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Towards Viable Quantum Computation for Chemistry

Abstract

Since its introduction one decade ago, the quantum algorithm for chemistry has been among the most anticipated applications of quantum computers. However, as the age of industrial quantum technology dawns, so has the realization that even "polynomial" resource overheads are often prohibitive. There remains a large gap between the capabilities of existing hardware and the resources required to quantum compute classically intractable problems in chemistry. The primary contribution of this dissertation is to take meaningful steps towards reducing the costs of three approaches to quantum computing chemistry. First, we discuss how chemistry problems can be embedded in Hamiltonians suitable for commercially manufactured quantum annealing machines. We introduce schemes for more efficiently compiling problems to annealing Hamiltonians and apply the techniques to problems in protein folding, gene expression, and cheminformatics. Second, we introduce the first adiabatic quantum algorithm for fermionic simulation. Towards this end, we develop tools which embed arbitrary universal Hamiltonians in constrained hardware at a reduced cost. Finally, we turn our attention to the digital quantum algorithm for chemistry. By exploiting the locality of physical interactions, we quadratically reduce the number of terms which must be simulated. By analyzing the scaling of time discretization errors in terms of chemical properties, we obtain significantly tighter bounds on the minimum number of time steps which must be simulated. Also included in this dissertation is a protocol for preparing configuration interaction states that is asymptotically superior to all prior results and the details of the most accurate experimental quantum simulation of chemistry ever performed.