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Quantum computing simulations: applications in physics and chemistry

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Abstract: Quantum computing is emerging as a new paradigm for the solution of a wide class of problems that are not accessible by conventional high performance computers based on classical algorithms. In particular, the simulation of the electronic structure of molecular and condensed matter systems is a challenging computational task as the cost of resources increases exponentially with the number of electrons when accurate solutions are required. In this talk, we will first introduce the basics of quantum computing using super-conducting qubits, focusing on those aspects that are crucial for the implementation of quantum chemistry algorithms. In the second part, we will briefly discuss the limitations of currently available classical approaches and highlight the advantages of the new generation of quantum algorithms for the solution of the many-electron Schrödinger equation in the ground and excited states.

Quantum computing and its applications in chemistry and physics

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Quantum computing is emerging as a new paradigm for the solution of a wide class of problems that are not accessible by conventional high performance computers based on classical algorithms. Quantum computers can in principle efficiently solve problems that require exponential resources on classical hardware, even when using the best known classical algorithms. In the last few years, several interesting problems with potential quantum speedup have been brought forward in the domain of quantum physics, like eigenvalue-search using quantum phase estimation algorithms and evaluation of observables in quantum chemistry, e.g. by means of the hybrid variational quantum eigensolver (VQE) algorithm.

The original idea that a quantum computer can potentially solve many-body quantum mechanical problems more efficiently than classical algorithms is due to R. Feynman who proposed to use quantum algorithms to investigate the fundamental properties of nature at the quantum scale. In particular, the simulation of the electronic structure of molecular and condensed matter systems is a challenging computational task as the cost of resources increases exponentially with the number of electrons when accurate solutions are required. With the deeper understanding of complex quantum systems acquired over the last decades this exponential barrier bottleneck may be overcome by the use of quantum computing hardware. To achieve this goal, new quantum algorithms need to be develop that are able to best exploit the potential of quantum speed-up [1,2]. While this effort should target the design of quantum algorithms for the future fault-tolerant quantum hardware, there is pressing need to develop algorithms, which can be implemented in present-day non-fault tolerant quantum hardware with limited coherence times [3].

In this talk, we will first introduce the basics of quantum computing using superconducting qubits, focusing on those aspects that are crucial for the implementation of quantum chemistry algorithms. In the second part, I will briefly discuss the limitations of currently available classical approaches and highlight the advantages of the new generation of quantum algorithms for the solution of the many-electron Schrödinger equation in the ground and excited states [4].

[1] B.P. Lanyon et al., *Nature Chem.* **2**, 106 (2010).
[2] N. Moll, et al., *Quantum Sci. Technol.* **3**, 030503 (2018).
[3] P. Baroutsos, et al., *Phys. Rev. A* **98**, 022322 (2018).
[4] M. Ganzhorn, et al., *arXiv:1809.05057* (2018).