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Dissipation in quantum time dependent mean field

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Abstract. We discuss an extension of Time dependent (TD) mean field theories such as TD Hartree Fock (TDHF) or TD Kohn-Sham (TDKS) in order to include dissipative effects as observed in many experimental situations. Applications to molecular problems are outlined. We present in particular a 1D model allowing to test a promising approach to include dissipative features in a quantum time dependent mean field. First results are presented in schematic cases.

1. Introduction

Mean field theory, and its time dependent (TD) extension, constitutes a sound starting basis for the description of numerous dynamical situations in a variety of many-fermion systems ranging from nuclei [1] to molecules and clusters [2]. Mean field theories in these systems have developed to a high level of sophistication, in particular in its stationary version, but dynamical versions thereof also attracted a lot of efforts especially for the description of low energy phenomena. In the nuclear context the keyword is Hartree Fock (HF) and its time dependent extension TDHF. Nuclear TDHF calculations have, to a large extent, been developed around effective density dependent functionals, typically Skyrme interactions, since several decades and have reached a high level of sophistication [3]. In clusters and molecules the underlying effective theory is Density Functional Theory (DFT) [4] and its Time Dependent extension TDDFT. The simplest mean field approximation thereof is known as Local Density Approximation (LDA and TDLDA), which again relies on a density dependent effective Hamiltonian [4]. Both nuclear TDHF and electronic TDLDA are thus using single particle density as a key input and thus bear strong formal resemblances, which actually reflect physical similarities in several observables [5]. One can mention as a typical example collective motion, in particular the Giant Dipole Resonance in nuclei [1] and its counterpart the Mie plasmon (or more generally speaking the optical response) in metal clusters [2].

Mean field theory constitutes a robust and sound basis for the description of many dynamical situations, but it fails to properly address dynamics beyond the linear regime, because it does not include dynamical correlations. Typical situations requiring such extensions are heavy-ion collisions in the Fermi energy range [6] or irradiation of clusters and molecules by intense laser fields [7, 8]. In spite of long standing efforts [9], the inclusion of dissipative effects via dynamical

correlations in a quantum mean field theory remains to a large extent an open issue. Several semi-classical approximations were developed, especially in the nuclear case over the last decades [10, 5], and more recently in the case of clusters [11]. However these latter approaches are limited to cases where a (semi) classical approximation is justified, or, in other words, to situations in which quantum shell effects can be safely neglected, typically when excitation energies are large enough, which excludes numerous physically relevant situations. Although not fully satisfying from the formal point of view, and in spite of some failures, the use of such semi classical approximations is probably acceptable in the case of heavy ion collisions in the Fermi energy domain [6, 5]. The situation is quite different for most molecular situations where quantum shell effects may play a leading role. The interest in these systems has been recently renewed following the accumulation of experimental evidence via imagining techniques, in particular in the case of irradiation of clusters and molecules by intense laser beams [8]. There is thus a recent renewed interest in this question of including dynamical correlations in quantum mean field, especially in the TDDFT community [12].

In the following, we propose a stochastic extension of TDHF/TDLDA which should allow to envision on short term the inclusion of dissipative effects in a quantum mechanical framework, and applications to realistic test cases both in the nuclear and the molecular contexts. After a brief reminder of the original theory, we outline a simpler form allowing test cases in model systems and outline the next steps to be performed along that line.

2. Theoretical framework

The formal starting point is Stochastic Time-Dependent Hartree-Fock (STDHF) originally formulated in nuclear dynamics [13], but which can be used in any systems where mean-field theory provides a sound description of low energy phenomena, as outlined above. STDHF proposes a description of dynamical correlations in terms of a stochastic ensemble of TDHF (mean-field) states. Originally, STDHF was formulated in terms of density matrices on the basis of the quantum Liouville equation [13]. STDHF can be reduced to a quantum kinetic equation (even accounting for fluctuations) and thus contains all ingredients for describing the path to thermalization and the thermal fluctuations around, as discussed in [13, 14]. But it has never been turned into a practical scheme. The aim of this paper is to propose a reformulation of STDHF, reducing correlations to 2 particles-2 holes ($2ph$) excitations, which allows a practical implementation of STDHF at acceptable expense, as will be illustrated on one example.

