Quantal Extension of Mean-Field Dynamics**

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Abstract

A method is presented for numerical implementation of the extended TDHF theory in which two-body correlations beyond the mean-field approximation are incorporated in the form of a quantal collision term. The method is tested in a model problem in which the exact solution can be obtained numerically. Whereas the usual TDHF fails to reproduce the long time evolution, a very good agreement is found between the extended TDHF and the exact solution.

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1 Introduction

The study of nuclei in out-of-equilibrium configurations in many-body quantum theory is a very complicated problem. However, due to their long mean-free path inside the nucleus and to their large amplitude zero point motion associated to a strong delocalization of their wave-packet, nucleons could be often regarded as independent fermions moving within a mean potential. Indeed, such theory, called Time-Dependent Hartree-Fock theory (TDHF), first applied to nuclear dynamics some twenty years ago by Bonche et al. [1], is able to reproduce quantitatively many properties of Heavy-Ion collisions [2]. However, in this theory, nucleons interact only through the mean-field and collisions between particles are neglected. It is difficult to believe that correlations induced by collisions do not play also an important role when highly dissipative processes are involved. For example, thermalization of single-particle degrees of freedom [3] and damping of collective motion [4, 5] could only be understood by the introduction of two-body correction. Furthermore, usual mean-field theory is not able to reproduce the large experimental width of mass produced during Heavy-Ion reactions at Intermediate energies.

In the extended Time-Dependent Hartree-Fock (ETDHF) theory, the description is improved beyond the mean-field approximation by incorporating correlations in the form of a quantal collision term [6]. Due to the numerical complexity, the applications of this theory on realistic situations remain a difficult problem, and therefore only a few approximate calculations have been performed so far [7]. In this paper, we describe the basic features of the ETDHF approach, propose a method for obtaining numerical solutions of the theory, and present an application of the method to an exactly solvable model.

2 Extended Time-Dependent Hartree-Fock Theory

The exact description of a quantum system is contained in the many-body density operator $\hat{D}(t)$ and its dynamical evolution is given by the Liouville-von Neumann equation

$$i\hbar \frac{d\hat{D}}{dt} = [\hat{H}, \hat{D}]$$

(1)
Since the system has a a priori a large number of degrees of freedom, the practical resolution of equation (1) is often impossible. The basic assumption of mean-field theory is to suppose that only one-body observables are important in the description of the system (neglecting, by the way, all correlations of order greater or equal to two). Usual mean-field theory neglect completely two-body dynamics and values of two-body observables are obtained assuming that they are equal to the least biased value when one-body observables are known[8]. In this approaches, all relevant information is contained in the one-body density operator \( \hat{\rho} \) and the dynamical evolution is replaced by[9]

\[
i\hbar \frac{d\hat{\rho}}{dt} = [\hat{h}, \hat{\rho}] \tag{2}
\]

where \( \hat{h} \) is the mean field associated to \( \hat{H} \). This approximate theory is already a many-body theory for out-of-equilibrium finite system. Note that, even if two-body dynamics are not explicitly included, non-trivial correlations between single particle states exists due to the reorganization of the mean-field during the time evolution.

However, this two-body correlation is not sufficient to reproduce the many facet of nuclei desexcitation. In particular, no dissipation, characteristic of the irreversible flow from collective motion to single particle degrees of freedom[3] and expected to be responsible of the thermalization of nuclei, is included. The next step towards extended mean-field is to include information about two-body correlation dynamics. This could be obtained in particular by a truncation of the BBGKY hierarchy[10] to the two first equations. This approaches assumed that TDHF is already a good approximation of the dynamics and two-body correlations are supposed only to act as a small perturbation added on top of the mean-field. This leads to a correction factor in the evolution of the one-body density operator[11]

\[
i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{h}, \hat{\rho}] + K(\hat{\rho}) \tag{3}
\]

with

\[
K(\hat{\rho}) = -\frac{i}{\hbar} \int_{-\infty}^{t} dt' t_2[V_{12}, U_{12}(t, t') \rho_1 \rho_2 \bar{V}_{12} (1 - \rho_1) (1 - \rho_2) U_{12}(t', t) - \bar{U}_{12}(t, t') (1 - \rho_1) (1 - \rho_2) \bar{V}_{12} \rho_1 \rho_2 U_{12}(t', t)] \tag{4}
\]

