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Dynamical treatment of dissipation in finite quantum electronic systems

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 but without no convincing fully quantum one. Therefore, many dynamical scenarios (where quantum effects still play a role in spite of dissipative trends) cannot be treated. Meanwhile, a strong experimental motivation, now in the case of nanostructures and molecules irradiated by intense lasers, has shown up. This motivated an increasing number of theoretical investigations, mostly on the basis of the well developed Time Dependent Density Functional Theory (TDDFT) 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 the (observed) electronic pattern. 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. 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 and first tests have been successfully led in a simplifed 1D model.

Biography

Phuong Mai Dinh received her PhD in 2002 in High Energy Nuclear Physics (Institute for Theoretical Physics in Saclay, France), and has been recruited in 2003 at the Laboratory for Theoretical Physics of Toulouse. She now works on the theory of multi-electronic systems (clusters, molecules) excited by intense electromagnetic fields (lasers, charged projectiles), within time-dependent density functional theory (TDDFT) and beyond. She is a Developer of the TDDFT code "TELEMAN". She has published 59 referred articles including 3 reviews and 3 book chapters, and has written 3 books. She is a Junior Member of the Institut Universitaire de France since 2012.

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