FEAST real-time propagation scheme for TDDFT with study of CNT's plasmonic effects

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We have developed a robust and accurate real-time and real-space all-electron-TDDFT simulator capable to obtain the excited states of molecules and small nanostructures with direct comparisons with experimental data. Using the standard formalism of dipole time-response from short-polarized impulses [1], the time propagations are then performed using a spectral based approach making efficient use of the FEAST eigenvalue software [2,3] (i.e. direct integration of the evolution operator at each time step). FEAST transforms the eigenvalue problem into solving a set of independent linear systems, and it then relies on a subspace-iteration procedure where convergence is reached in a single iteration at each step of the time propagation. In comparison with a Crank-Nicolson scheme where small time intervals are needed and the linear systems need to be solved one after another, our spectral approach allows for larger time intervals and requires only one linear system to be solved by interval using a parallel implementation of FEAST. Similarly to the linear response theory, extended states need to be computed for performing the spectral decomposition at each time step. Within the real-space and real-time framework, however, the system matrices are sparse and linear parallel scalability can easily be obtained using multiple search intervals for FEAST and an appropriate parallel computing power. Several numerical results on molecules will be presented including the optical response of short CNTs. We have obtained the plasmonic excitations including some evidence of a 1-D Luttinger plasmon excitation peak from which the plasmon velocity can be calculated.

[1] K. Yabana, T. Nakatsukasa, J.-I. Iwata, and G. F. Bertsch, *Real-time, real-space implementation of the linear response time-dependent density-functional theory.* Phys. Stat. Sol. (b) 243,No. 5 , pp11211138 (2006).

[2] E.Polizzi, *Density-Matrix-Based Algorithms for Solving Eigenvalue Problems*, Phys. Rev. B. Vol 79, 115112 (2009)

[3] FEAST solver, *http://www.ecs.umass.edu/∼polizzi/feast*,