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Dissipation in Quantum Mean Field

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Abstract. We discuss an extension of Time Dependent Hartree Fock (TDHF) to include dissipative effects. We propose a simple model to test a stochastic extension of TDHF. Applications to nuclear and molecular problems are outlined.

Mean field constitutes a sound starting basis for the description of numerous dynamical situations in a variety of systems ranging from nuclei [1] to molecular systems and clusters [2]. Mean field has been indeed developed in these fields and raised to a high level of sophistication. In the nuclear context it is well known under the acronym Hartree Fock and the time dependent extension thereof (TDHF). Nuclear TDHF calculations have, to a large extent, been developed around effective density dependent functionals, typically Skyrme interactions [1]. In clusters and molecules the leading effective theory is Density Functional Theory [3] and its Time Dependent extension TDDFT, which again relies on a density dependent effective Hamiltonian [2]. Both TDHF and standard TDDFT are thus using single particle density as a key input and thus bear strong formal resemblances. These resemblances actually reflect physical similarities in several observables [4]. Let us cite as a typical example here collective motion, in particular the Giant Dipole Resonance in nuclei and its counterpart the Mie plasmon (or more generally speaking the optical response) in metal clusters [2].

Although mean field constitutes a robust and sound basis for the description of many dynamical situations, it is well known that it for example fails to properly address dynamics beyond the linear regime. A way out is to include dissipative effects which mock up dynamical correlations not accounted for at mere mean field level. In spite of long standing efforts [5], the inclusion of dissipative effects in a quantum mean field remains to a large extent an open issue. Several semi classical approximations were developed, especially in the nuclear case over the last decades [4, 6], and more recently in the case of clusters [7], but these approaches are limited to cases where a (semi) classical approximation is justified. This may be partially true in the case of heavy ion collisions in the Fermi energy domain [4, 8] but certainly hard to envision for most molecular

situations. There is thus a recent renewed interest in this question, especially in the TDDFT community, the move being triggered by the accumulation of experimental evidence for dissipative effects in many situations, in particular in the case of irradiation of clusters and molecules by intense laser beams [9].

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

1 Stochastic TDHF

1.1 General outline

Although the question of extending TDHF to account for dissipation (via "two body collisions") was attacked several decades ago [5] no convincing approach was finally developed in the fully quantal context. The 1980's saw in turn, the development of semi classical approximations, leading to approaches based on kinetic theory [6]. The next move was to include quantum features in the dynamics. The most convincing approach is probably the method proposed in the early 1990's and known as FMD (Fermionic Molecular Dynamics) or AMD (antisymmetrized Molecular Dynamics) in which a degraded version of TDHF is complemented by a classical collision term, in the spirit of kinetic theory [10]. Still such approaches heavily rely on semi classics and further developments have shown the necessity of including more and more quantal features [11].

An alternative, both to kinetic equations and to the molecular dynamics methods, was proposed in the early 1990's but never made practical, mostly for computational reasons. The Stochastic TDHF approach [12] aims at providing a theoretical framework for stochastic extensions of TDHF, but without recurring to the kinetic equation stage. STDHF is based on two basic assumptions :

- a perturbative treatment of the residual interaction V on a well chosen time interval τ, around a TDHF trajectory; this delivers correlated states built around the TDHF one.
- projection of the correlated states on an ensemble of TDHF determinants.

A key ingredient of STDHF, as of most stochastic approaches, is the typical time scale (here τ) on which correlations are building up and loss of coherence becomes possible, justifying a stochastic treatment. The hypothesis of a perturbative treatment on a time interval τ, on the basis of TDHF, now imposes that

$$\tau_{\rm coll} \ll \tau \ll \tau_{\rm m.f.} \tag{1}$$

While dynamics has to remain dominated by mean-field ($\tau_{\rm m.f.}$), the residual interaction should be efficient enough to allow a sufficient number of transitions

between states of the system ($\tau_{\rm coll}$) to justify a statistical hypothesis. In the framework of STDHF, the notation $\tau_{\rm coll}$, which refers to the duration of an elemetary collision, does not exist directly but allows to grasp the essence of the process.

