

Some Recent Mathematical Advances in Coupled-Cluster Theory

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In this talk, I will address mathematical developments of coupled-cluster theory based on strong monotonicity [1] and topological degree theory [2,3] as well as algebraic investigations [4]. In the single-reference coupled-cluster theory, by means of the exponential ansatz, the Schrödinger equation is reformulated into a polynomial system (system of nonlinear equations). The unknowns are the cluster amplitudes that may correspond to ground- or excited states. Strong monotonicity is limited to the description of ground states, other theoretical tools can be used to analyze excited states. Results include establishing existence and error estimates of approximate solutions and moreover highlighting some of the numerically observed behavior [5].

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