Minicolloque n° 30 **X Oral** **☐ Poster**

Baptiste ANSELME MARTIN[a,b*], Marko J. RANČIĆ, Pascal SIMON[b]

a. Total S.A., NanoInnov, 91120 Palaiseau
b. Laboratoire de Physique des Solides, 91405 Orsay

* email : baptiste.anselme-martin@total.com

Quantum computers hold many promises in solving complex problems intractable for classical computers. The simulation of quantum electronic systems is expected to be one of the first applications of near-term quantum computers. However noise and decoherence strongly limits current quantum hardware. To circumvent those limitations hybrid quantum-classical methods have been proposed that delegate only a part of the algorithm to the quantum computer. Among those, the Variational Quantum Eigensolver (VQE) has been proposed and implemented experimentally on small size quantum computers [1], where the quantum computer produces a parametrized state, whose energy is minimized classically. The design of efficient ansätze that both produce relevant variational states and are robust to noise is a very active topic in quantum computing. In this work we investigate the simulation of correlated fermionic systems like the Hubbard model on a quantum computer using the Variational Hamiltonian Ansatz (VHA) [2], a problem-tailored ansatz inspired from the time-evolution operator under the Hamiltonian of interest, the time steps being replaced by variational parameters, potentially providing a way of short-cutting adiabatic evolution. We explore the implementation of VQE targeting strongly correlated ground states for the 1D Hubbard chain. We attempt to qualify how short circuit depth affect the quality of optimized parametrized states in terms of fidelity with exact solutions and physical properties. We show that despite low fidelity (< 90 %), short VHA ansätze are still able to capture qualitatively the main features of the 1D Hubbard model with strong Coulomb repulsion such like the decreasing number of doubly occupied sites or spin correlations, indicating that the variational states lie in a physically relevant subspace of the total Hilbert space.

[1] A. Peruzzo, Nature Communications, 5(1):4213 (2014)
[2] D. Wecker, Phys. Rev. A, 92 :0423303 (2015)

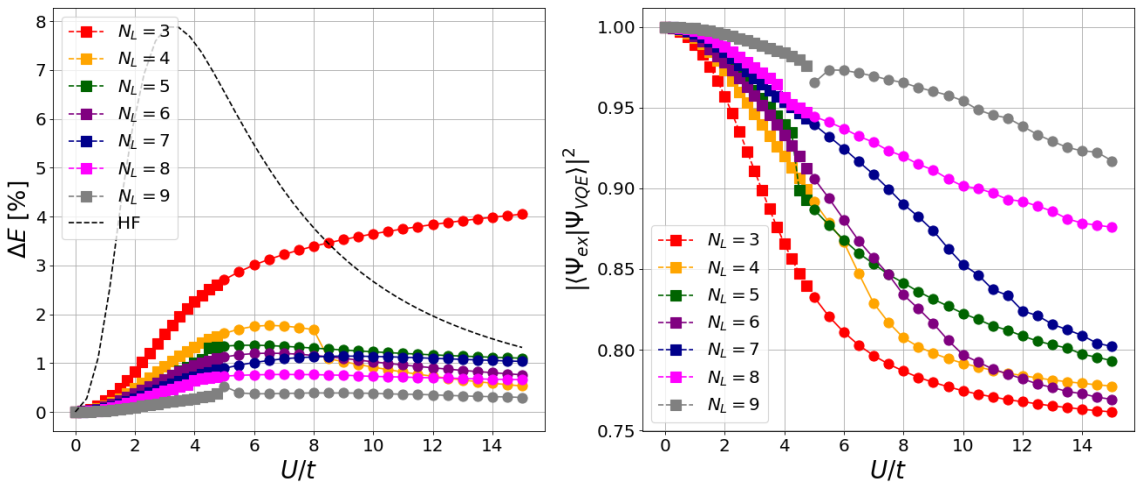

Figure 1 : Classical simulation of the VQE algorithm applied to the 1D Hubbard model with 8 sites. On the left, the energy error at different circuit depth. On the right, the overlap of the output state with the exact groundstate.