Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

The particle-particle random phase approximation and beyond – insight from the superconductive Gorkov perspective and implications of an efficient truncation scheme DU ZHANG, WEITAO YANG, Duke University, WEITAO YANG GROUP TEAM — As an excited-state electronic structure method, the particle-particle random phase approximation (ppRPA) satisfactorily resolves many challenges for the time-dependent density functional theory (TDDFT)/particle-hole (ph) RPA, e.g. absence of double excitations, diradicals, singlet-to-triplet instability, etc. Given that the ppRPA equation has been derived from the pairing potential linear response, we derive it using the propagator approach using the superconductive Gorkov formalism. Systematic higher-order contributions are added to the ppRPA, yielding the pp Bethe-Salpeter equation (BSE). This development can be combined with our recently proposed truncation scheme, which makes typical ppRPA calculations up to 100 times faster than the Davidson's algorithm. Since the electron correlation is important in yielding good excitation energies for the ppRPA (the superiority of DFT reference states over Hartree-Fock ones, esp. for large systems), combining the two developments allows us to add the electron correlation into the ppRPA calculation at a modest formal scaling of O(N4), pushing the excitation energy calculations towards both larger systems and higher accuracy.

Du Zhang
Duke University

Date submitted: 06 Nov 2015 Electronic form version 1.4