Theoretical Quantum Physics

Group Seminar

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The geometric aspect of electronic structure theory

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Abstract

Approximate wave functions for the ground electronic state can be obtained by standard methods of electronic structure, for instance, Hartree-Fock, Configuration Interaction, or Coupled Cluster theories. In these methods the approximate wave function is obtained as an optimal point, according to some criterion, of a subset of the set of all possible wave functions. What is the importance and what do we know about the geometry of these subsets? In this talk we will argue that much can be learned from this geometric aspect, and we will show our initial progresses (and expectations!) of our research on this subject. We will discuss: How the geometry of the Grassmannian can be used to find the Slater determinant with maximum overlap to a correlated wave function; The application to understand entanglement and correlation in electronic systems; And have a glimpse at the manifold associated to the coupled-cluster theory.

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