University of Louisville
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Literature Seminar

When: October 13, 2022
Time: 2:30 p.m.
Location: CBLL-16

Complex Analysis in Electronic Structure Theory Application

Abstract:
Recent developments in theoretical chemistry have made use of analytic continuity into the complex plane for a number of applications, *e.g.* in the design of optical meta-materials [1-2], the study of topological phenomena in optical systems [3-6], and investigation of molecular electronic devices [7]. Additionally, complex analysis can be used in electronic structure theory to build new models and that make use of non-Hermitian operators to computationally solve the Schrödinger equation. As a result, the use of the complex plane not only extends the system from real space to imaginary space, but allows for understanding of significant phenomena in molecular systems. For example, conical intersections can be described and interpreted in a new way by making use of complex domain. In this talk I will discuss three developments that make use of the complex plane to describe strongly correlated many-electron systems -- holomorphic-modified Hartree-Fock [8], the connection of different Hartree-Fock solutions across the complex plane, which provides a mean field description of conical intersection type phenomena [9], and the development of a complex-plane coupled-cluster theory that can be used to compute conical intersection type phenomena which is used to investigate degenerate metastable resonance states in anionic molecules [10].

Keywords—complex analysis, non-hermitian operators, holomorphic functions, exceptional points

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