Quantum computation for quantum chemistry and chemical dynamics

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The exact solution of the quantum many-body problem has an exponential computational complexity on any classical computer. Most of the quantum chemistry methods, perhaps with the exception of full configuration interaction or the density matrix renormalization group approach, could be summarized as the collection of methods and their applications to solve the equation efficiently, yet approximately. It was for the specific purpose to simulate quantum systems that Richard Feynman proposed the use of a quantum computer or quantum device to simulate quantum many-body systems. Feynman's proposal led to the development of the field of quantum computation. Quantum computer algorithms have demonstrated exponential speedup for the factoring of prime numbers, a quadratic speedup in the search of random databases, and exponential speedup in some graph-theoretical problems, amongst other applications. In 2005, we introduced a quantum algorithm for the solution of the full configuration interaction problem in polynomial time using a quantum computer [1,5]. We have extended the algorithm to the calculation of excited states and better preparation of initial states by employing multi-configurational self-consistent field (MCSCF) initial trial wave functions [2]. We recently introduced a quantum algorithm for the direct simulation of the dynamics of electrons and nuclei with a quadratic cost in the number of quantum gates and a linear cost in terms of the quantum bits [3]. Since then, we have increased the efficiency of the algorithm towards the ultimate limit of scaling with system size [6]. More recently, we carried out the first quantum chemistry calculation on a quantum computer in collaboration with Andrew White's group at the University of Queensland, Australia [4]. In this talk, I will provide a brief introduction to quantum computation, summarize the FCI and quantum dynamics algorithms, and describe the experimental realization.

References

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