Stochastic treatment of electronic dissipation on top of a mean-field approach.

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Résumé

The quantum description of dissipative mechanisms in finite quantum systems is a long standing question in physics. It was originally addressed in nuclear physics, in particular a few decades ago, with the development of classical and semiclassical approaches. Meanwhile, a strong experimental motivation, now in the case of nanostructures and molecules irradiated by intense lasers, has shown up. This has motivated an increasing number of theoretical investigations in finite electronic systems, mostly on the basis of the well developed Time Dependent Density Functional Theory (TDDFT) that provides a robust effective mean field description of many low energy dynamical scenarios. Still, these TDDFT approaches fail to account for dissipative effects leading to observed electronic patterns. There is thus a crucial need for a formal and practical route to account for dissipative/thermalization features on top of quantum mean field.

We propose here a formalism allowing to describe the collisional correlations responsible for thermalization effects in finite quantum electronic systems. The approach is built as a stochastic extension of TDDFT, coined Stochastic Time-Dependent Hartree-Fock (STDHF). Dynamical correlations are treated in time-dependent perturbation theory and stochastic loss of coherence is assumed at some time intervals. This theory was formulated long ago for density matrices but never applied in practical cases because of its computational involvement. With a recent reformulation of the theory, applications are now conceivable. We obtained results in a 1D model and a full 3D sodiium cluster that satisfactory led to dissipative features in the electronic response of the system after an initial excitation.

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Mots-Clés: TDDFT, mean, field, stochastic TDHF, electronic dissipation