The basic idea of STDHF is to build correlations perturbatively around TDHF/TDLDA trajectories. Starting from an initial time $t_0 = 0$ we expand the time dependent correlated state $|\psi(t)\rangle$ into n-particle-n-hole (nph) excitations around the underlying Slater state $|\Phi\rangle$:

$$|\psi(t)\rangle = |\Phi\rangle + \sum_{pp'hh'} c_{pp'hh'} \hat{a}_p^\dagger \hat{a}_{p'}^\dagger \hat{a}_{h'} \hat{a}_h |\Phi\rangle + ... \tag{1}$$

where all ingredients on r.h.s. ($|\Phi\rangle$, $\hat{a}_p^\dagger$, $\hat{a}_h$, c) depend explicitly on time t. The nph basis has the great advantage that all states in the expansion (1) are ortho-normalized. The first non vanishing term of the expansion is the $2ph$ excitation around mean field, as the $1ph$ excitation is already included in the TDHF propagation. Assuming that the $2ph$ excitations indeed correspond to the leading contribution we truncate the expansion to this first ($2ph$) term. There remains to compute the $2ph$ expansion coefficients $c_{pp'hh'}$ which account for the dynamical correlations beyond the mean field state built up during time evolution.

To that end, we consider not too large time intervals τ so that we can describe the built-up of correlations in time dependent perturbation theory. Following standard steps of derivation we finally obtain transition probabilities in terms of Fermi Golden rule as

$$|c_{pp'hh'}(\tau)|^2 \simeq \tau \delta(\varepsilon_{p'} + \varepsilon_p - \varepsilon_{h'} - \varepsilon_h) |\langle \Phi_{pp'hh'} | \hat{V}(\tau) | \Phi \rangle|^2 \tag{2}$$

where $|\Phi_{pp'hh'}\rangle$ denotes one particular $2ph$ excitation on top of $|\Phi\rangle$. The single particle (sp) energies ε_j are taken here as the expectation values $\varepsilon_j = \langle\varphi_j(t)|\hat{h}(t)|\varphi_j(t)\rangle$ where $\hat{h}(t)$ is the instantaneous mean field associated to state $|\Phi\rangle$.

Equation (2) can be read as the probability of transition from the state $|\Phi\rangle$ to the $2ph$ state $|\Phi_{pp'hh'}\rangle$ due to the residual interaction $\hat{V}$ not accounted for in the mean field. In fact, it is the probability accumulated during an interval τ of propagation. The δ function plays the role of a energy selection rule, where only $2ph$-transitions fulfilling (up to some small uncertainty) energy conservation are allowed, and give nonzero transition probabilities.

Practically speaking we propagate an ensemble of Slater states according to TDHF/TDLDA and occasionally (every τ) evaluate jump probabilities. At each time jump probabilities are evaluated we sample the thus computed jump probabilities and choose a new state of the system according to the sampling (namely a $2ph$ excited state) or keep the actual state, depending on the probability sampling. The process is repeated in time for each member of the ensemble and this produces *one* realization of STDHF (one event). The whole procedure is then repeated for each member of the ensemble thus producing an ensemble of STDHF events, the ensemble itself representing the correlated evolution of the system. The ensemble then provides the necessary content to compute relevant observables as is illustrated below.

