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Research Seminar

When: March 31, 2022
Time: 12:00 p.m.
Location: CBLL-16

Exploring the Self-Consistent Field (SCF) Energy Landscape as a Tool for Identifying New Forms of Reference Wavefunctions

Abstract

Global elucidation of SCF (self-consistent-field) solutions is an extension of global optimization in which the goal is the identification of all solutions. The value of identifying multiple SCF solutions is to use as reference wavefunctions, for example as shown in our group's difference projected double-hybrid density functional theory approach[1], or as linear combinations in nonorthogonal multireference configuration interaction[2] (NOMRCI) and nonorthogonal multiconfigurational SCF (NOMCSCF)[3] wavefunction models. However, global elucidation is NP-hard[4,5], and the high-dimensional space over which to search combined with the relatively high cost of local SCF optimization causes difficulty in efficiently searching over the full SCF space. To address the technical issues of high-dimensionality and nonlinearity, a Lie algebraic description[6] of electronic structure combined with a stochastic basin hopping approach[7] has been used. In this presentation, different parameters are explored to achieve the best efficiency of our proposed methods and interesting features of located SCF solutions are discussed. These results proved our proposed methods are reliable within 100 basis functions. Furthermore, extension to the larger molecular systems can be done using `Divide and conquer` strategy. To achieve this goal, we further propose our new developments to reduce the dimensionality of the problem and improve the local optimization method. We use active space models combined with a constraint built into the Fock matrix through a Lagrangian approach to define subspaces in SCF space. Thus, through a divide and conquer approach we can efficiently partitioning the mean-field electronic structure problem into relevant subspaces that can efficiently be examined to identify SCF solutions

References

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