COMPUTATIONAL RESEARCH in BOSTON and BEYOND SEMINAR

Numerically exact electron-phonon dynamics: projecting away instabilities in the hierarchical equations of motion

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ABSTRACT:

Coupled electron-phonon dynamics span a rich array of chemical and physical phenomena that includes energy and charge mobility in polar semiconductors, spectroscopic signatures in organic molecular crystals, dynamics in biological light-harvesting complexes, and superconductivity. Yet, models of such dynamics remain challenging to solve. One popular computational approach for solving these models exactly is the hierarchical equations of motion (HEOM). We have found that HEOM contains inherent instabilities that grow exponentially in time. In the case of continuous-bath models, these instabilities are routinely delayed to later times by increasing the hierarchy dimension; however, for systems coupled to discrete, nondispersive modes, increasing the hierarchy dimension does little to alleviate the problem. We show that these instabilities can also be removed completely at a potentially much lower cost via projection onto the space of stable eigenmodes; furthermore, we find that for discrete-bath models at zero temperature, the remaining projected dynamics computed with few hierarchy levels are essentially identical to the exact dynamics that otherwise might require an intractably large number of hierarchy levels for convergence. Recognizing that computation of the eigenmodes might be prohibitive, we also present a Prony filtration algorithm that may be useful as an alternative for accomplishing this projection when diagonalization is too costly. We present results demonstrating the efficacy of HEOM projected via diagonalization and Prony filtration.

THURSDAY, MAY 30, 2019
12:00 PM – 1:00 PM
Building 32 Room 141
STATA

Pizza and beverages will be provided.

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