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Use of a Quantum Annealer in optimization problems

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Quantum computing is becoming a new paradigm in computational physics, with two complementary emerging approaches, the circuit-based technology and the quantum annealers such as D-Wave. To better understand the software and the hardware performances of these new technologies, we have started to investigate how to solve a general optimization problem with the Quantum Annealer D-Wave thanks to a 2021 grant by Q@TN (Quantum Science and Technology in Trento) for Access to the CINECA Quantum Computing facility. As a first use case, we have selected the physics of phase transitions in two systems: the well known Frustrated Ising Model \[1\] and the more challenging Graphene honeycomb lattice \[2\]. The solution of these problems, presented in this work, open the possibility to master these new computing techniques and to extended them to other problems of interest for the INFN community. The Quantum Annealer can be exploited for particles and nuclear physics problems and in principle for any minimization task, both in fundamental and applied studies.

The Ising model with nearest-neighbor interactions on the two-dimensional (2D) square lattice is the simplest model to study the ferromagnetic to paramagnetic transition. On the D-Wave, we have implemented a more complex Ising model with the addition of competing antiferromagnetic interactions between the diagonal neighbors with two coupling constants J_1 and J_2. With this configuration, the Hamiltonian is represented as a graph which is embedded into the D-Wave hardware topology with a given connectivity degree. This embedding is crucial since the D-Wave topology is different from the topology of the starting graph: moreover each calculation is performed with different connections among the qubits and gives a slightly different result. We study the behaviour of the solution with different annealing parameters, such as the chain strength and the annealing time. The magnetization plot in Fig. 1 is promising, since we can identify the phase transition by varying the ratio between the ferromagnetic and antiferromagnetic couplings.

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Fig. 1 caption: Magnetization transition phase. The plot shows a conventional behavior when a material has a transition phase. Near the transition point, the lattice reaches its maximum complexity, and the error associated with the measure increases in value. The quantum annealing simulations are performed on two dimensional square lattice with L=20x20.

We propose to apply the same technique to study the magnetism of Graphene with a Hubbard-like Hamiltonian: the mapping of such a complex Hamiltonian to an Ising form is a new, emerging and not trivial activity. First results have been obtained for simple molecules \[3\] by rewriting the second quantization Hamiltonian in terms of Pauli spin matrices: this technique, that relies on the use of ancillary qubits in addition to the original lattice, has been recently proposed for a Fermi-Hubbard problem \[4\]. The use of a Quantum Annealer to explore the unique properties of Graphene could also speed up the theoretical investigation of the properties of this material for innovative sensors and detectors \[5\].

\[1\] Park & Lee, *Phase transition of Frustrated Ising model via D-wave Quantum Annealing Machine*, arXiv:2110.05124v1 (2021)

\[2\] 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)

\[3\] R. Xia et al., *Electronic structure calculations and the Ising hamiltonian,* The Journal of Physical Chemistry B 122 (2017) 3384

\[4\] R. Levy et al., *Towards solving the Fermi-Hubbard model via tailored quantum annealers*, arXiv:2207.14374v1.

\[5\] Shang-Yung Wang, *Graphene-based detectors for directional dark matter detection*, arxiv:1509.08801v3 (2019).

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