A quantum circuit algorithm for simulating artificial graphene

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In this work we develop an algorithm for quantum computers to obtain the ground state and ground energy of the free moving electrons in artificial graphene (AG). Additionally, the algorithm is simulated for small AG sheets. For our simulations we use HPC resources, since in quantum matter simulation the cost in classical computing resources grows exponentially as the size of the system increases. We focus our research on graphene analogues: 2D materials based on honeycomb lattice potentials. These lattices give rise to Dirac electrons and the main electronic properties of graphene while offering much more tunable platforms, allowing for larger electron-electron interactions or spin-orbit couplings and to explore new phases of matter.

Our algorithm consists of a quantum circuit simulating an adiabatic (gradual) evolution moving from an AG system with non-interacting electrons, which is easy to solve and prepare in our quantum circuit, to one with arbitrary Coulomb interactions, for which we don't know the solution. Electrons in AG are modeled with the 2D Fermi-Hubbard Hamiltonian, including kinetic, spin-orbit, and Coulomb terms. We first map the AG orbitals to a 1D string of qubits —or quantum bits, the minimal unit of quantum information— using the Jordan-Wigner transform. Each site of the lattice is mapped to a pair of qubits, one for each possible spin. To prepare the initial, non-interacting state, we use Gaussian state preparation, which scales as $O(N)$ [1]. The evolution part of the circuit is based on previous strategies developed for square lattices [2] which reduce the scaling to $O(N_x)$, with N_x the shortest dimension of the lattice. Thus, the size and depth of the quantum circuit grow linearly with the size of the system. All parts of the circuit, including measurement, involve only nearest neighbor quantum gates.

Simulations of the quantum circuit for lattices with up to four hexagons are run using the Openfermion package [3] and Cirq [4] and qibo [5] simulators and with the aid of structured tensor networks (TN) and quimb [6] on Marenostrum 4 supercomputer at Barcelona Supercomputing Center. This work also takes advantage of the recently developed TN distributed library RosneT [7] to scale up the simulations to larger lattices. We study, for different hexagonal lattices, the efficiency of both the quantum algorithm, namely the cost in number of qubits and depth of the circuit, and of its classical simulation, in terms of computer memory and time, with HPC. These simulations serve to test the quantum algorithm and to optimize the speed of the adiabatic evolution, allowing us to estimate optimal circuit depths for larger, more costly systems. They also explore the efficiency of TN algorithms for simulating Fermi-hubbard models based on quantum circuits, providing insight into the actual complexity of these systems along the way.

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