\footnote{In this expression, usually, an additional term exist due to the propagation of initial correlations. In this paper, we suppose that, initially, we have uncorrelated states.}
Taken same notations as in ref.[11], the label 1 and 2 refers to first and second particles, for example

\[ \langle ij | \rho_1 \rho_2 | kl \rangle = \langle i | \hat{\rho} | k \rangle \langle j | \hat{\rho} | l \rangle \]  

(5)

\( U_{12} \) is the propagator of two independent particles associated to the mean-field:

\[ U_{12} = U_1 \otimes U_2 \]  

(6)

with

\[ U_1(t,t') = T \left( \exp \left( -\frac{i}{\hbar} \int_{t'}^{t} h(\rho(s)) ds \right) \right) \]  

(7)

and \( tr_2 \) is the partial trace taken over the second particle whereas \( \tilde{V}_{12} \) includes the antisymmetrization.

Eq. (4) is the starting point of most of the theories that goes beyond TDHF. For example, all semi-classical applications which include collision effects[12] (namely BUU approaches) can be derived from it, by developing the Wigner transform of (3) up to first order in \( \hbar \). Over the past decade, significant progresses have been made on the description of nuclear dynamics within semi-classical transport theories and extension of mean-field seems to be a promising tool for describing dynamics. However, nuclei are quantum objects even under extreme conditions and important physical component are missing in a semi-classical treatment. Some attempts in order to treat the collision term in a quantum picture already exists[7, 14]. Nevertheless, due to the complicated expression of \( K(\rho) \), these investigations have been carried out under strong approximations.

Here, we describe a procedure for treating the collision term (4) with minimum bias and which may be adapted for solving the ETDHF equation in realistic situations under reasonable numerical approximations.

### 3 Re-examination and numerical algorithm

In a single particle bases, the one-body density operator reads

\[ \hat{\rho} = \sum_{\lambda, \lambda'} | \lambda \rangle n_{\lambda, \lambda'} \langle \lambda' | \]  

(8)
and the evolution equation take the form

\[ \begin{aligned}
   i\hbar \frac{\partial}{\partial t} |\lambda\rangle &= \hbar(\rho) |\lambda\rangle \\
   \frac{d}{dt} n_{\lambda, \lambda'} &= -\frac{1}{\hbar^2} \left( F_{\lambda, \lambda'} + F_{\lambda'}^{*} \right)
\end{aligned} \tag{9} \]

with

\[ F_{\lambda, \lambda'} = \sum_{\alpha, \alpha', \beta, \beta', \gamma, \delta, \delta'} \langle \lambda \delta' | V_{12} | \alpha \beta \rangle \int_{-\infty}^{t} dt' \langle \alpha' \beta' | V_{12} | \gamma \delta \rangle |t'\rangle \]

\[ n_{\gamma \lambda} n_{\delta \delta'} (\delta_{\alpha \alpha'} - n_{\alpha \alpha'}) (\delta_{\beta \beta'} - n_{\beta \beta'}) \]

\[ -n_{\alpha \alpha'} n_{\beta \beta'} (\delta_{\gamma \lambda} - n_{\gamma \lambda}) (\delta_{\delta \delta'} - n_{\delta \delta'}) \tag{10} \]

\[ + n_{\alpha \alpha'} n_{\beta \beta'} (\delta_{\gamma \lambda} - n_{\gamma \lambda}) (\delta_{\delta \delta'} - n_{\delta \delta'}) \tag{11} \]

This expression is the most general one could extract from (4). We know from work of [14], that approximations in (11) leads to important change in physical results. In particular, the time integration is often replaced by a conservation of energy based on a Markovian approximation of the collision but we know that this memory effect is important since it creates the non-trivial coupling between collective and single particle motions. Furthermore, we are obligated to consider the non-diagonal part of (11) which will give the coherent evolution of single-particle states.

A direct resolution of (11) needs a large numerical effort. However, in the following, we will see that it could be considerably simplified without losing its generality.

