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On the Chemical Basis of Trotter-Suzuki Errors in Quantum Chemistry Simulation RYAN BABBUSH, JARROD MCCLEAN, Harvard University, DAVE WECKER, Microsoft Research, ALÁN ASPURU-GUZIK, Harvard University, NATHAN WIEBE, Microsoft Research — Although the simulation of quantum chemistry is one of the most anticipated applications of quantum computing, the scaling of known upper bounds on the complexity of these algorithms is daunting. Prior work has bounded errors due to Trotterization in terms of the norm of the error operator and analyzed scaling with respect to the number of spin-orbitals. However, we find that these error bounds can be loose by up to sixteen orders of magnitude for some molecules. Furthermore, numerical results for small systems fail to reveal any clear correlation between ground state error and number of spin-orbitals. We instead argue that chemical properties, such as the maximum nuclear charge in a molecule and the filling fraction of orbitals, can be decisive for determining the cost of a quantum simulation. Our analysis motivates several strategies to use classical processing to further reduce the required Trotter step size and to estimate the necessary number of steps, without requiring additional quantum resources. Finally, we demonstrate improved methods for state preparation techniques which are asymptotically superior to proposals in the simulation literature.

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