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Orthogonal wave function dynamics in heavy-ion collisions

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Summary. — A rich variety of phenomena characterises dissipative heavy-ion collisions, ranging from equilibration processes to the disintegration into fragments and nuclear clusters. The description of such a complex behaviour requires to track at the same time the evolution of the nuclear mean field and the effect of nucleonic degrees of freedom. We illustrate a solution to combine these two aspects within a unique theoretical framework, starting from the time-dependent Hartree-Fock scheme and by introducing a dynamical basis of orthogonal fermionic wave functions.

1. – Introduction

Several ongoing and planned experiments explore the properties of the nuclear interaction in combination with the dynamics of heavy-ion collisions [1]. To describe a broad range of energy regimes, from low (a few MeV per nucleon) to Fermi and intermediate energies (a few hundred MeV per nucleon), microscopic models should handle a large variety of mechanisms, resulting from the combination of the collective behaviour of the mean-field potential and the effect of nucleonic degrees of freedom. Even though several approaches have been developed [2, 3], they all rely on very similar approximations. In particular, crude approximations on the quantum character of nucleonic wave functions are imposed. In the following, we start by presenting the connection and the usual approximations which link the present transport approaches for heavy-ion collisions. We then illustrate how a dynamical basis of orthogonal fermionic wave functions could dismiss a number of usual approximations and, at the same time, allow to combine the nuclear mean-field description and the effect of nucleonic degrees of freedom.

2. – Current scheme of transport models and usual approximations

As sketched in fig. 1, current transport models for heavy-ion collisions are typically presented in a layout ordered in two groups, mean-field and molecular-dynamics approaches. Yet, such arrangement reflects the use of a scheme of approximations which, as discussed thereafter, could be revisited.

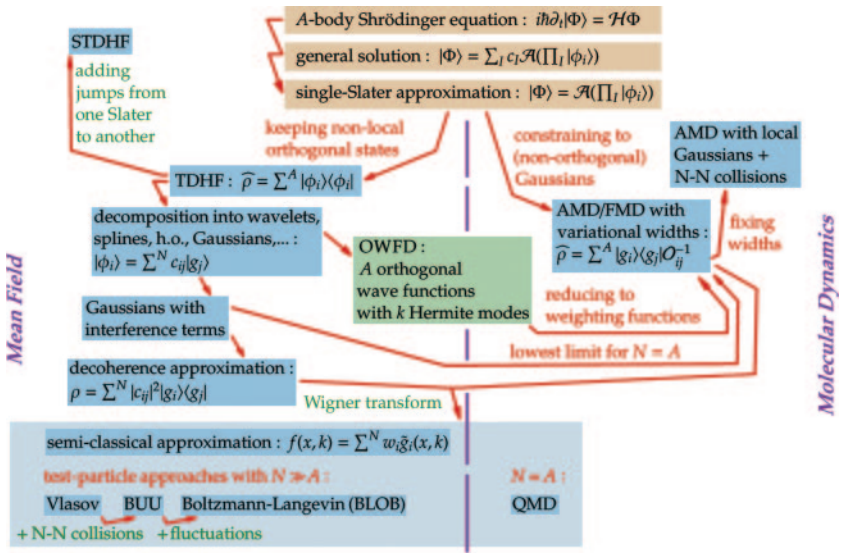

Fig. 1. – Scheme of transport approaches with their connections and approximations. See text.

Mean-field models can be seen as extensions or reductions of the time-dependent Hartree-Fock (TDHF) theory [4]. A characteristic property of TDHF is that, when wave functions are constructed from an orthogonal basis, orthogonality persists all the way throughout the evolution of the system [5]. Within this picture, a level scheme could be handled in relation with nuclear-structure features. An usual reduction is the Wigner transform from TDHF to its semiclassical counterpart, the Vlasov equation [6], which favours efficient numerical implementations, like the test-particle method [7]. Although wave function features are lost, the semiclassical counterpart of mean-field models has the advantage of preserving a reliable description of bulk properties and collective motion. It is also the avenue to phase-space–based semiclassical approaches and Fermi-liquid theories [8]. Common extensions can be elaborated by taking into account correlations beyond mean field in terms of the BBGKY hierarchy [9,10]. In the TDHF framework for heavy-ion collisions, extensions are introduced to describe quantum fluctuations and explore a wider landscape of mean-field trajectories [11, 12]. In the semiclassical framework, proceeding from the Vlasov equation, extensions towards and beyond the Boltzmann equation introduce two-body dissipation through a nucleon-nucleon collision term [13], or fluctuations through stochastic jumps related to nucleonic degrees of freedom [14,15], or clustering through three-body collision terms [16,17], also related to nucleonic degrees of freedom. Like any mean-field theory, Boltzmann approaches lack nucleon-nucleon correlations, even if single test particles used in the integration procedure are localised and can be used to introduce an average contribution corresponding to two-body nucleon-nucleon collisions. In order to introduce the effect of nucleon-nucleon correlations in such approaches, a possible strategy is to continuously analyse phase space and redefine effective nucleonic correlation contributions iteratively, at each time step of the mean-field evolution, leading to exploitable solutions of the Boltzmann-Langevin equation [10,15].

