Determinstc Quantum Algorithm for the Graph Isomorphism Problem

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The development of qubit and bosonic based algorithms for solving the computatonal task of finding molecular substructures is central to a solving a wide range of problems in chemistry, including molecular docking and search of retrosynthetc pathways. By representng molecular structures with graphs, the molecular substructure search can be formulated in terms of the so- called *subgraph isomorphism problem*, already proven to be NP-complete. We propose a qubit- based circuit to solve the graph isomorphic problem, inspired by the well-known Bernstein – Vazirani algorithm, and currently rely on efficient classical algorithms to sample all subgraphs. This qubit-based approach enjoys numerous advantages. Due to the determinstc nature of the Bernstein – Vazirani algorithm, the correct answer is always theoretcally obtained, preferable to the probabilistc nature of variatonal quantum algorithms. Additonally, the circuit architecture involved does not require tuning the quantum gates' parameters for different graphs of the same size, but only change how the qubits are initalized. This allows the screening of large numbers of ligands of the same size without changing the circuit, rendering a practical approach. Future directons include the experimental realizaton for small-scale graphs on near term devices and exploraton of algorithms for hybrid architectures for solving the subgraph isomorphism problem with both qubits and bosonic modes.