Electronic structure via coherent control of time dependent quantum dynamics

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Abstract

Ab-initio Chemistry is a highly developed field of science with immense success in predicting and characterizing the force fields governing the motion of atoms and molecules. Yet, even to date, challenges remain. The properties of excited electronic states are difficult to treat accurately. In this talk I will present a new approach aimed at obtaining a quick and accurate evaluation of eigenvalues of very large matrices which are ubiquitous in Quantum Chemistry.

The philosophy upon which this proposal is based is the method of coherent control whereby one attempts to influence the outcome of a molecular process, by controlling the underlying quantum coherences. We suggest using the same strategy, but the process to be optimized is the determination of the lowest energy of the system. We find that the eigenvalues spanned by an initial wavefunction are uniquely determined by the coherent control time parameters which minimize the energy. These observations, coupled with a numerical solution of the time dependent Schrödinger equation lead to a new \( N^2 \) scaling method of obtaining the eigenvalues and eigenfunctions of atoms and molecules. Numerical results will be presented for the He and C atoms.