### 3.1 Coarse-Graining in time

Supposing that we know the one-body density at time \( t \):

\[ \hat{\rho} = \sum_{i} |\Phi_{i}\rangle n_{i} \langle \Phi_{i}| \tag{12} \]

From information theory, it means that we have access to the least biased description of our system when only one-body observables are known. We can have a geometrical picture of the information reduction. One-body space could be represented by a manifold in a bigger space (see fig. [4]). Suppose that we start from one point on this manifold. The exact dynamical evolution could be represented schematically by a trajectory in this space. Due to the
presence of two-body correlations, the trajectory will not remain in the one-body space. Nevertheless, the exact trajectory is associated to a path in the one-body space which reproduce the one-body dynamics of the exact evolution. The goal of using mean-field theory is to predict this trajectory. In the one-body space, the TDHF theory corresponds also to a trajectory. However, due to the neglected two-body correlations dynamics, usual mean-field is not able to reproduce the long-time evolution of the system. This is symbolized in fig. 1, by a strong departure of the TDHF theory from the best one-body trajectory. The goal of ETDHF is to correct the mean-field evolution in order to be a much better approximation of the best trajectory.

Figure 1: Geometric picture of TDHF and EXACT evolution. The Initial condition is supposed to be contained in the one-body space. The exact trajectory is symbolised by a path in the total space. In particular, due to the presence of two-body correlations, this trajectory do not remain in the one-body manifold. The best associated trajectory in the one-body space is represented in dashed-line whereas the TDHF evolution is represented in solid line. The neglected two-body correlation dynamics in TDHF, implies that this theory do not corresponds to the best trajectory for long time evolution.

However, some remarks are in order:
- Whereas TDHF fails to reproduce the long time evolution due to accumulated errors on two-body observables, one-body dynamics remains dominant. It implies that it exists a typical macroscopic time interval $\Delta t$ during which mean-field is a good approximation of the dynamics. This time interval is of the order of the time between two collisions. Note that, a basic assumption of ETDHF and TDHF is that this time interval is large compared to the typical time-scale of mean-field evolution.

- For time greater or equal to $\Delta t$, two-body correlations appear as a small correction to the mean-field and could be treated in perturbation.

It enable us to coarse-grain the time evolution for the extended mean-field dynamics. Instead of solving equation (3) in time, we will divide the evolution into two step:

- The Hartree-Fock states will be evolved through the usual TDHF equation between $t$ and $t + \Delta t$

\[
\begin{aligned}
  i\hbar \frac{\partial}{\partial t} |\Phi_i\rangle &= h(\rho) |\Phi_i\rangle \\
  \frac{d}{dt} n_i &= 0
\end{aligned}
\]  

(13)

- We then use the perturbation theory in order to correct the one-body density by the error accumulated during $\Delta t$ associated with (9). We then find the new density operator $\hat{\rho}'$ (see fig. 2)

\[
\hat{\rho}'(t + \Delta t) = \hat{\rho}(t + \Delta t) + \Delta \rho
\]

\[i\hbar \frac{\partial}{\partial t} = [h, \hat{\rho}] \text{ Integrated Effect of collision}
\]  

(14)

The new one-body density is then diagonalize and the procedure is iterated (see fig. 3),
Figure 2: Schematic representation of ETDHF evolution within the coarse-graining time framework. The two steps procedure is represented. In solid line, the usual TDHF is first performed. After a time $\Delta t$, a correction is applied (small dashed line) in order to account for two-body correlations propagation.

### 3.2 Determination of a Basis

In order to express different operator matrices elements, we need a priori a complete basis of the single-particle space. However, this could rarely be obtained in a problem with a huge number of degrees of freedom. On the other hand, if we suppose to have such a basis, only few of the states will be necessary in order to have the main information about the system (the rest corresponding to configuration which are not accessible). In a previous application\cite{14}, the author proposes to include only a part of the Hartree-Fock bases (including all occupied states ("hole states") and few unoccupied states ("particle states")) and to follow them with time. However, the system could reach many different configurations and single-particle states that were not included at the initial time could become important. It is thus difficult to believe that one can choose the basis at the initial time. Conversely, at each coarse-grained time step $\Delta t$, we will construct a bases that contains the important information about different configurations accessible to the system between a given time $t$ and $t + \Delta t$. According to this procedure,

- At a given time $t$, we suppose to have the Hartree-Fock basis $|\Phi_i(t)\rangle$. 

