UNIVERSITY AT ALBANY
State University of New York

College of Arts and Sciences
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Colloquium

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Algebraic Varieties in Quantum Chemistry

Friday, September 29, 2023
3:00 p.m. in Massry 221

Abstract. We develop algebraic geometry for the coupled cluster (CC) theory of quantum many-body systems. Coupled cluster theory provides a large class of high-accuracy methods that are widely employed in the computational many-body community. In this ansatz, the high-dimensional eigenvalue problem that encodes the electronic Schrödinger equation is approximated by a hierarchy of 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 present the state of the art in solving the CC equations.