3. Results

For simplicity, we work on a 1D dimensional system mocking up the scales of a typical molecular system (actually close to metallic). The associated mean field Hamiltonian in x representation is given by

$$\hat{h}_N = -\frac{\Delta}{2m} + V_{\rm conf}(x) + \kappa\rho(x)^\alpha \tag{3}$$

where κ and α are parameters parametrizing the consistent component of the mean field (here we have chosen $\kappa = 3$ and $\alpha = 1$). The confining potential $V_{\rm conf}$ is chosen harmonic with frequency $\hbar w = 0.06Ry$ which delivers a rather dense spectrum with a large density of states thus a priori allowing numerous $2ph$ transitions even in a 1D system. We choose as residual interaction for two-body collisions a simple zero-range force

$$V_N(x,x') = \delta(x-x')V_0 \quad . \tag{4}$$

with $V_0 = 3Ry$ and reflecting boundary conditions. Starting from the ground state of the system we inject excitation energy E^* at initial time by applying some multi particle-hole excitation. The thus deposited excitation energy serves as seed for the branching of dynamical correlations which are evaluated each $\tau = 0.5fs$. We checked, by varying τ from half to double value, that the detailed choice of τ has minor effect. We propagate simultaneously 10 occupied wave functions (which constitute the actual Slater states) and 17 empty states which provide the reservoir for evaluating $2ph$ transitions. The examples presented below gather about 50 events.

As an illustrative example of how STDHF events do evolve in time we plot in Figure 1 the time evolution of single particle energies following an initial $3ph$ excitation delivering an excitation energy of a bit less than 2 Ry. The figure nicely shows how $2ph$ transitions do occur in the course of time. Of course, the figure is only illustrative to the extent that other events will deliver another sequence of $2ph$ transitions. But on the average the total number of $2ph$ transitions is a rather robust quantity (at least for such an excitation energy) and only varies little form one event to the next. The dense spectrum in that case allows a sizable number of such transitions and thus ensures an efficient dissipative scenario.

A key quantity to analyze dissipation and mixing are occupation numbers. This quantity can be evaluated from the ensemble of STDHF events via the one body density matrix $\hat{\rho}$ constructed

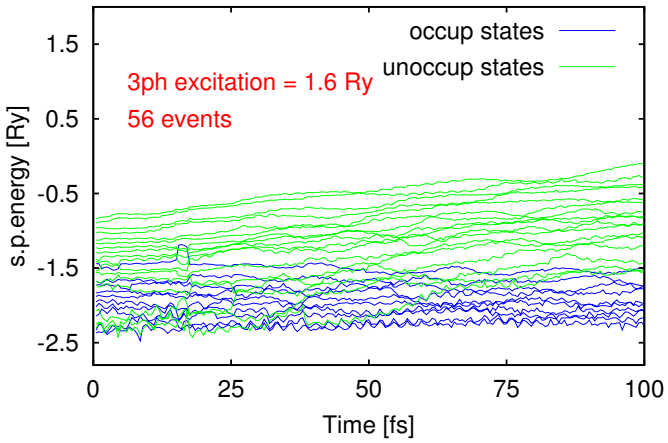

Figure 1: Time evolution of sp energies for one particular event. The excitation energy is 1.6 Ry in that case.

as the average of the one body density matrice of each event $\hat{\rho}_i$ as :

$$\hat{\rho} = \frac{1}{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} \hat{\rho}_i \tag{5}$$

where $\mathcal{N}$ is the total number of events. The one body density matrix for a given event i is obtained by summing over the occupied states as

$$\hat{\rho}_i(x, x') = \sum_{\alpha=1}^{N} \varphi_\alpha^*(x')\varphi_\alpha(x) \tag{6}$$

where N represents the total number of occupied states. The density matrix (5), thus constructed, is then diagonalized and its eigenvalues provide the occupation numbers $n(\varepsilon)$ which can be plotted as a function of time to analyze the path to thermalization.

The time evolution of occupation numbers is illustrated in Figure 2 in the case of an initial $3ph$ excitation delivering $E^* = 1.6$ Ry. In the early times the figure nicely exhibits traces of the initial excitation with spiky structures. These structures are progressively smoothed as a consequence of the relaxation process. The asymptotic state finally exhibits a smooth profile resembling a Fermi distribution

$$n(\varepsilon) = \frac{1}{\exp(\frac{\varepsilon - \varepsilon_F}{k_B T}) + 1} \tag{7}$$

which signals a thermal equilibrium state. We have fitted the distribution finally reached in the STDHF propagation to the equilibrium profile (7), see figure 3. The agreement is satisfying in view of the small system under consideration. The fit allows to extract a temperature. In that it is $k_B T =\sim 0.17 Ry$, which represents a significant fraction of the actual Fermi energy when measured from bottom of the potential well. We thus have clearly reached a thermal state. This statement can be corroborated by looking at the time evolution of the sp entropy (not shown here). It is found that the entropy increases steadily and levels of asymptotically with an exponential convergence rate.

