Towards quantum chemistry on quantum computers

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Quantum computers have a potential to change the way quantum chemistry is done. For example, they are able to efficiently find the exact solution of many-body Hamiltonian eigenvalue problem [1]. As was shown in the seminal work by Aspuru-Guzik et. al. [2], quantum computers, if available, would be able to perform the full configuration interaction (FCI) energy calculations with only a polynomial scaling, in contrast to conventional computers where FCI scales exponentially. Of course, experimental realization of large enough quantum computers is an extremely difficult task. However, first step towards this goal, calculation of H_2 in a minimal basis on a real quantum computer, has been reported recently by Lanyon et al. [3]

This lecture will summarize our work in the field of interconnection of quantum chemistry and quantum computing [4]. Improved version of the quantum full configuration interaction (QFCI) method, which uses the iterative phase estimation algorithm and its application to non-relativistic as well as relativistic configuration interaction (CI) energy calculations will be presented.

As far as non-relativistic CI calculations are concerned, simulations (on a conventional computer) of QFCI calculations of the four lowest lying electronic states of methylene molecule (CH_2), which exhibit a multireference character were performed [4]. It has been shown that with a suitably chosen initial state of the quantum register, one is able to achieve the probability amplification regime of the iterative phase estimation even for nearly dissociated molecule. Concerning the relativistic calculations, we have performed simulations of the quantum computing analogue of the Kramers-restricted CI calculations for the SbH molecule. A minimalistic example of a quantum circuit performing such a calculation, which might become experimentally realizable in the near future, will be presented. Last but not least, possible use of genetic algorithms in the design of quantum circuits for QFCI calculations will be discussed.

References

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