Dissipation in Quantum Time Dependent Mean Field

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Mean field provides an essential starting point to understand the dynamics of numerous many-body systems ranging from nuclei to molecules, clusters and nano structures. Beyond structural or low energy properties, the analysis of dynamical processes, especially beyond the linear response domain requires the account of correlations beyond mean field, especially incoherent ones. The topic has been widely explored in nuclear dynamics with major efforts devoted to the development of semi-classical approximations, leading to Boltzmann type kinetic equations [2, 3]. Recent developments in laser technology now allow to analyse in some detail the response of clusters and molecules in short intense laser fields which typically lead to dissipative effects, beyond means field. Semi-classical approaches have also been explored in the field [1, 5] but are restricted to simple metals at sufficiently high excitations, which represents a strong limitation. There is thus a growing interest in the inclusion of dissipative features in current mean field theories in the case of electronic systems. The underlying mean field theory is here provided by Density Functional Theory (DFT) in its simplest Local Density Approximation (LDA), which is recognised as a robust and flexible approach for such systems, at least at moderate excitations [4, 5, 7].

We discuss in the present work some extensive studies we have led to include incoherent correlations on top of Time Dependent LDA or Time Dependent Harthree Fock (TDHF) approaches which represent archetypical mean fields approaches in the time domain. We briefly discuss available methods such as Trajectory Surface Hopping [8] and Time Dependent Current Density Functional Theory (TDCDFT, [9]), which turn out not to be adapted to the excitation energy domain we are interested in, both for formal and practical reasons. We next propose two alternative routes to solve the problem. We propose a quantum Relaxation Time Ansatz (RTA) providing an approximate quantum kinetic treatment [10] and a stochastic extension of mean field, know as Stochastic TDHF [6]. The RTA has allow us too access realistic laser irradiation scenarios and study in particular the impact of dissipation on electron emission in moderate size clusters. The STDHF (or Stochastic TDLDA) approach is much richer but still at a more schematic level. We have nevertheless explored it in simple molecular systems and been able to analyse its capabilities in detail [11, 12]. We have also tested it in a schematic 2 level model and are currently exploring simplifications of the theory to make them computable in realistic molecular and cluster cases.

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