Magnetism in graphene

- Graphene exhibits nontrivial magnetic properties
- At nanoscale magnetism stems from imbalances in the two sublattices induced by defects or strain
- Different phase transitions are under investigation
- Example [2]: graphene nanoflake with transition from paramagnetic to anti-ferromagnetic phase (left plot)





Kane-Mele-Hubbard Model

- The KMH Hamiltonian includes terms for Coulomb interaction and spin-orbit coupling to describe graphene as a topological insulator:

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

- Three phases in example above (right plot): gapless semimetal (SM), topological band insulator (TBI), antiferromagnetic insulator (AFI)
- Problem currently solved with Mean Field Theory. We are making an attempt to solve it on D-Wave [3]

Outlook

These results open the possibility to extend the solution of optimization problems to HEP applications: to **pattern recognition**, **track reconstruction**, **particle identification** and **similar minimization problems**

[1] Park & Lee, *Phase transition of Frustrated Ising model via D-wave Quantum Annealing Machine*, arXiv:2110.05124v1 (2021)
[2] T.T. Phung, *Numerical studies of magnetism and transport properties in graphene nano-devices*, PhD. Thesis 2019
[3] R. Xia et al., *Electronic structure calculations and the Ising hamiltonian*, The Journal of Physical Chemistry B 122 (2017) 3384

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