With the assumption Eq.(1) one can propagate an initially uncorrelated state $D_N = |N\rangle\langle N|$ (Slater determinant) between an instant 0 and τ, within accounting for the residual interaction. It leads to express the density matrix of this, now correlated, state $\mathcal{D}_N$, as a statistical superposition of uncorrelated states D_M (TDHF states):

$$\mathcal{D}_N(\tau) = (1 - \sum_{M\neq N} W_{MN}) D_N(\tau) + \sum_{M\neq N} W_{MN} D_M(\tau) \tag{2}$$

The weights W_{MN}, which are the key ingredients, can then be expressed from Fermi golden rule [12] (on the time interval $t = 0 \rightarrow t = \tau$):

$$W_{MN} = \frac{2\pi}{\hbar} |\langle N|\hat{V}_N|N\rangle|^2 \delta(E_M - E_N)\tau \tag{3}$$

where $\hat{V}_N$ is the residual interaction for state $|N\rangle$ and $E_{N(\rm resp. M)}$ the total energy of state N (resp. M). The matrix element is evaluated at time $t = 0$. One furthermore expects that the dominant terms in the above expansion are the ones corresponding to 2 particles$-$2 holes ($2ph$) excitations with respect to $|N\rangle$.

The elementary propagation Eq.(2) then allows to build an ensemble of stochastic trajectories

$$\left\{ \begin{array}{ccccc} D_N & \stackrel{\tau}{\rightarrow} & \{D_M, W_{MN}\} & & \\ & & D_{M_0} & \stackrel{\tau}{\rightarrow} & \{D_L, W_{M_0 L}\} \\ & & & & \cdots \end{array} \right\}_{N=1,\ldots} \tag{4}$$

Practically speaking, starting from a pure TDHF state D_N one chooses, after the first STDHF time step (by sampling according to the W_M weights) a new pure TDHF state D_{M_0}. The process is then iterated starting with D_{M_0} which progressively builds up one trajectory. And an ensemble of trajectories built this way constitutes the STDHF ensemble representation of the whole dynamical process.

1.2 Critical discussion

There are several interests to this approach, once it is made practical. Let us briefly mention the most salient ones.

- STDHF is a fully quantal approach, at least as much as TDHF is quantal;
- it relies on a full TDHF formulation, thus without recurring to approximate TDHF states such as those used in elaborate molecular dynamics methods;

- it avoids the difficult question of treating a collision term directly, which by construction is an involved high dimensional integral, even in the classical case;

- it goes beyond kinetic theory as it also includes stochastic effects. It can actually be shown that it may be reduced to a stochastic extension of kinetic equations [12].

Of course STDHF has to be made practical. That is certainly a difficult question and several problems need to be overcome. Let us briefly mention a few of them. The major difficulty is of computational nature. Direct simulations of ensembles of TDHF states remain quite demanding. The nuclear case, though, is certainly simpler as typical realistic dynamical situations may be considered on rather short time scales (in natural time scales), namely involving only some hundreds or thousands of time steps, no more. This is typically the case of heavy ion collisions in the Fermi energy domain [8]. The situation is much less forgiving in the electronic case where realistic scenarios involve typically 2 or more orders of magnitude longer times (again in natural time scales) than nuclear ones, thus making the simulations of realistic ensemble basically unreachable. Even if we thus can use direct simulations of STDHF in the nuclear case we shall have to develop a simplified version thereof for application to the electronic case. In the mean time it will certainly be highly interesting to consider model systems as will be discussed in the following. Finally one should also keep in mind the intrinsic limitations connected to the validity of the whole approach, essentially what concerns the identification of τ and the approximations on which time dependent perturbation theory implicitly relies. In the following we shall nevertheless consider that these latter aspects are under control.

2 Towards Testing STDHF in a Simple Model

2.1 STDHF in a $2ph$ picture

We denote by $|N\rangle$ a typical Slater state following original notation of STDHF derivation. The label N should not be confused with the number of particles present in the system, which we denote by $\mathcal{N}$. The $|N\rangle$ sSater state thus reads

$$|N\rangle = \mathcal{A}_{1\ldots\mathcal{N}} \prod_{i=1}^{\mathcal{N}} [|\phi_{i,N}\rangle] \tag{5}$$

introducing the antisymmetrization operator $\mathcal{A}_{1\ldots\mathcal{N}}$. Note that we keep the index N on each single particle (s.p.) state $|\phi_{i,N}\rangle$ to specificy the link to the Slater state $|N\rangle$.

