Beyond mean-field description of break-up, transfer and fusion.

D. Lacroix, M. Assié, S. Ayik, G. Hupin, J.A. Scarpaci and K. Washiyama

1GANIL, CEA and IN2P3, Boîte Postale 5027, 14076 Caen Cedex, France
2Institut de Physique Nucléaire, Université Paris-Sud-11-CNRS/IN2P3, 91406 Orsay, France
3Physics Department, Tennessee Technological University, Cookeville, Tennessee 38505, USA.

Abstract

Microscopic theories beyond mean-field are developed to include pairing, in-medium nucleon-nucleon collisions as well as effects of initial fluctuations of one-body observables on nuclear dynamics. These theories are applied to nuclear reactions. The role of pairing on nuclear break-up is discussed. By including the effect of zero point motion of collective variables through a stochastic mean-field theory, not only average evolution of one-body observables are properly described but also fluctuations. Diffusion coefficients in fusion as well as mass distributions in transfer reactions are estimated.

1 Introduction

Time-Dependent Energy Density Functional (TD-EDF) provides a suitable microscopic framework to treat both nuclear structure and reactions along the nuclear chart [1,2]. In most of current applications, an effective interaction (of Skyrme or Gogny type) is introduced to provide an energy functional, denoted $\mathcal{E}(\rho)$, where $\rho$ is the one-body density matrix. Then, guided by the Hamiltonian case, equations of motion are written in terms of the one-body density evolution

$$i\hbar \frac{\partial}{\partial t} \rho = [h[\rho], \rho],$$

where $h[\rho] \equiv \partial \mathcal{E}(\rho) / \partial \rho$ denotes the mean-field Hamiltonian. Although this approach is traditionally called Time-Dependent Hartree-Fock (TDHF), it should not be confused with TDHF derived from a two-body Hamiltonian. At least because of the parameters of the effective vertex are directly adjusted to experimental observations, EDF incorporates much more correlations than a pure Hartree-Fock theory. TD-EDF has been improved significantly in the past decades and could now be applied without assuming specific symmetries in space and includes all terms of the effective interactions used in the static EDF [1].

Starting from a pure independent particle state, the one-body evolution described by Eq. (1) can be replaced by the evolution of a single Slater determinant. As a

\footnote{This is due to the fact that $\rho^2 - \rho$ is preserved along the mean-field trajectory.}
consequence it misses important physical effects which are accounted for in “state of the art” EDF dedicated to nuclear structure. These effects are (i) Pairing correlations usually treated by considering quasi-particles trial states instead of Slater determinants. (ii) Fluctuations of one-body observables and correlations induced by restoration of broken symmetries which are generally incorporated using configuration mixing methods, leading to the so-called Multi-Reference EDF (MR-EDF) [3-5]. Due to the numerical effort, Time-Dependent Energy Density Functional devoted to nuclear dynamics generally neglects these correlations and fails to account for the richness of phenomena taking place in nuclear dynamics [6]. Recently, we have developed two transport theories dedicated to effect (i) and (ii) respectively. Highlights and applications of these new approaches are given below.

2 Time-Dependent EDF with pairing correlations

Guided by the Hamiltonian case, different extensions of mean-field theory have been proposed starting from a generalization of the one-body density equation of motion:

\[
\frac{i\hbar}{\partial \rho}{\partial t} = [h[\rho], \rho] + \frac{1}{2} \text{Tr}_2[\tilde{v}_{12}^c, C_{12}],
\]

where \( \tilde{v}_{12}^c \) denotes the anti-symmetric effective vertex in the correlation channel. \( \text{Tr}_2(.) \) is the partial trace on the second particle while \( C_{12} = \rho_{12} - \rho_1 \rho_2 (1 - A_{12}) \) denotes the two-body correlation matrix defined from the two-body density \( \rho_{12} \). Here, indices refer to the particle on which the operator is applied while \( A_{12} \) is the permutation operator. Eq. (2) should be complemented by the equation of motion for the two-body correlation. It is written here as

