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High accuracy many-body calculations on quantum computers¹

JAMES FREERICKS, JEFFREY COHN, KHADIJEH NAJAFI, Georgetown University, FOREST YANG, University of California, Berkeley — Quantum computers have the potential to revolutionize simulations of many-body physics. But currently available quantum computers are often noisy and subject to rapid decoherence. How can we extract the most accurate result from a digital quantum simulation? In this talk, we describe how to improve the accuracy of current quantum chemistry calculations and of proposed many-body Green's function calculations by employing the quantum computer to directly calculate the many-body self-energy. Then, a conventional computer is employed with an exact noninteracting Green's function, to construct the fully interacting Green's function and extract quantities of physical interest like the ground-state energy. We illustrate how one would perform the measurement in the quantum computer and how one would post-process that data to extract the physical quantities of interest. Since the self-energy is a rather smooth and often small quantity, it is more robust to errors than extracting the full Green's function or the total energy. This allows us, in the spirit of high precision AMO experiments, to greatly improve the accuracy of the quantum computer. We end with a discussion of what the requirements are to implement these types of algorithms on currently available hardware.

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