Figure 3: With the same convention as in fig.1, the schematic evolution through the numerical resolution of ETDHF is represented. Each $\Delta t$, a correction is applied to the mean-field evolution. The ETDHF procedure is expected to follow the best trajectory in the one-body manifold.
We only perform the evolution of occupied states between \( t \) and \( t + \Delta t \).

- At time \( t + \Delta t \), we complete the hole states (\( |\Phi_i(t + \Delta t)\rangle \)) by a limited ensemble of particle states (\( |p_j(t + \Delta t)\rangle \)). This states are constructed in order to be a good approximation of eigenstates of \( h(t + \Delta t) \) with an energy smaller than a given energy \( \varepsilon_{Max} \). In the following, we will discussed in detail the construction of the basis and the choice of \( \varepsilon_{Max} \).

\[ \Rightarrow \text{Between } t \text{ and } t + \Delta t, \text{ two single-particle states (1-2) could collide.} \]

As a consequences, new states could be populated. In a simplified vision of collision\( \text{ii} \), we can assume that the transition probability from (1-2) to two new states (3-4) is important when

\[ \varepsilon_1 + \varepsilon_2 \sim \varepsilon_3 + \varepsilon_4 \]

The maximum accessible energy \( \varepsilon_{Max} \) is obtained when 1 and 2 are the hole state with highest energy \( E_{Max} \) and 3 or 4 is the hole state with lowest energy \( E_{Min} \). This give the natural truncation energy for the basis:

\[ \varepsilon_{Max} = 2E_{Max} - E_{Min} \]

\[ \Rightarrow \text{In order to find states with low energy, we apply an imaginary time method to Hartree-Fock states. This method, explained in APPENDIX A, provides finally a truncated basis: } \{ |\Phi_i(t + \Delta t)\rangle \otimes |p_j(t + \Delta t)\rangle \} \text{ where all different matrices could be expressed. This basis will be called ”instantaneous basis” and noted generically } \{ |\lambda\rangle \} \text{ in the following.} \]

- In order to include the memory effect in the collision terms. The instantaneous basis is evolved backward self-consistently.

4 Re-organization of occupation numbers and single-particle wave-functions.

The collision term introduce a small correction to the density at each macroscopic time step \( \Delta t \), see expression (14). In the following, we will treat \( \Delta \rho \) in

\(^2\text{Here, the simplification is contained in the fact that, in general, states (1-2) are not eigenstates of } h \text{ which is the condition of having an exact conservation of energy.}\)
first order perturbation theory. In this case, the new density operator could be expressed as:

\[ \hat{\rho}' = \sum_i |\Phi_i\rangle n_i' \langle \Phi_i| \]  

where new states are obtained through the following procedure

- **New occupation numbers:** In first order perturbation, only diagonal elements of \( \hat{\Delta \rho} \) are necessary to calculate the new eigenvalues \( n_i' \) of \( \hat{\rho}' \). The time evolution of this diagonal elements between \( t \) and \( t + \Delta t \) is given by a *master equation* (see APPENDIX B)

\[ \frac{dn_\lambda}{dt} = (1 - n_\lambda) W^+ - n_\lambda W^- \]  

with initial condition

\[ n_i'(t) = n_i(t) \]  

During \( t \) and \( t + \Delta t \) the gain and loss term, respectively \( W^+ \) and \( W^- \), are considered constant. In this case, the equation (16) is exactly solvable and reads:

\[ n_i(t + \Delta t) = n_i(t) \exp \left( -\Delta t \left( W^+ - W^- \right) \right) \]

\[ + \frac{W^+}{W^+ + W^-} \left( 1 - \exp \left( -\Delta t \left( W^+ - W^- \right) \right) \right) \]  

- **Reorganization of states:** The new states are given in perturbation theory by

\[ |\phi_i'(t + \Delta t)\rangle = |\lambda\rangle + \sum_{\lambda' \neq \lambda} \frac{1}{n_{\lambda'} - n_{\lambda}'} |\lambda'\rangle \langle \lambda' | \Delta \rho | \lambda \rangle \]  

It is important to note, that, not only previously occupied states but also part of unoccupied states are included at each macroscopic time-step in the dynamics. In a previous application, Tohayama argued that non-diagonal elements in the density matrices are important. In our approach, they are explicitly included since the first order perturbation is equivalent to a approximate diagonalization of \( \hat{\rho}' \). However, here we do not fixe the basis at the initial time and the system will dynamically choose which configuration will be accessible.
In this section, we have described the scheme we will use in order to extend TDHF. In the following, we will apply it to a model that could be exactly solved numerically.

