RICE QUANTUM GROUP MEETING SEMINAR SERIES

Guo P. Chen

Prof. Gustavo E. Scuseria group

December 15, 2023, Friday

4PM, SST 300

Robust and Efficient Quantum Chemistry Methods for Dynamic and Static Electron Correlations

***Abstract*:**

Electron correlation underlies a wide range of chemical and physical phenomena, and its accurate and efficient description is one of the central goals of modern quantum chemistry. Dynamic or weak correlations arise from instantaneous polarization of the system due to quantum fluctuations, whereas static or strong correlations are typically associated with spontaneous symmetry breaking in mean-field. In this talk, I will present recent theoretical and algorithmic advances in treating these two types of electron correlations. For dynamic correlations, I will show that finite-order many-body perturbation theory is inadequate in describing large, polarizable systems, for which an infinite-order method such as random-phase approximation (RPA) is necessary. I will also discuss how we can improve upon RPA through renormalized perturbative corrections and how the resulting method can be made computationally efficient without sacrificing accuracy. For static correlations, I will focus on symmetry-projected Hartree-Fock-Bogoliubov (PHFB) theory, which is a black-box variational method with mean-field computational cost, as opposed to other multiconfigurational methods. Until recently, robust implementations of PHFB were impeded by numerical issues associated with computing matrix elements between Hartree-Fock-Bogoliubov (HFB) states. I will present a robust reformulation of Wick's theorem that resolves these issues. These advances in treating dynamic and static correlations will facilitate future developments of high-accuracy methods for large-size systems across all correlation regimes.

***Bio*:**

Guo P. Chen is a postdoctoral researcher in the group of Prof. Gustavo E. Scuseria. He obtained his B.S. and M.S. degrees in chemistry from Tsinghua University with Prof. Jun Li and his Ph.D. in chemistry from the University of California, Irvine with Prof. Filipp Furche. His work focuses on unconventional approaches to electronic structure theory, such as random-phase approximation methods and nonorthogonal multireference methods based on symmetry-projected mean-field theory. His research interests include correlated wavefunction methods, computational spectroscopy, low-scaling parallel algorithms, and computational rare-earth and actinide chemistry.

Snacks and Coffee will be served during the event Wine & cheese will be served after the talk. Everyone is welcome to stay around after the seminar for further informal discussions.