Symmetry-preserving unitary product states for quantum computation

Hugh. G. A. Burton

Yusuf Hamied Department of Chemistry, University of Cambridge, U.K.

Emerging quantum electronic structure algorithms require new wave function approximations that can be efficiently implemented using shallow quantum circuits on near-term devices. However, combining gate efficiency and the preservation of physical symmetries has proved difficult using existing techniques, particularly since traditional approximations are not easily translated onto a quantum device. This talk will describe how these these challenges can be overcome using a well-defined Unitary Product State constructed from spin-adapted one-body operators and paired two-body operators with local qubit connectivity. I will describe how a product of unitary operations can be considered as a new class of wave function approximations, and how we can intuitively understand the preparation of correlated electronic states. Furthermore, by exploiting orbital optimisation and drawing connections with generalized valence bond theory, I will demonstrate that highly-accurate quantum wave functions can be constructed with gate-efficient and symmetry-preserving quantum circuits, paving the way for a new generation of quantum-compatible wave function approximations.