5 Application

We have considered two distinguishable particles in a one-dimensional anharmonic potential. The total Hamiltonian reads

\[ H = \sum_i \left( \frac{\hat{p}_i^2}{2m} + U_i \right) + \sum_{i<j} V_{ij} \]  

(20)

where the one-body external field is

\[ U_i = \frac{1}{2} k \hat{x}_i^2 + \frac{1}{4} k' \hat{x}_i^4 \]  

(21)

and the non-local two-body interaction \( V_{ij} \) is taken as

\[ V_{i,j} = \frac{t_0}{\sqrt{2\pi\sigma}} \exp -\frac{(\hat{r}_i - \hat{r}_j)^2}{2\sigma^2} \]  

(22)

This problem, which seems simple in appearance contains already different features of many-body physics and is a good benchmark for ETDHF since it could be compared with the exact solution.

5.1 Initial conditions and evolution

We consider the system initially heated and constrained. The initial two-body density operator is written as a statistical equilibrium

\[ \hat{\rho}^{ini} = \frac{1}{Z} \exp -\frac{1}{k_B T} \left( \hat{H} - \lambda \hat{Q} \right) \]  

(23)

where \( \hat{Q} \) is a one-body operator and \( \lambda \hat{Q} \) is the initial constraining field. At initial time, the constraint is relaxed and the system evolve. In fig. 4, we show the one-body external field part of \( \hat{H} \) in r-space (solid line) and the equivalent constrained field \( \hat{H} - \lambda \hat{Q} \) (dashed line). After relaxation of the constraint, three different evolutions are compared:
Figure 4: One-body part of the external field in r-space, with the initial constraint (dashed line) and without the initial constraint (solid line).
• **EXACT evolution:** For the exact evolution, we solve exactly the von Neumann equation for the two-body density operator:

\[
\text{i} \hbar \frac{d \hat{D}}{dt} = [\hat{H}, \hat{D}] \tag{24}
\]

• **TDHF:** The equation of motion is

\[
\text{i} \hbar \frac{\partial \rho}{\partial t} = [\hbar, \rho] \tag{25}
\]

Note that occupation numbers remains unchanged during the evolution

\[
\frac{d n_i}{dt} = 0 \tag{26}
\]

• **ETDHF:** For the ETDHF, we apply the procedure described above. In this case, occupation numbers evolve in time and new states are mixed to initial one during the dynamics.

For both TDHF and ETDHF, the initial density is the one-body that corresponds to the exact one

\[
\rho^{ini} = \text{tr}_2 \hat{D}^{ini} \tag{27}
\]

### 5.2 Results and Discussion

#### 5.2.1 Prediction of one-body dynamics:

In fig. 5, we have represented the dynamical evolution of the diagonal part of the one-body density in r-space. At initial time, the one-body density has been imposed to be the same for all calculations. We see that usual TDHF (dashed line) calculation is a good approximation of the exact one-body dynamics (circles) for time smaller than 100 fm/c. However, for longer time, we observe strong differences between TDHF prediction and the expected result. On the same graphic, the equivalent evolution is reported for ETDHF simulations (solid curve). The ETDHF prediction of the one-body density operator follow closely the exact one even for long time evolution.

