Stochastic Time-Dependent Hartree-Fock for heavy-ion collisions in the Fermi energy domain

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We present the first realization of Stochastic TDHF, a theory which goes beyond pure mean-field dynamics, embracing dissipation as well as fluctuations. Applications to heavy-ion collisions in the Fermi energy domain are given and analyzed in terms of dissipative features and Intermediate Mass Fragment production.

Since its early introduction in quantum dynamics TDHF [1] is the basic selfconsistent theory for many dynamical processes in physics and chemistry. In nuclear physics, it has found since long widespread and fruitful applications in collective motion and heavy-ion reactions [2–5]. Recently, a new field of applications to the nonlinear electron dynamics in metal clusters has opened up [6–8] which brings up challenging questions in connection with new experimental investigations [9–12].

Mere TDHF is nevertheless too restricted in its degrees-of-freedom if one goes beyond the regime of low-energy (collective) dynamics. For example, TDHF becomes insufficient for the description of central heavy-ion collisions in the Fermi energy domain [13]. But it is just these collisions which have unravelled a bunch of exciting phenomena, particularly from the generation of experiments using 4π multidetectors [13], and there exists up to now no theoretical tool which is definitively validated in this field [16].

Extensions of TDHF to include dynamical correlations are formally and computationally feasible [14,17,18]. But these extensions still remain restricted to the low-energy regime, where only few channels are active in the dynamics. Statistical approaches are more appropriate for higher energies and there exist attempts to complement the TDHF equation by a collision term [19,20]. This raises, however, considerable technical difficulties due to the large number of rarely occupied orbitals needed in such an approach. Moreover, such a collisionally extended TDHF is still bound to one mean path and grossly underestimates the large statistical fluctuations of the mean field.

The semiclassical variant of collisional TDHF, the Boltzmann - Uehling - Uhlenbeck (BUU) approach, has been more successful in describing average trends in medium-energy heavy ion collisions [21,22]. But it suffers also from insufficiencies, particularly when considering experiments in which fluctuations are playing a crucial role such as in the formation of Intermediate Mass Fragments (IMF’s) [13] or in the production of rare particles well below threshold [23]. The Boltzmann-Langevin equation (BLE) has thus been introduced as an extension of BUU which incorporates (possibly large) dynamical fluctuations by switching to a full ensemble description. It should allow a pertinent description of variances and widths of observables [24]. But huge computational (and even some formal) difficulties hinder up to now large scale applications of these BLE approaches.

A related theory for generating and propagating an ensemble of quantum states is Stochastic Time-Dependent Hartree-Fock (STDHF). It goes back to the basic quantal mean field dynamics and treats dynamical correlations in Markovian approximation by occasional jumps from one TDHF trajectory to another one, thus generating an ensemble of TDHF trajectories in the course of time [25].

The key issue in the STDHF scheme is an efficient selection of the jumps. Strategies have been proposed, based on the principle of maximum overlap with the corresponding correlated state and evaluated practically with linear response techniques [26,27,28]. But before attacking the problem with these elaborate (and costly)
achieved by the transformation 

\[ \int \sigma_{\text{eff}} \frac{1}{\pi} \mathrm{d} \alpha \mathrm{d} \beta \] 

where \( \sigma_{\text{eff}} \) is the effective cross section as in BUU. A spatial filtering function \( V \) is used to select the particles to be included in the collision. We need now to modify the phase profile of the single particle wavefunctions \( \varphi_\alpha(r,t) \) and \( \varphi_\beta(r,t) \) such that local average over \( V^{(i)} \) produces the new momenta \( (\vec{p}_\alpha, \vec{p}_\beta) \). This is achieved by the transformation 

\[ \varphi'_\alpha(r,t) = \exp\left(-i(\vec{p}'_\alpha - \vec{p}_\alpha) \cdot \mathbf{r} \right) \varphi_\alpha(r,t) \] 

and similarly for \( \varphi_\beta \).

As in BUU, the collision may end up in a region of phase space where particles are already present. This is measured by the overlap of the old \( |\Phi\rangle \) and new \( |\Phi'\rangle \) TDHF states. The Pauli blocking factor is the amount of still available space, which is then simply \( 1 - |\langle \Phi' | \Phi \rangle|^2 \). This blocking factor is sampled by Monte-Carlo techniques. In contrary to the classical BUU scheme we need here two more steps for a final clean-up. First, the new single particle wavefunctions \( \varphi'_\alpha \) and \( \varphi'_\beta \) are each orthogonalized on all other \( \varphi_\gamma \). And second, we need to restore the original value of the total energy because we find a slight modification of the total energy (although most of the energy matching has been accounted for by conserving the "classical" kinetic energy in the collision). This is achieved by energy rescaling with an iterative imaginary time step \( |\Phi'\rangle \rightarrow (1 - \delta h)^n |\Phi'\rangle \) where \( h \) is the actual mean field Hamiltonian and \( \delta \) a (small) shift parameter to be chosen such that total energy is recovered in a few iterations \( n \approx 4 - 5 \). This altogether accomplishes the stochastic jump of the TDHF trajectories.

The scheme can be simplified for the initial stages of a collision of two small nuclei. The single particle wavefunctions in each one of the colliding nuclei are initially well localized, such that we can skip the subdivision into test volumes and treat the collision with respect to the straightforward averages \( \bar{r}_\alpha \) and \( \bar{p}_\alpha \) of the single particle wavefunctions. This amounts to letting the space-filtering factor \( G^{(i)} \rightarrow 1 \) and the trivial renormalization factor \( \nu = (N^{(i)}_\alpha N^{(i)}_\beta)^{1/2} \rightarrow 1 \). This simplification is surely applicable for the initial stages of the collision where most of the statistical ensemble is built up and where most dissipation takes place. It may overestimate collision rates after the compound stage. But this is mostly a quantitative problem. The description will remain pertinent at least at a qualitative level.

