Unitary product states: A quantum-compatible approach for strong correlation

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The preparation of systematically improvable electronic wave functions for treating strong electron correlation is a key challenge for quantum chemistry applications using emerging quantum computers. For near-term devices, these wave functions must achieve high-accuracy with shallow quantum circuits and simple numerical optimisation. It has been shown theoretically that an arbitrary wave function can be constructed using a product of unitary one- and two-body fermionic operators. However, because this product depends on the choice and ordering of fermionic operators, we do not know how to construct these wave functions in practice. In this presentation, I will explore the systematic construction of near-exact quantum-compatible wave functions using the minimum number of quantum operators. I will show how we can build and optimise a product of unitary operators taken from a minimal pool containing only one-body and paired two-body fermionic operators. Using discrete optimisation techniques, I show how the selection and ordering of these operators can be systematically improved to identify the most accurate and compact fermionic wave function. This approach obtains highly-accurate energies for strongly correlated systems using significantly fewer quantum operators than current state-of-the-art techniques, and provides a new route to numerically investigate the properties of future quantum-compatible wave function approximations.