A quantum alternating operator ansatz with hard and soft constraints for lattice protein folding

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Gate-based universal quantum computers form a rapidly evolving field of quantum computing hardware technology. In previous work, we presented a quantum algorithm for lattice protein folding on a cubic lattice, tailored for quantum annealers. In this paper, we introduce a novel approach for solving the lattice protein folding problem on universal gate-based quantum computing architectures. Lattice protein models are coarse-grained representations of proteins that have been used extensively over the past thirty years to examine the principles of protein folding and design. These models can be used to explore a vast number of possible protein conformations and to infer structural properties of more complex atomistic protein structures. Numerous classical computational methods exist for the determination of protein structure from an arbitrary input sequence, although all of these techniques have significant computational limitations. We formulate the problem as a quantum alternating operator ansatz, a member of the wider class of variational quantum/classical hybrid algorithms. The algorithm consist of a fixed-length sequence of parametrizable quantum gates that alternate between applying the cost and mixer Hamiltonian whilst the gate parameters are variationally optimized by a classical computer. These algorithms have been shown to be reasonably robust against certain types of errors which makes them promising candidates for practical use on small noisy near-term quantum computers. On the circuit level, the cost Hamiltonian encodes the optimization problem whose expectation value we wish to maximize whilst the mixer Hamiltonian is meant to mix the amplitudes between different solution states. Recent work by Hadfield et. al (2017) described how the mixer Hamiltonian can be used to constrain the search to the feasible subspace of solutions that satisfy certain hard constraints. To increase the probability of sampling the ground state, we propose splitting the optimization problem into hard and soft constraints. In this work, we describe how to one-hot encode the lattice protein folding problem as an Ising-type Hamiltonian and how different components of the cost Hamiltonian can be integrated into the mixer Hamiltonian. In combination with the introduction of a problem specific initial state we threefold the ground state probability for all definitions of the mixer Hamiltonian. All three proposed mixer Hamiltonians outperform the traditional X mixer at depth p = 1 and p = 2 by a constant factor.