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Moments-based ground-state energy estimation for pre-fault tolerant quantum hardware and beyond

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Ground-state energy estimation of chemical systems is perhaps one of the most promising applications of emerging quantum processors. However, the presence of noise makes near-term implementation of quantum algorithms challenging, while fault-tolerance at the scale required for useful computation remains a medium-term prospect. We present Hamiltonian moments-based approaches to ground-state energy estimation that aim to bridge the gap between near-term variational methods and fault-tolerant quantum phase estimation. The methods avoid the challenges faced by variational methods stemming from iterative trial-state optimisation, while the quantum circuits are both shorter and more robust to noise than those necessary for phase estimation. Our proof-of-principle quantum hardware demonstrations combined with numerical and analytic investigations give insight into the requirements for scaling to treatment of larger systems as hardware improves and enters the fault-tolerant regime. Since the error correction overheads required for phase estimation prohibit near-term or early fault-tolerant implementation for chemical systems of meaningful sizes, alternatives, such as moments-based methods, are much more promising pathways to achieving a useful quantum advantage in the near- or medium-term.

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