\[
\frac{i\hbar}{\partial \rho}{\partial t} = [h_1[\rho] + h_2[\rho], C_{12}]
+ (1 - \rho_1)(1 - \rho_2)\tilde{v}_{12}^c \rho_1 \rho_2 - \rho_1 \rho_2 \tilde{v}_{12}^c (1 - \rho_1) (1 - \rho_2) \Rightarrow B_{12}
+ (1 - \rho_1 - \rho_2)\tilde{v}_{12}^c C_{12} - C_{12} \tilde{v}_{12}^c (1 - \rho_1 - \rho_2). \Rightarrow P_{12}
+ \text{Higher orders.}
\]

(3)

\( B_{12} \) and \( P_{12} \) contain correlations associated to in-medium nucleon-nucleon collisions and pairing respectively. Higher-order terms (not shown here) contain in particular three-, four-... body effects. When correlations between more than two particles are neglected, the resulting theory is known as the Time-Dependent Density-Matrix (TDDM) (see for instance [7]). Even in that case, prohibitory numerical efforts are needed due to the explicit treatment of two-body matrices. Guided by the BCS approximation, we recently proposed to reduce the complexity by assuming that components of \( \tilde{v}_{12}^c \) and \( C_{12} \) are non-zero only between pairs of time-reversed states. This approximation, called hereafter TDDMP, leads to important simplifications: (a) the number of correlation matrix elements to be calculated is significantly reduced, and (b) \( H_{12} \) cancels out and only \( B_{12} \) and \( P_{12} \) contribute to the correlation
evolution. The TDDM$^P$ theory has been recently applied to the nuclear break-up of

correlated systems. Figure 1 illustrates the evolution of the one-body density in a
$^{16}$O as a $^{208}$Pb collision partner passes by. The perturbation by the external nuclear
passing potential induces an emission to the continuum. The one nucleon emission
has been extensively studied in ref. [9]. With the TDDM$^P$ theory, one can extend
the study of one nucleon case to the two nucleons emission for initially correlated
nucleons. In left side of figure 1, the relative angle between two nucleons emitted
in coincidence has been extracted for initially correlated or anti-correlated systems.
As expected intuitively [8,10], in the former case small relative angles are obtained
while larger relative angles are seen in the latter case. Our study clearly points out
that coincidence measurements using nuclear break-up can be used as a tool to infer
correlation properties inside nuclei.

3 Proper treatment of one-body observables fluctuations

Besides the absence of pairing correlation discussed in previous section, mean-field
transport theory given by Eq. 1 provides a good description of mean values of one-
body observables in low energy reactions. However, it completely fails to describe fluctuations of one-body observables. This can directly be traced back to the use of a single Slater determinant as a building block. Indeed, as it is well known in the static case, the independent particle picture is unable to describe properly the zero point motion in collective space pleading for multi-reference approaches where several Slater determinants (or quasi-particle states) are considered simultaneously. During the past decades, large efforts have been devoted to develop transport theories that are able to describe not only mean-values but also fluctuations (for a review see [6,11]). However, even 30 years after the first application of TD-EDF, no practical solution simple enough to be applied to many different physical phenomena has been really proposed so far. Recently, we have shown that the theory introduced in ref. [12] and based on stochastic initial values in one-body space might provide such a solution. The underlying principle is the following:

