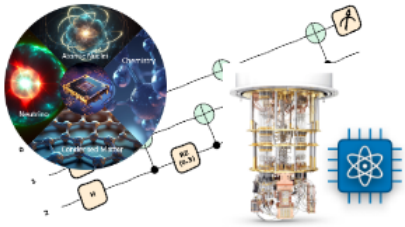

Contribution ID: **58** Type: **Contributed Talk (45min including questions)**

Molecular property simulations on quantum computers: Derivation, implementation, and hardware experiments

Thursday, November 20, 2025 3:50 PM (45 minutes)

Molecular simulation has been identified as one of the first practical applications where quantum computers could demonstrate utility, prompting extensive research into quantum algorithms for chemistry. Here, we go beyond ground state energy simulation and present various works related to obtaining molecular properties on quantum computers. These works are inspired by classical quantum chemistry knowledge, formulated in a hybrid quantum/classical algorithm framework, and go beyond "ideal simulator"studies, investigating shot and device noise. Crucially, we present first proof-of-concept hardware experiments of our algorithms on real quantum devices.

First, we present quantum algorithms for modelling spectroscopic properties by studying the response of matter to light. Classical linear response theory in a multi-configurational self-consistent field framework is reformulated for quantum computing. We explore different qLR formalisms, leveraging reduced density matrices, subspace approaches, and polarizable embedding. We showcase ideal simulator and noise study results of absorption spectra and electronic circular dichroism.[1-4]

Second, our in-house developed quantum computational software is introduced.[5] Here, we combine implementation of common wave function Ansätze with our property algorithm development. We use qubit-wise commutativity, on-the-fly Pauli savings, circuit grouping, Ansatz-based read-out and error mitigation, Pauli twirling, and dynamic decoupling. The software interfaces directly to Qiskit and IBM Quantum allowing shot and device noise simulations as well as cloud-based quantum hardware access. To showcase these developments, we present experimental results of absorption spectrum calculated on IBM quantum hardware using our in-house developed software to run qLR with novel error mitigation techniques.[6]

Third, we introduce a proof-of-concept study of electron spin resonance isotropic hyperfine coupling constants using unrestricted oo-qubit-ADAPT. We present hardware results using a combination of error suppression, mitigation, and post-selection schemes.[7]

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[5] Kjellgren and Ziems. SlowQuant, https://github.com/erikkjellgren/SlowQuant
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[7] Jensen, Hedemark, Ziems, Kjellgren, Reinholdt, Knecht, Coriani, Kongsted, Sauer, arXiv:2503.09214

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