MAR14-2013-008821

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

TDDFT and RPA for mesoscopic systems with thousands to millions of electrons: understating the red-shift in silver clusters absorption around 5nm

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Two quantum approaches for describing mesoscopic quantum systems with TDDFT will be described: The first, in collaboration with G. Lu and colleagues, is a single-orbital Madelung-like TDDFT propagation incorporating the correct homogenous electron gas dependence of the susceptibility on frequency, wavevector and density. We used this approach to understand the red-shift in the absorption of silver clusters around 5nm diameters. The second, in collaboration with R. Baer and E. Rabani, obtains the exact TDDFT and RPA results by stochastic averaging where the system's time-dependent density and potential is obtained by propagating small set of randomly chosen stochastic-orbitals, each of which is initially a random combination of the system's occupied orbitals. For large systems $\sim$ 10-40 orbitals are sufficient to get the correct dynamics regardless of the number of electrons.