Recursive unitary ansatz for near-term quantum computers: ground and excited states

Rahul Maitra
Department of Chemistry,
Indian Institute of Technology Bombay,
Powai, Mumbai 400076, India
rmaitra@chem.iitb.ac.in

In this talk, I will briefly outline a novel many-body approach to accurately incorporate high-rank correlation effects via a low rank parametrization of the wavefunction ansatz. With a few physically motivated approximations of an effective Hamiltonian that otherwise contains exponentially large number of terms, we propose several variants that strike the right balance between accuracy and computational affordability[1]. Motivated by these developments of the many-body theory in the context of classical computing, I will propose a recursive unitary version of the same that allows us to simulate strongly correlated molecular systems with the help of the hybrid quantum-classical variational quantum eigensolver algorithm. I will demonstrate that the proposed recursive unitary forms the basis of a *partially disentangled* wavefunction ansatz in which arbitrarily high rank excitations are implicitly included through the appearance of a series of nested commutators[2]. Based on the ideas of energy sorting and operator commutativity pre-screening, I will introduce COMPASS, an automated toolkit towards on-the-fly fabrication of a variable structured wavefunction ansatz. COMPASS ensures minimal number of parameters and quantum gates to accurately simulate strongly correlated electronic systems in the Noisy Intermediate Scale Quantum (NISQ) devices. Extensions towards the treatment of excited states in the Quantum Equation of Motion (QEOM) framework would also be discussed.

[1] Tribedi, S.; Chakraborty, A.; Maitra, R. J. Chem. Theory Comput. 2020, 16, 6317

[2] Halder, D; Prasannaa, V. S.; Maitra, R. J. Chem. Phys. 2022, 157, 174117