Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Coupled-Cluster and Linear-Response Time-Dependent Density-Functional Theory Perspectives on Particle-Particle Random-Phase Approximation DEGAO PENG, HELEN VAN AGGELEN, STEPHAN STEINMANN, YANG YANG, WEITAO YANG, Duke Univ, DUKE UNIVERSITY TEAM — The particle-particle random-phase approximation (pp-RPA) recently attracts extensive interests in quantum chemistry recently. Pp-RPA is a versatile model to calculate ground-state correlation energies, and double ionization potential/double electron affinity. We inspect particle-particle random-phase approximation in different perspectives to further understand its theoretical fundamentals. Viewed as summation of all ladder diagrams, the pp-RPA correlation energy is proved to be analytically equivalent to the ladder coupled-cluster doubles (ladder-CCD) theory. With this equivalence, we can make use of various well-established coupled-cluster techniques to study pp-RPA. Furthermore, we establish linear-response time-dependent density-functional theory with pairing fields (TDDFT-PF), where pp-RPA can be interpreted as the mean-field approximation to a general theory. TDDFT-PF is closely related to the density-functional theory of superconductors, but is applied to normal systems to capture exact N plus/minus 2 excitations. In the linear-response regime, both the adiabatic and non-adiabatic TDDFT-PF equations are established. This sets the fundamentals for further density-functional developments aiming for pp-RPA. These theoretical perspectives will be very helpful for future study.

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Date submitted: 15 Nov 2013

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