Since the one-body density matrices govern the evolution of all one-body observables, it means that the extension of mean-field enable us to predict one-body dynamics with a good accuracy. Indeed, if we look to one particular one-body observable, for example the center of mass motion (denoted \(\langle X \rangle\), fig. 6), we observe a very good agreement between exact calculation and ETDHF prediction whereas TDHF fails to reproduce the long-time dynamics.
Figure 5: Evolution of the one-body density operator in r-space. Three different simulations are displayed: Exact (small circle), TDHF (dashed line) and ETDHF (solid line).
Figure 6: Center of mass motion \( \langle X(t) \rangle \) of the two-particle in interaction. The three different simulations are represented: Exact (small circle), TDHF (dashed line) and ETDHF (solid line).
5.2.2 Variation of occupation numbers

In fig. 7, we have plotted the variation of occupation numbers (i.e. the eigenvalues of $\hat{\rho}$) in the exact (circles) and ETDHF treatment (dashed line). Due to the presence of a residual two-body interaction, we observe a reorganization of occupation numbers in the exact evolution. The numerical procedure we have developed in order to extend the mean-field dynamics is able to reproduce this complicated behavior. This demonstrate in particular that two-body correlation dynamics is properly taken into account through the method we have used. It is important to note that reorganization of occupation numbers is accompanied by an evolution of the relevant single-particle states and that no bias exists in our approach, in the choice of this relevant states. This is one of the major improvement contained in our procedure.

5.2.3 Conclusion and outlook

In this article, we have discussed the possibility of extending mean-field in quantum dynamics in order to include two-body correlations. Such theory, is numerically much more complicated to apply than usual TDHF simulations. As a result, only few applications have been carried out up to now. These applications often rely on important simplifications made in the collision term. We propose here, a procedure to solve numerically this problem. In our approach, no additional bias is introduced by the simulation and the collision effect is treated in all its generality. The method is then tested on a simple model that could be exactly integrated numerically. This model of two particle interacting one with the other already contains many facet of many-body problems. In particular, the two-body interaction leads to a strong reorganization of occupation numbers during the dynamics and affect considerably the long-time evolution. As expected, usual mean-field dynamics is not able to account accurately for this complicated behavior. On opposite, the inclusion of two-body correlation dynamics into the mean evolution improve considerably the prediction of one-body observables.

The ETDHF seems to be a very promising tool for the description of nuclei under extreme conditions. In forthcoming work, we will apply the numerical procedure to realistic nuclei. The inclusion of two-body correlations will considerably improve our knowledge about the nuclear dynamics. In particular, this many-body theory includes the possibility for collective motion to dissipate energy through an irreversible flow to single-particle de-
Figure 7: Occupation numbers evolution. Circle represents the exact evolution of occupation numbers and dashed line represents evolution predicted by ETDHF. The TDHF simulation (not represented) predicts fixed occupation numbers.
degrees of freedom. This will certainly ameliorate the prediction of damping of giant resonances. On the other hand, this extended theory is needed for the understanding of thermalization of nuclei.

6 APPENDIX A: Determination of the instantaneous basis.

The instantaneous basis is constructed in order to be a good approximation of part of the eigenvectors of the mean-field Hamiltonian \( h \) at time \( t + \Delta t \). Noting \( |\xi_\alpha\rangle \) this eigenvectors, we have

\[
\hat{h}[\rho(t+\Delta t)] |\xi_\alpha\rangle = \varepsilon_\alpha |\xi_\alpha\rangle
\]  

Determining all \( |\xi_\alpha\rangle \) is not possible in general since it imply the inversion of huge matrices. However, the \( |\xi_\alpha\rangle \)'s form a complete basis of the single particle space. In particular, Hartree-Fock states could be expressed in this basis

\[
|\Phi_i\rangle = \sum_\alpha C_i^\alpha |\xi_\alpha\rangle
\]  

Using the imaginary time method, consists in applying the operator \( \exp (-\beta \hat{h}) \) to the state:

\[
|\Phi'_i\rangle = \exp (-\beta \hat{h}) |\Phi_i\rangle
\]

where \( \beta \) is a real number. The interest of such operator leads in the following:

\[
(\exp (-\beta \hat{h}))^n |\Phi_i\rangle = \exp (-\beta n \varepsilon_0) \sum_\alpha C_i^\alpha \exp (-\beta n (\varepsilon_\alpha - \varepsilon_0)) |\xi_\alpha\rangle
\]  

which shows that

\[
(\exp (-\beta \hat{h}))^n |\Phi_i\rangle \xrightarrow{\beta \to \infty} |\xi_0\rangle
\]

