APS March Meeting 2021

View Abstract

CONTROL ID: 3505316

TITLE: Conditional wavefunction approach to the structure and dynamics of quantum systems

Abstract Body: The interacting conditional wavefunction approach is a recently introduced method for performing quantum dynamics simulations that is multiconfigurational by construction and that is able to capture quantitative accuracy for situations where mean-field theory fails. The technique is highly parallelizable and reformulates the traditional “curse of dimensionality” by using a stochastic wavefunction ansatz that is based on an interacting set of single-particle conditional wavefunctions. Here, we put forth an imaginary-time version of the method and demonstrate its ability for capturing correlated properties in systems made of interacting electrons and nuclei. This is illustrated for three highly-correlated problems: a model system of electron-Hydrogen scattering, a photo-excited proton-coupled electron transfer problem, and the strong-field ionization dynamics of a model H_2 molecule. These examples highlight the ability of the method to capture electron-electron, electron-nuclear and field-induced correlations respectively. This work paves the way for applications to systems driven out of equilibrium.

Funding Acknowledgement: We acknowledge funding from the ERC through the QSpec-NewMat Project

Special Instructions: My collaborator Kevin Lively and I would like to present our talks in the same session, preferably
back to back. His submission is entitled: "Vibronic Spectra from First Principles: Capturing the Franck-Condon Effect without Born-Oppenheimer Surfaces"

PRESENTATION TYPE: Oral

UNIT: 16.0 GENERAL THEORY, COMPUTATIONAL PHYSICS (DCOMP)

SORTING CATEGORY: 16.01.04 First-principles modeling of excited-state phenomena in materials (DCOMP, DCP, DMP) [same as 05.01.14]

Category Type: Computational

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Teams: (none)

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