Imagine a correlated system, and some one-body observable $Q$ with mean-value $\langle Q \rangle$ and fluctuation $\sigma_Q = \langle Q^2 \rangle - \langle Q \rangle^2$. A single Slater determinant (SD) that minimizes the EDF is generally able to reproduce the mean-value but strongly underestimates fluctuations, i.e. $\sigma_{Q,SD}^2 \ll \sigma_Q$, where $\sigma_{Q,SD}^2$ denotes the Slater determinant expectation value. If instead, a statistical ensemble of Slater determinants is used. Each SD leads to a quantum expectation value $\bar{\sigma}_\lambda^2$, where $\lambda$ labels the SD under interest. One can then optimize the statistical ensemble in such a way that $\bar{\sigma}_\lambda^2 \simeq \sigma_Q$ where $\bar{\langle X \rangle}$ denotes the statistical average over quantum expectation values. The statistical assumption described above provides a practical solution to mimic initial zero point motion in collective space. Then, the system evolution is performed by evolving each SD independently from the others, therefore neglecting interference between different trajectories. This approach, that can be regarded as the first step towards multi-reference TD-EDF, has been shown (i) to incorporates the one-body dissipation and associated fluctuation mechanism in accordance with the quantal dissipation-fluctuation relation, (ii) to give dispersion of one-body observables that is identical to a previous formula derived from the Balian-Vénéroni variational principle [13,14].

In practice, initial fluctuations are simulated by an ensemble of initial single-particle density matrices, each of them associated to a single SD [12]:

$$\rho^\lambda(\mathbf{r}, \mathbf{r}', t_0) = \sum_{ij} \Phi_i^*(\mathbf{r}, t_0) \rho_{ij}^\lambda \Phi_j(\mathbf{r}', t_0),$$

(4)

where summation $i$ and $j$ is made over a complete set of single-particle states $\Phi_i(\mathbf{r}, t_0)$, and $i$ implicitly contains spin and isospin quantum numbers. Components of density matrices, $\rho_{ij}^\lambda$ are time-independent random Gaussian numbers with mean value $\bar{\rho}_{ij}^\lambda = \delta_{ij} n_i$ and a variance of the fluctuating part $\delta \rho_{ij}^\lambda$ is specified by,

$$\overline{\delta \rho_{ij}^\lambda \delta \rho_{j'i'}^\lambda} = \frac{1}{2} \delta_{jj'} \delta_{ii'} [n_i(1 - n_j) + n_j(1 - n_i)].$$

(5)
The great advantage of the Stochastic Mean-Field (SMF) theory is that each Slater determinant $\lambda$ evolves independently from each other following the time evolution of its single-particle wave-functions in its self-consistent mean-field Hamiltonian, denoted by $h(\rho^\lambda)$, according to

$$ih\frac{\partial}{\partial t}\Phi_i(\mathbf{r}, t; \lambda) = h(\rho^\lambda)\Phi_i(\mathbf{r}, t; \lambda).$$

(6)

with the boundary condition $\Phi_i(\mathbf{r}, t; \lambda) = \Phi_i(\mathbf{r}, t_0)$. Time evolution of mean-values and dispersion then express as

$$Q(t) = \sum_{ij} \langle \Phi_i(t; \lambda) | Q | \Phi_j(t; \lambda) \rangle \rho_{ij}^\lambda \equiv Q^\lambda(t), \quad \sigma_Q = (Q^\lambda(t) - Q(t))^2,$$

(7)

where the average is made over initial conditions.

### 3.1 Application to fusion and transfer reactions

The powerfulness and applicability of the SMF have been recently illustrated in fusion reactions by extending the work of ref. [15,16]. Using a macroscopic reduction of the stochastic mean-field evolution, central collisions leading to fusion have been mapped to a one-dimensional macroscopic Langevin evolution on the relative distance $\dot{R}$ between the two nuclei given by [17]:

$$\dot{P}^\lambda = -\partial_R U(R^\lambda) - \gamma(R^\lambda)\dot{R}^\lambda + \xi^\lambda_P(t).$$

(8)

$U(R^\lambda)$ and $\gamma(R^\lambda)$ denote the nuclear+coulomb potential and dissipation associated to one-body friction respectively and are already present at the mean-field level [15,16]. $\xi^\lambda_P(t)$ is a Gaussian random force acting on the relative motion reflecting stochasticity in the initial value. This fluctuating part leads to diffusion in collective space which can be approximated by $\xi^\lambda_P(t)\xi^\lambda_P(t') \simeq 2\delta(t - t')D_{PP}(R)$ where $D_{PP}(R)$ denotes the momentum diffusion coefficient. The latter term is nothing but the one that is missing in the original theory and is of primer importance to properly describe observables fluctuations. An example of reduced friction $\beta(R) \equiv \gamma(R)/\mu(R)$ and diffusion coefficients $D_{PP}(R)$ estimated from the macroscopic reduction of SMF is given in figure 2 for the head-on $^{40}$Ca+$^{40}$Ca collision.

