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Algebraic Varieties in Quantum Chemistry

THURSDAY, May 30th, at 4:00 PM
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ABSTRACT

We discuss the algebra and geometry behind coupled cluster (CC) theory of quantum many-body systems. The high-dimensional eigenvalue problems that encode the electronic Schröedinger equation are approximated by polynomial systems at various levels of truncation. The exponential parametrization of the eigenstates gives rise to truncation varieties. These generalize Grassmannians in their Plücker embedding. We explain how to derive Hamiltonians, we offer a detailed study of truncation varieties and their CC degrees, and we discuss the solution of the CC equations. This is joint work with Fabian Faulstich and Svala Sverrisdóttir.