For a first exploration, we have implemented the above scheme in its simplified version (using global averages rather than local ones) into a 3D nuclear TDHF code without any symmetry restriction. The mean field Hamiltonian is generated from a Skyrme force with a density-dependent zero-range interaction, as used in BUU studies. As a test case, we consider \( ^{16}\text{O} \) on \( ^{16}\text{O} \) collisions.

Figure 2 shows the results for a head-on collision \( ^{16}\text{O} + ^{16}\text{O} \) at 50 MeV/\( \text{u} \) beam energy. The TDHF scheme has been carried up to an ensemble of 100 trajectories. The upper panel shows the time evolution of the ensemble average momentum quadrupole moment \( Q_{20} = \langle k^2 Y_{20} \rangle \). It is known to provide a robust indicator of the dissipative phase leading to the formation of an excited compound nucleus (distinguished by a small deformation) [22,23]. A TDHF and a BUU result are also plotted for comparison. The TDHF calculation leads in this case to a perfect transparency which is reflected by...
typical mean-field oscillations of $Q_{20}$. In contrast, the STDHF calculation, as BUU, leads to the formation of a compound nucleus as can be seen from the damping of $Q_{20}$ to 0. The damping rate $\tau_c$ in STDHF, however, is somewhat larger than in BUU. This rate may be further analysed by considering the number of successful two-body collisions $n_c$ as a function of time, see lower panel of Figure 1. Two-body collisions are peaked around $t = 30 \text{ fm/c}$, which roughly corresponds to the time of maximum overlap of the two colliding nuclei. The BUU calculation provides a smaller peak value of $n_c$, but a broader peak, such that, after all, the integrated number of two-body collisions during the overlap phase is comparable to the result of STDHF.

It is interesting to note here the difference between BUU and STDHF, before overlap. While in STDHF Pauli blocking is perfectly effective, leading to exactly no two body collisions ($n_c = 0$), there remains a residual background of 2-body collisions in the BUU case, due to the approximate treatment of Pauli blocking and to the fact that the test particle sampling only provides approximate ground states, even with large numbers of test particles per nucleon. Finally, the middle panel of Figure 1 displays the variance $\sigma_{20}$ associated to the quadrupole moment $Q_{20}$, as calculated from the ensemble of computed events. Note that $\sigma_{20}$ exhibits a marked bump at the time of maximum overlap. Such a bump in variance is characteristic for a transient regime as demonstrated in BLE-based calculations [24,33].

As stressed above, a major advantage of STDHF is the fact that it provides at once an ensemble of TDHF trajectories, which contain the proper (possibly large) fluctuations of the mean-field. As a first illustration of the capabilities of STDHF, we analyze the emerging ensemble in terms of the formation of IMF’s. The IMF identification is done with a percolation-type algorithm applied to the density of matter inside the computing box, as in [34]. This analysis allows to evaluate, mass, charge, velocity,... of the IMF’s. The upper panel of Figure 2 shows the fraction $f_1$ of events leading to incomplete fusion (1 fragment) as function of time. Results from four different $^{16}\text{O}+^{16}\text{O}$ collisions at beam energies 50 and 75 MeV/u and impact parameters $b=0$ and 2 fm are shown. Just after touching ($t \sim 2 \text{ fm/c}$), $f_1$ goes to 1 which corresponds to the overlap phase. In a later stage ($t \geq 40 - 50 \text{ fm/c}$) the system evolves to either incomplete fusion ($f_1 = 1$), fission (2 IMF’s), or fragmentation (3 or more IMF’s). At 50 MeV/u, both impact parameters lead to almost 100% incomplete fusion (average mass $<A> \sim 22 \pm 1$ and charge $<Z> \sim 11 \pm 1$). Note that isospin symmetry (N=Z) is preserved here, without being enforced. At 75 MeV/u, fission and even fragmentation mechanisms take over. The detailed division into various fragments is shown for the most ”fragmenting” case in the lower panel of Figure 2. Fission seems still to dominate. But there is a sizeable amount of events with three fragments and occasionally more than that.

It should finally be noted that the computational effort involved in one STDHF event is comparable to the effort required for performing an acceptable BUU calculation. This has to be put in perspective with the differences in the physical contents of the 2 approaches (quantal versus semi-classical, full fluctuations versus average description).
FIG. 2. Time evolution of the fraction of events (100 events ensembles for each reaction) leading to incomplete fusion (upper panel) and to fission of fragmentation (lower panel) for $^{16}$O+$^{16}$O collisions with impact parameters $b = 0$ and 2 fm at 50 and 75 MeV/u beam energy.

We have presented a first application of STDHF as a propagation scheme which is capable of describing collisions and fluctuations beyond a mean-field approach by generating an ensemble of TDHF trajectories through occasional jumps. An intuitively motivated and well manageable jump algorithm was developed in close analogy to the semiclassical cousin of collisional TDHF, the BUU equation. The first results for collisions $^{16}$O+$^{16}$O are very encouraging. We see a physically reasonable damping of collective motion leading to formation of a compound nucleus. This proves that STDHF is an efficient way of sampling a collision term in the case of quantum propagation. Beyond that, STDHF generates at the same time an ensemble of trajectories with the capability of embracing large mean-field fluctuations, which corresponds to the Boltzmann-Langevin treatment in the semiclassical domain. This also allows a reliable description also of variances. The results of our test case show nicely the growth of the variance related to strong dissipation. Moreover, these results have been obtained with much less expense but more physics than needed for a comparable BLE calculation.

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