MAR06-2005-030034

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

Turbocharging time-dependent density-functional theory with Lanczos chains

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Using a super-operator formulation of linearized time-dependent density-functional theory, the dynamical polarizability of a system of interacting electrons is represented by a matrix continued- fraction whose coefficients can be obtained from the non-symmetric block- Lanczos method. The resulting algorithm, which is particularly convenient when large basis sets are used, allows for the calculation of the full spectrum of a system with a computational workload only a few times larger than needed for static polarizabilities within time-independent density-functional perturbation theory. The method is demonstrated with calculation of the spectrum of benzene and of fullerene, and prospects for its application to the large-scale calculation of optical spectra are discussed.