A quantum-circuit algorithm for simulating artificial graphene

Adrián Pérez-Salinas
Axel Pérez-Obiol, Sergio Sánchez-Ramírez, B. G. Moraes, Artur Garcia-Saez

Barcelona Supercomputing Center (BSC), Barcelona 08034, Spain

adrian.perezsalinas95@gmail.com

In this work, a quantum algorithm for attaining the ground state and energy of free moving electrons in an artificial graphene (AG) lattice is developed. This work thus lies in the intersection of condensed-matter physics and quantum computing, and makes use of HPC resources to perform simulations.

The AG is modeled via the 2D Fermi-Hubbard Hamiltonian including hopping, Coulomb and spin-orbit terms. The algorithm to obtain this ground state is carried in three steps. First, the lattice is mapped to a quantum computer using the Jordan-Wigner mapping. Second, an easy-to-prepare initial state is created in the quantum computer. This initial state does not consider any interacting electrons [1]. Finally, adiabatic evolution is performed to include all elements in the model of interest. The exact implementation is based on previous works for square lattice [2], adapted and improved to this problem. The algorithm is efficiently performed, requiring a linear number of operations with respect to the system size both for the initial state preparation and for each step in the adiabatic evolution.

The algorithm is simulated using simulators quantum circuits build upon exact statevector [3] and Matrix Product States (MPS) [4]. Calculations are made in supercomputer MareNostrum 4 at BSC. Exact simulation is performed for systems up to 32 qubits, while MPS methods permit to arrive up to 36 qubits with fidelities over 99%. With a sufficient amount of resources, the errors in the final energy can be bounded below 1% with respect to the initial one, see Fig. 1. Future extensions of this work aim to use distributed computing to increase the size of addressable systems.

References:
[1] Jiang, Zhang, et al., *Physical Review Applied* 9.4 (2018): 044036.
[2] Cade, Chris, et al., *Physical Review B* 102.23 (2020): 235122.
[3] Efthymiou, Stavros, et al., *Quantum Science and Technology* 7.1 (2021): 015018.
[4] Sánchez-Ramírez, Sergio, et al., *IEEE/ACM Second International Workshop on Quantum Computing Software* (2021).

Figures:

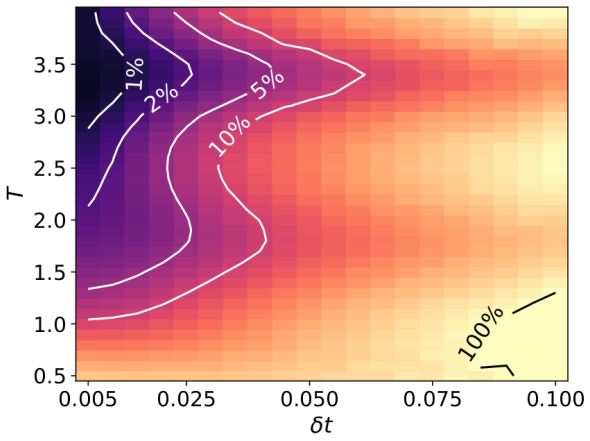

Figure 1: Error in the obtained energy with respect to the initial one for a sample system depending on adiabatic evolution time (T) and time steps (δt).