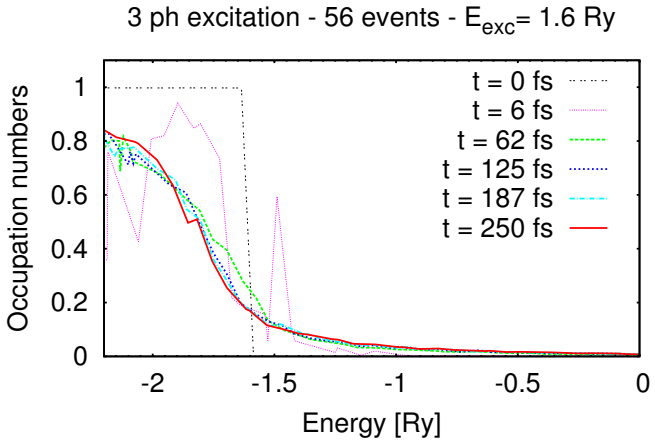

Figure 2: Snapshots of occupation numbers $n(\varepsilon)$ as a function of sp energy ε at selected times for 1.6 Ry excitation energy.

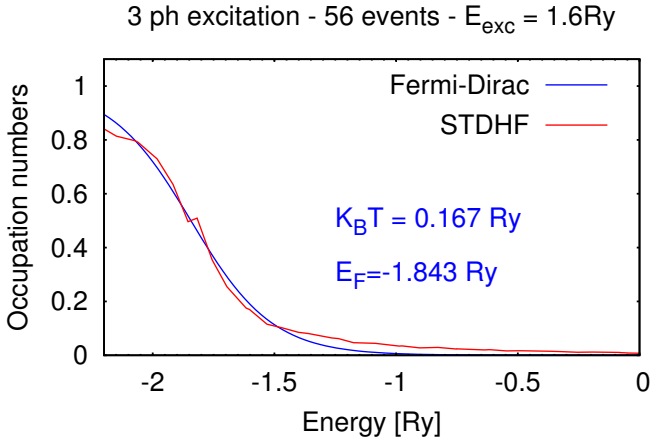

Figure 3: Fit of the final distribution of the example in figure 2, see red line, to a Fermi distribution (7), see blue line.

4. Conclusions and perspectives

We have introduced a stochastic approach to include dissipation (and fluctuations) on top of time dependent mean field theories. This approach treats correlations in time dependent perturbation theory on short time. Dynamical correlations are then sampled to provide an ensemble description of the dynamics, in terms of pure mean field states. We have illustrated this approach on a simple 1D model mocking up typical molecular situations. The first results obtained in this framework show that the adopted strategy is very promising. In spite of the 1D restriction the density of states is large enough to allow a significant number of $2ph$ transitions which are at the source of our dissipative mechanism. The system is excited at initial time by a random multi ph excitation which immediately deposits a (possibly large) excitation energy. The correlated one body density matrix obtained as the ensemble average of pure mean field density matrices displays the expected features of a system driven towards thermal equilibrium as expected in the cases explored in this study. This exploratory case raises a large number of questions. They concern for example analysis tools to be further developed in particular

single particle entropy and associated relaxation times towards equilibrium, correlated two body density matrix..., to mention a few. It also concerns some technical issues on the preservation of conservation laws (total energy, centre of mass...) which are presently only preserved in average. They also concern formal developments to be performed in particular a reformulation of the theory in terms of mixed states to allow the treatment of low energy cases where the stochastic sampling reaches its limits in terms of statistics. These various aspects are presently being considered.

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