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Energy Landscape of Electronic Structure Theory

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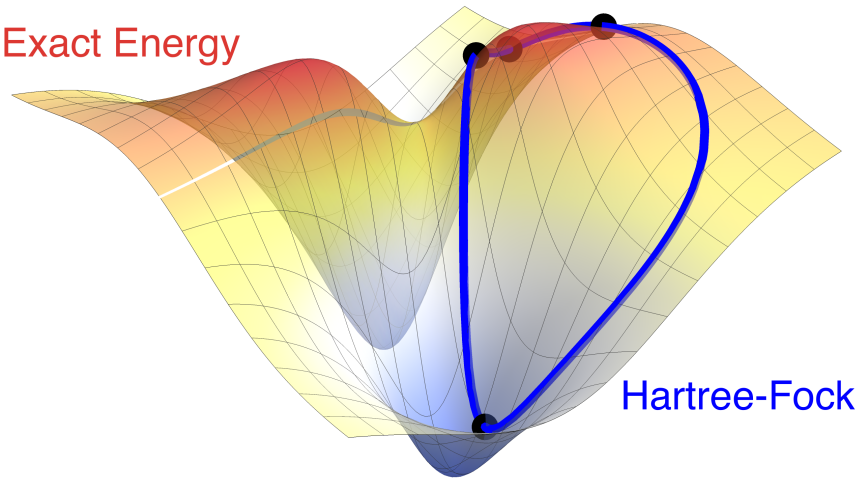

Electronic structure methods are generally built around iterative self-consistent equations, matrix eigenvalue problems, or corrections based on perturbation theory. In many cases, these methods use a single Slater determinant to define a reference wave function upon which electron correlation can be added. However, these “single-reference” approximations still face significant challenges for systems with many competing electronic configurations or difficult charge-transfer excited states. In this talk, I will introduce an alternative perspective on these challenges by considering the electronic structure problem as a parametrised energy landscape. Starting with exact full configuration interaction, I will describe the fundamental properties of this electronic structure landscape and explain how exact ground and excited states emerge from this representation. Using Hartree-Fock theory as an example, I will then show how approximate methods can be understood through the landscape perspective, including the origin of spin symmetry breaking for strongly correlated electrons, the properties of higher-energy excited-state solutions, and the divergence of perturbation theory. Finally, I will consider how the electronic landscape perspective can be extended to understand and improve more advanced theoretical methods such as quantum variational algorithms based on unitary coupled cluster theory.