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A quantum relaxation-time approximation for finite fermion systems

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ABSTRACT

We propose a relaxation time approximation for the description of the dynamics of strongly excited fermion systems. Our approach is based on time-dependent density functional theory at the level of the local density approximation. This mean-field picture is augmented by collisional correlations handled in relaxation time approximation which is inspired from the corresponding semi-classical picture. The method involves the estimate of microscopic relaxation rates/times which is presently taken from the well established semi-classical experience. The relaxation time approximation implies evaluation of the instantaneous equilibrium state towards which the dynamical state is progressively driven at the pace of the microscopic relaxation time. As test case, we consider Na clusters of various sizes excited either by a swift ion projectile or by a short and intense laser pulse, driven in various dynamical regimes ranging from linear to strongly non-linear reactions. We observe a strong effect of dissipation on sensitive observables such as net ionization and angular distributions of emitted electrons. The effect is especially large for moderate excitations where typical relaxation/dissipation time scales efficiently compete with ionization for dissipating the available excitation energy. Technical details on the actual procedure to implement a working recipe of such

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a quantum relaxation approximation are given in appendices for completeness.

1. Introduction

The analysis of the non-linear response of finite fermion systems subject to strong perturbations constitutes a central issue in many areas of physics. Prominent examples are low energy nuclear physics and fission [1,2] as well as excitation of clusters and molecules by intense laser pulses [3,4]. But similar situations are also encountered elsewhere, for example, in trapped Fermi gases [5] or electron transport in nano systems [6]. The case of irradiated clusters and molecules has become particularly interesting due to recent progress in experimental techniques at the side of photon sources [4,7] as well as at the side of detection accessing more and more detailed information from the decaying system. Particularly useful observables are from the distributions of emitted electron (kinetic energy, angular distributions, ...) through elaborate imaging techniques such as Velocity Map Imaging (VMI) [8,9]. These highly sophisticated measurements call for elaborate theoretical modeling to reconstruct the underlying dynamics of both the irradiation and de-excitation process. The choice of models ranges from a highly detailed quantum description to macroscopic rate equations [4]. Each one of these approaches is valid in a limited range of dynamical scenarios. The robust and rather versatile Time-Dependent Density Functional Theory (TDDFT), mostly realized at the level of the Time-Dependent Local-Density Approximation (TDLDA), [10–12] certainly provides one of the best compromises in the domain of quantum dynamics from the linear regime up to highly non-linear processes [4,13,14]. Still TDLDA basically remains a mean-field approach and misses by construction dissipative effects from electron–electron collisions which are expected to play a role in the course of violent excitation/de-excitation scenarios. This limits the range of applicability of TDLDA to moderate excitations and/or the entrance phase of the dynamics. A step beyond TDLDA is the GW approximation which allows to account for coherent two-body correlations and it has been used already for estimating electronic lifetimes in clusters [15]. But also this extension remains limited to low excitations. There is thus a strong interest to extend TDLDA by collisional dynamics in order to push the limits farther out. It is the goal of this paper to investigate such an extension by including the effect of collisional correlations (or dynamical correlations). The notion of "collisional correlations" is taken from Fermi liquid theory [16] with incoherent reduction of two-body correlations to two-Fermion collisions. As a first example of application, we discuss the case of irradiated metal clusters. But we emphasize that the strategy outlined here is applicable to any many-fermion system where TDLDA is a good starting point, namely where it provides a good description of low energy dynamics.

The much celebrated Boltzmann equation constitutes the prototype approach to collisional dynamics in classical systems [17]. In quantum systems, one has to account for the Heisenberg uncertainty relation and the Pauli principle. Pauli blocking can be accounted for by extending the Boltzmann collision term to the Boltzmann–Uehling–Uhlenbeck (BUU) form [18]. This semi-classical BUU approach (also known as Vlasov–Uehling–Uhlenbeck (VUU) equation) provides an acceptable picture at sufficiently large excitations where quantum shell effects can be ignored. It has been extensively used in nuclear physics [19,20] and also explored in metal clusters [21,22] in a high excitation domain. A further limitation of the BUU/VUU approach appears in the case of clusters: it is not clear that it could be used in systems others than simple alkalines, where electron wave functions are sufficiently delocalized and smooth to allow a semi-classical treatment [23]. This hinders, e.g., an application to C_{60} which is one of the systems attracting the most elaborate analysis of dissipative dynamics so far [7,24]. It should finally be noted that even in the high-excitation domain a major de-excitation channel is ionization which may quickly take away large amounts of excitation energy cooling the system down into a regime where quantum effects cannot be neglected any more. This limits BUU/VUU often to the initial stages of a dynamical process. All this shows that there is an urgent need for a quantum description augmented by relaxation effects.