We thus see that, application of the imaginary-time operator to any state converge towards the lowest state in energy. More generally, this operator remove the space pertained by states with high energy on profit of low energy states. Using this property, new states are constructed with following steps:
• **Application of** \( \exp(-\beta h) \): from each Hartree-Fock state, a series of state is constructed:\(^3\)

\[
\begin{align*}
\left| \psi_i^{(0)} \right\rangle &= |\Phi_i\rangle \\
\left| \psi_i^{(n)} \right\rangle &= \mathcal{N}^{(n)} \left\{ \exp(-\beta h) - \left\langle \psi_i^{n-1} | \exp(-\beta h) | \psi_i^{n-1} \right\rangle \right\} |\psi_i^{(n-1)}\rangle
\end{align*}
\]

The number of states per Hartree-Fock states will determine the precision of the evaluation of the collision term. In practice, we observe that only few extra states are necessary to be included between two times separated by \( \Delta t \).

• All states are grouped and orthonormalized. Note that the Hartree-Fock basis remains unchanged.

• Instead of considering directly this basis, we diagonalize the projected Hamiltonian:

\[
(1 - \hat{P}) h [\hat{p}] (1 - \hat{P}) |p_j\rangle = \varepsilon |p_j\rangle
\]

with

\[
\hat{P} = \sum_i |\Phi_i\rangle \left\langle \Phi_i \right| 
\]

• Finally states with energy \( \varepsilon \) greater than the energy \( \varepsilon_{\text{Max}} \) are rejected. Note that, all created new states belongs to the kernel of \( \hat{\rho}(t + \Delta t) \) which will simplify considerably the expression of the collision term.

7 **APPENDIX B: Expression of transition elements.**

In our instantaneous basis, the density is diagonal, the coefficients of eq. \( \Box \) reads

\[
F_{\lambda,\lambda'} = \sum_{\alpha,\beta} \langle \lambda \delta | V_{12} | \alpha \beta \rangle_{A} |t
\]

\(^3\)Note that, the use of a field \( h' = h + \delta h \) where \( \delta h \) is a small external stochastic field improve this method.
\[
\int_{-\infty}^{t} dt' (n_{\lambda} n_{\delta}(1-n_{\alpha})(1-n_{\beta}) - n_{\alpha} n_{\beta}(1-n_{\lambda})(1-n_{\delta}))
\]
\[
\langle \alpha\beta|V_{12}|\lambda\delta \rangle_{A} |t'\rangle
\]

In order to express the integral in time, we applied a backward mean-field evolution (where we have neglected the correlation part). In this case, occupation numbers are constant, however, a finite life-time $\tau$ (equivalent to the Landau beating time) has been added in order to properly calculate the integral (we have fixed $\tau$ in order to not biased the integral value).

- **Diagonal elements:** The equation of motion is written as equation (18) where

\[
W^{-} = \frac{4}{\hbar^{2}} \sum_{\alpha,\beta,\delta} n_{\alpha} n_{\beta}(1-n_{\delta}) \text{Real} \{ \langle \lambda\delta|V_{12}|\alpha\beta \rangle_{A} |t \rangle
\]
\[
\int_{-\infty}^{t} dt' \exp\left(\frac{t'-t}{\tau}\right) \langle \alpha\beta|V_{12}|\lambda\delta \rangle_{A} |t'\rangle\}
\]
\[
W^{+} = \frac{4}{\hbar^{2}} \sum_{\alpha,\beta,\delta} (1-n_{\alpha})(1-n_{\beta})n_{\delta} \text{Real} \{ \langle \lambda\delta|V_{12}|\alpha\beta \rangle_{A} |t \rangle
\]
\[
\int_{-\infty}^{t} dt' \exp\left(\frac{t'-t}{\tau}\right) \langle \alpha\beta|V_{12}|\lambda\delta \rangle_{A} |t'\rangle\}
\]

We have checked that the lost term and the gain term are almost constant during each time interval $\Delta t$

- **Non-diagonal elements:** The non-diagonal elements are necessary in order to express the mixing of states. The integrated effect of collision is simply taken as

\[
\langle \lambda|\Delta \rho|\lambda' \rangle = \frac{-\Delta t}{\hbar^{2}} (F_{\lambda,\lambda'} + F_{\lambda',\lambda}^{*})
\]

(35)

**References**

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