

Algebraic Varieties in Quantum Chemistry

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We discuss the algebra behind coupled cluster (CC) theory of quantum many-body systems. The high-dimensional eigenvalue problems that encode the electronic Schrödinger equation are approximated by a hierarchy of polynomial systems at various levels of truncation, for example CCD and CCSD. This leads us to a class of projective varieties which generalize Grassmannians in their Plücker embedding. We offer a detailed study of truncation varieties and their CC degrees, a complexity measure for solving the CC equations for a given truncation. Also we present the state of the art in solving the polynomial systems numerically. This is joint work with Fabian Faulstich and Bernd Sturmfels.