Interpretation and Optimization of Orbital Spaces in Real-Time Coupled Cluster

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Computing induced electromagnetic properties via frequency-domain approaches (e.g. response theory) typically involves considering many excited states individually. Real-time methods, on the other hand, often treat all possible excited states simultaneously, leading to ambiguous interpretations of spectral features. Additionally, understanding the leading-order contributions to these properties would allow for the accurate truncation of the virtual orbital space, resulting in significant computational savings. The nature of key excited states may be explored by decomposing individual spectral features into their orbital contributions via Fourier transformation of the time-dependent wave function parameters. This decomposition is explored for canonical and localized orbital spaces with the goal of improving efficiency in real-time coupled cluster simulations through local correlation schemes.