We assume that we have propagated for a while a time dependent Slater state $|N\rangle = |N(t)\rangle$ according to the Hamiltonian $\hat{h}_N(t)$. The point is to compute the transition matrix elements $\langle M|\hat{V}_N|N\rangle$ where we further impose $|M\rangle$ to be a $2ph$

state built on the (time dependent) $|N\rangle$ state, i.e.

$$|M\rangle = \hat{a}^\dagger_{\alpha_{p'}} \hat{a}^\dagger_{\alpha_p} \hat{a}_{\alpha_h} \hat{a}_{\alpha_{h'}} |N\rangle \tag{6}$$

where p, p' belong to "particle" states and h, h' belong to "hole" states. The formally simplest choice to take the hole states from those s.p. states occupied in $|N\rangle$ and the particle states from the unoccupied ones. One then has for energies

$$E_N = \langle N|\hat{h}_N|N\rangle \tag{7}$$

and

$$E_M = \langle M|\hat{h}_N|M\rangle \approx E_N + \varepsilon_p + \varepsilon_{p'} - \varepsilon_h - \varepsilon_{h'} \tag{8}$$

where the ε_i are the single particle energies associated to $|N\rangle$ state.

The two-body interaction $\hat{V}_N$ can be expanded as

$$\hat{V}_N = \frac{1}{2} \sum_{i_1<i_2, j_1<j_2} (\alpha_{i_1}\alpha_{i_2}|V_N|\widetilde{\alpha_{j_1}\alpha_{j_2}}) \hat{a}^\dagger_{\alpha_{i_1}} \hat{a}^\dagger_{\alpha_{i_2}} \hat{a}_{\alpha_{j_2}} \hat{a}_{\alpha_{j_1}} \tag{9}$$

where $|\widetilde{\alpha_{j_1}\alpha_{j_2}})$ is an anti-symmetrized state of two independent Fermions. This then yields

$$\langle M|\hat{V}_N|N\rangle = \frac{1}{2} \sum_{i_1<i_2 j_1<j_2} (\alpha_{i_1}\alpha_{i_2}|V_N|\widetilde{\alpha_{j_1}\alpha_{j_2}}) \langle M|\hat{a}^\dagger_{\alpha_{i_1}} \hat{a}^\dagger_{\alpha_{i_2}} \hat{a}_{\alpha_{j_2}} \hat{a}_{\alpha_{j_1}}|N\rangle \quad . \tag{10}$$

With $|M\rangle$ given as in Eq. (6) the above summation reduces to

$$\langle M|\hat{V}_N|N\rangle = (pp'|V_N|hh')\langle M|\hat{a}^\dagger_p \hat{a}^\dagger_{p'} \hat{a}_{h'} \hat{a}_h|N\rangle = (pp'|V_N|hh') \tag{11}$$

with

$$(pp'|V_N|hh') = \int \mathrm{d}x \mathrm{d}x' \phi^*_p(x)\phi^*_{p'}(x') V_N(x,x') \phi_h(x)\phi_{h'}(x') \tag{12}$$

In the basic transition element of STDHF, we have to evaluate

$$|\langle M|\hat{V}_\mathrm{N}|N\rangle|^2 \delta(E_M - E_N) \approx |\langle M|\hat{V}_\mathrm{N}|N\rangle|^2 \delta(\varepsilon_p + \varepsilon_{p'} - \varepsilon_h - \varepsilon_{h'}) \tag{13}$$

and this implies to give a practical definition to the Dirac δ-function. In a space of discrete spectra, we employ a finite-width δ function

$$\delta(E) \longrightarrow \delta_w(E) = \frac{1}{\omega\sqrt{\pi}} \exp\left(-\frac{E^2}{w^2}\right) \quad . \tag{14}$$

One possible motivation for finite width is that one has used a finite sampling time $\tau = \Delta t$ associated with a width $w = \Delta t^{-1}$. This is however conceptually not easy to assess. It is more plausible to relate the width to the uncertainty in the s.p. energies as will be discussed later.

2.2 A 1D example

For simplicity, we start with considering a 1D system. The associated mean field Hamiltonian is denoted $\hat{h}_N$ which we shall choose as (in x representation)

$$\hat{h}_N = -\frac{\Delta}{2m} + V_{\rm ext}(x) + \kappa\rho(x)^\alpha \tag{15}$$

where κ and α are parameters mocking up the self consistent component of the mean field and $V_{\rm ext}(x)$ is a well chosen one-body external potential, typically a Woods-Saxon as a starter. This model (15) is close to a typical situation in molecular or cluster physics where the ionic background provides a spatially fixed external potential. An alternative simulating self-bound system, as drops of liquid ^{3}He or nuclei, is a Skyrme-like Hamiltonian

$$\hat{h}_N = -\frac{\Delta}{2m} - \kappa_1\rho(x)^\alpha + \kappa_2\rho(x)^\beta \quad . \tag{16}$$

In any case, we choose as a residual interaction for two-body collisions a simple zero-range force

$$V_N(x,x') = \delta(x-x')V_0 \quad . \tag{17}$$

This choice differs from the TDDFT residual interaction according to the mean fields (15) or (16). It is legitimate and reasonable that the collision term need not to use the same residual interaction as TDDFT or RPA (which is $\delta\hat{h}_N/\delta\rho$). Note also that in actual computations, we shall complement $\hat{h}_N$ by an external perturbing field $V_{\rm perturb}$ driving the system out of equilibrium (laser, initial boost, ...).

