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Double, Rydberg and Charge Transfer Excitations from Pairing Matrix Fluctuation and Particle-Particle Random Phase Approximation YANG YANG, Duke Univ, HELEN VAN AGGELEN, Ghent Univ and Duke Univ, WEITAO YANG, Duke Univ — Double, Rydberg and charge transfer (CT) excitations have been great challenges for time-dependent density functional theory (TDDFT). Starting from an $(N \pm 2)$-electron single-determinant reference, we investigate excitations for the N-electron system through the pairing matrix fluctuation, which contains information on two-electron addition/removal processes. We adopt the particle-particle random phase approximation (pp-RPA) and the particle-particle Tamm-Dancoff approximation (pp-TDA) to approximate the pairing matrix fluctuation and then determine excitation energies by the differences of two-electron addition/removal energies. This approach captures all types of interesting excitations: single and double excitations are described accurately, Rydberg excitations are in good agreement with experimental data and CT excitations display correct 1/R dependence. Furthermore, the pp-RPA and the pp-TDA have a computational cost similar to TDDFT and consequently are promising for practical calculations.

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