Polaritonic Quantum Chemistry: Exact Ansatz for Quantum Devices and a Quantum Algorithm

SPEAKER:
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A key challenge in quantum science is the efficient preparation of eigenstates of quantum many-body systems which typically span exponentially large Hilbert spaces. A popular and powerful approach to address this complexity is the use of exponential ansätze that attempt to capture the essential structural features of the many-body wavefunctions. However, their operational form is, in general, system-dependent, making it difficult to draw broad conclusions across different physical systems. In this talk, I will present a universal methodology for learning the exact ansatz of polaritonic quantum chemistry that can be implemented on quantum devices. This novel approach is based on a generalization of the contracted Schrödinger equation for electronic systems, which allows the ansatz to retain the same number of degrees of freedom as the original many-body Hamiltonian. In addition to discussing the theoretical foundations of the approach, I will provide explicit numerical examples of model and molecular polaritonic quantum systems and compare the method's performance with (polaritonic) coupled-cluster theory. At the end of the talk, I will present a quantum algorithm for near intermediate-scale quantum hardware by computing the dissociation curve of molecular systems strongly coupled to a bosonic bath.

The talk is mainly based on: "Exact Ansatz of Fermion-Boson Systems for a Quantum Device", Physical Review Letters 133 (8), 080202 (2024).

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