2.3 Some practical details

Practically one is thus left to evaluate possible $2ph$ transitions as built on $|N\rangle$. There is a huge space of choices for the $2ph$ states. Possible options are:

1. One propagates more s.p. states than initially occupied in $|N\rangle$ and considers $2ph$ states within this basis of propagated s.p. states. This is topologically simple as these states are immediately ortho-normal. But then the s.p. energies have some uncertainty $\Delta\varepsilon_i$ because the propagated s.p. states are not necessarily eigenstates of $\hat{h}_N$. One may minimize the uncertainties by diagonalizing the occupied states with respect to $\hat{h}_N$ and also the unoccupied ones (but not across particle to hole states).

2. One defines $2ph$ states with respect to the instantaneous Hamiltonian $\hat{h}_N$. A problem here is that the occupied states in $|N\rangle$ are not the eigenstates of $\hat{h}_N$. Thus one has to orthogonalize the eigenstates on the given occupied states of $|N\rangle$.

3. One optimizes new $2ph$ states from a maximum jump probability principle.

The most efficient choice is probably point 3. But it would still have to be worked out and will certainly be formally involved. The most straightforward and plausible is strategy 1. We will follow this line in the first studies.

The problem here is that the s.p. energies ε_i have some uncertainty $\Delta\varepsilon_i$. We turn it into an advantage by choosing the width of the energy conserving δ function in the rate (13) from s.p. variances $\Delta\varepsilon_i$. An important quantity here is provided by the total variance

$$\Delta {h_N}^2 = \langle N| \left(\hat{h}_N - \langle N|\hat{h}_N|N\rangle\right)^2 |N\rangle = \sum_{i=1}^{\mathcal{N}} \Delta {\varepsilon_i}^2 \tag{18}$$

where the summation runs over occupied s.p. states ($\varepsilon_i = \langle\phi_{i,N}|\hat{h}_N|\phi_{i,N}\rangle$). The average s.p. variance is then $\overline{\Delta\varepsilon^2} = \Delta {h_N}^2/\mathcal{N}$. There are now at least two options for choosing the width

$$w = 2\Delta h_N/\mathcal{N} \quad \text{or} \tag{19}$$

$$w = \left[\Delta {\varepsilon_p}^2 + \Delta {\varepsilon_{p'}}^2 + \Delta {\varepsilon_h}^2 + \Delta {\varepsilon_{h'}}^2\right]^{1/2} \quad . \tag{20}$$

The form (20) employs only the variances of the s.p. states actually encountered in the jump. Thus each term in the rate Eq. (13) is associated to a different width. Much simpler is the form Eq. (19) which uses an average width for each term. In a first round, we should choose the simplest version Eq. (19).

There remains to add a few words of caution concerning energy and momentum preservation during such simulations. There is presently no control over momentum conservation in the rate (13) and energy conservation is not perfect either due to the finite energy width in the rates. This has to be tested numerically and we have to see whether fluctuations and/or drift of momentum and energy remains acceptable. If not, we can easily augment the scheme by projectors on momentum and energy.

Another open question is also the capability of a 1D model to provide sufficient $2ph$ phase space to justify statistical arguments. Again, we have to test this practically. If we find the phase space insufficient, we may extend the studies a multi-channel 1D model.

3 Next steps

The next steps will consist in pursuing the studies on the model 1D test case and, in parallel, explore more realistic 3D nuclear cases, again within restricting excitations to $2ph$ as outlined above. A key aspect is certainly the exploration of the $2ph$ density of state which will control the capability of the system to explore transitions. This density of state will of course depend on the actual physical situation and correlatively on the perturbing potential used to simulate that, thus including implicitly the amplitude of the perturbation. Indeed too small a perturbation will not allow the full development of a sufficiently large number of transitions between states, thus inhibiting a statistical treatment. In turn,

too large an excitation may impose, in order to preserve the perturbative nature of the description, to reduce considerably the time step on which the perturbative analysis has to be performed. It is hard to predict the behavior of realistic systems in such respect and the next urgent step is thus to start computational explorations. Work along that line is already in progress.

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