Quantum computing for applications in physics and chemistry

Ivano Tavernelli
IBM Quantum, IBM Research - Zurich, 8803 Rüschlikon, Switzerland

The original idea that a quantum *machine* can potentially solve many-body quantum mechanical problems more efficiently than classical computers is due to R. Feynman who proposed the use of quantum computers to investigate the fundamental properties of nature at the quantum scale. In particular, the solution of problems in electronic structure, many-body physics, and high energy physics (just to mention a few) is a challenging computational task for classical computers as the number of needed resources increases exponentially with the number of degrees of freedom. More recently, the possibility of obtaining quantum speedup for the solution of classical optimization problems has opened up new research avenues in, e.g., classical statistical mechanics, machine learning and finance.

Thanks to the recent development of quantum technologies, we have now the possibility of addressing these classes of problems with the help of quantum computers. To achieve this goal, several quantum algorithms able to best exploit the potential quantum speedup of state-of-the-art, noisy, quantum hardware have been proposed [1,2].

After a short introduction on the state-of-the-art of digital quantum computing from a hardware and software prospective, I will present applications in many-body and high energy physics, focusing on those aspects that are relevant to achieve quantum advantage with near-term and fault tolerant quantum computers. In particular, I will focus on recent results in electronic structure calculations [3], lattice gauge theory [4], and quantum dynamics [5].

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[2] A. Kandala et al., *'Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets'*, *Nature*, **549**, 242 (2017).
[3] P. Baroutsos, et al., *'Quantum algorithms for electronic structure calculations: Particle-hole Hamiltonian and optimized wave-function expansions'*, *Phys. Rev. A*, **98**, 022322 (2018); P. Ollitrault et al., *'Quantum equation of motion for computing molecular excitation energies on a noisy quantum processor'*, *Phys. Rev. Res.*, **2**, 043140 (2020).
[4] S.V. Mathis, G. Mazzola, I. Tavernelli, "Toward scalable simulations of lattice gauge theories on quantum computers", *Physical Review D* 102, 094501 (2021); G. Mazzola, S.V. Mathis, G. Mazzola, I. Tavernelli, "Gauge-invariant quantum circuits for U(1) and Yang-Mills lattice gauge theories", *Physical Review Research* 3, 043209, (2021).
[5] P.J. Ollitrault, et al., *'Nonadiabatic molecular quantum dynamics with quantum computers'*, *Phys. Rev. Lett.*, **125**, 260511 (2020). P.J. Ollitrault, et al., *'Molecular Quantum Dynamics: A Quantum Computing Perspective'*, *Acc. Chem. Res.*, **54**, 4229 (2021). P.J. Ollitrault, et al., *'Quantum algorithms for grid-based variational time evolution'*, arXiv:2203.02521 (2022).