The possibility to estimate transport coefficients associated to fluctuation and dissipation from a fully microscopic quantum transport theory is a major breakthrough. However, to be really convincing, one should in addition prove that the increase of fluctuations is consistent with experimental observations. To prove that SMF can be a predictive framework, we have recently considered transfer reactions [18]. Fragment mass distributions deduced from Heavy-Ion reactions have been extensively studied. It is seen that the dispersion in mass scales approximately with the average number of exchanged nucleons. While mean-field properly describes the latter, it
miserably fails to account for the dispersion. This phenomena is rather well understood in macroscopic models but has not been yet reproduced microscopically. To address this issue, we have considered head-on collisions below the Coulomb barrier. In that case, nuclei approach, exchange some nucleons and then re-separate. Similarly to the relative distance case, a macroscopic reduction onto the projectile (resp. target) mass, denoted by $A_P^\lambda$ (resp. $A_T^\lambda$) can be made leading to:

$$\frac{d}{dt} A^\lambda_P = v(A^\lambda_P, t) + \xi^\lambda_A(t),$$  \hspace{1cm} (9)

where $v(A^\lambda_P, t)$ denotes the drift coefficient for nucleons transfer. Again, the fluctuating term $\xi_A^\lambda(t)$ is linked to the diffusion in mass through $\xi^\lambda_A(t)\xi^\lambda_A(t') = 2\delta(t-t')D_{AA}$. Mass dispersion can then directly be estimated using:

$$\sigma_{AA}^2(t) \simeq 2 \int_0^t D_{AA}(s) ds. \hspace{1cm} (10)$$

An illustration of $\sigma_{AA}^2(t)$ for $^{40}\text{Ca}+^{40}\text{Ca}$ reactions is given in Fig. 3.1 and compared to the number of exchanged nucleons, denoted by $N_{ex}$. In all cases, both quantities are very close from each other and lead to much higher dispersion than the original mean-field. Indeed, the estimated asymptotic values in the latter case are 0.004, 0.008 and 0.008 from low to high energy and are much less than the final number of exchanged nucleons that are equal to 0.43, 1.44 and 3.63 respectively. On opposite, the predicted asymptotic mass dispersions are equal to 0.73, 1.72 and 3.79 and is much closer to $N_{ex}$ (see also figure 3.1). This numerical test provides a strong support for the validity of the stochastic mean-field approach.

Figure 2: (Color online) Evolution of reduced friction (left) and diffusion coefficient (right) as a function of the relative distance for the head-on $^{40}\text{Ca}+^{40}\text{Ca}$ collision at center of mass energy $E_{\text{c.m.}} = 100$ MeV.
Figure 3: (Color online) Evolution of $\sigma_{AA}^2$ calculated in SMF approach for $^{40}\text{Ca} + ^{40}\text{Ca}$ (top) at different center of mass energies. Number of exchanged particles is superimposed by the filled-circles, filled-squares, and filled-triangles from high to low energies. (Adapted from [?])

4 Summary

Two different approaches have been presented that include correlations beyond mean-field. These approaches differ in the strategy and in the types of correlation that are included. The TDDM$^P$ formalism is appropriate to account for pairing effects in a reasonable numerical time. An illustration on break-up reactions clearly points out the importance of such correlations in nuclear reactions. The SMF theory with initial random conditions can be seen as the first step towards the inclusion of collective variables zero point motion. Applications to fusion and transfer reactions could be of particular interest to treat fluctuations around an average mean-field path.

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