Molecular-dynamics, in antisymmetrized form (AMD and FMD), could be obtained from TDHF by reducing the wave function basis to Gaussians and by fixing as many wave functions as the nucleons present in the system [18-20]. Since Gaussian functions

do not constitute an orthogonal set, antisymmetrization cannot be disregarded. To introduce localisation properties, the variance of Gaussian functions is constrained to a fixed value. A notable advantage of molecular dynamics is the inherent persistence of nucleonic correlations, which can be used as a foothold to implement nuclen-nuclen collisions in a BUU-like scheme and introduce two-body dissipation, clustering and large-amplitude fluctuations. Still, this advantage comes with the drawback of a simplified mean-field representations, due to the schematic wave function description.

In this survey outlined in fig. 1, starting from the general solution of the A-body Schrödinger equation, we have been going through several approximations such as reducing to a single-Slater, imposing decoherence to avoid non-local effects, operating a Wigner transform to replace quantum operators by phase space, limiting to a simple-basis decomposition (Gaussians) with the drawback of losing orthogonality, or freezing the variance of wave functions to further reduce non-local effects.

3. – Dropping usual approximations, early attempts

On the borderline between TDHF and semiclassical theories, an early attempt to construct a richer mean-field description for heavy-ion collisions was proposed in the form of the Dywan model [21], where the system was sampled by an orthogonal set of weighted wavelets. In a first numerical realisation, however, the wavelet basis was replaced by a (non-orthogonal) Gaussian basis $|g_j\rangle$, so that each nucleonic wave function ϕ_i was represented by several Gaussian functions of different amplitude, initially fitted to the Hartree-Fock states [22, 23], leading to the decomposition

$$|\phi_i\rangle = \sum^{N} c_{ij}|g_j\rangle. \tag{1}$$

In order to introduce a BUU-like collision term in phase-space through a master equation, a decoherence approximation followed by a Wigner transform was applied. This realisation resulted essentially into a semiclassical approach (see bottom box in fig. 1), similar to BUU, with the difference that the full phase-space density distribution was represented by a sum of Gaussian functions with variable width in phase space rather then a sum of test particles (*i.e.*, delta functions or functions with fixed width and weight).

In a second numerical realisation, both the decoherence approximation and the Wigner transform were dismissed. Several Gaussian functions per nucleon where used again to sample the density distribution with the difference that, in this new framework ("Gaussians with interference terms" in fig. 1), they could interfere constructively and destructively by introducing a time-dependent complex amplitude [24, 25]. In particular, the coefficient c_{ij} in eq. (1) could have negative sign and the Gaussian function, with variational position $\vec{r}_j$ ($\vec{k}_j$) and width $\vec{\chi}_j$ ($\vec{\phi}_j$) in configuration (momentum) space, was

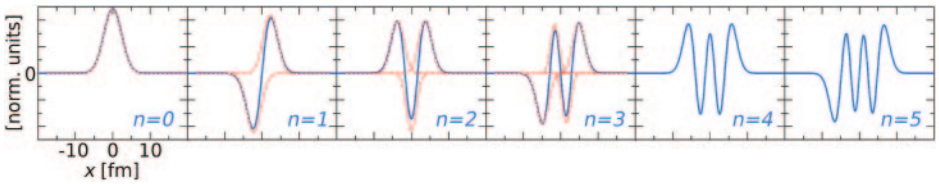

Fig. 2. – Harmonic oscillator states (blue) and decomposition into a superposition of Gaussian base functions (dashed red, up to $n = 3$).

parameterised as

$$
\begin{aligned}
g_j(\vec{r}) &= g_{x_j}(x) g_{y_j}(y) g_{z_j}(z); \\
g_{x_j}(x) &= \left(\frac{1}{2\pi\chi_j}\right)^{1/4} \exp\left(-\xi_j \frac{(x-x_j)^2}{2} + ik_j(x-x_j)\right),
\end{aligned}
\tag{2}
$$

where $\xi_j = \frac{1}{2\chi_j} - 2i\gamma_j$, $\gamma_j = \frac{\sigma_j}{2\chi_{x_j}}$, $\chi_j\phi_j - \sigma_j^2 = \frac{1}{4}$. In fig. 2 some harmonic-oscillator states are decomposed into a superposition of Gaussian functions with adapted width and amplitude.

On the one hand, this approach is closer to TDHF and handles delocalization while, on the other hand, if the number of Gaussian functions is reduced to equal the number of nucleons in the system, it recalls molecular dynamics with variational widths (FMD [18]). The difficulty of treating overlaps among several Gaussian functions is a mayor issue in the numerical implementation, especially when an effective nucleon-nucleon collision term has to be defined. Although some quantum features could be recovered, this model ranks among the mean-field approaches and lacks nucleonic degrees of freedom.

4. – Orthogonal wave function dynamics: concept and examples

With the purpose of mantaining Hartree-Fock states throughout the time evolution and introducing effective nucleonic degrees of freedom, a newer formalism was worked out [26]. Departing from early attempts, the Gaussian scheme was dismissed in favour of a set of Hermite polynomials. In this implementation, while the number of nucleonic wave functions equals the number of nucleons A in the system, each nucleonic wave function is parameterised as a sum of Hermite polynomials sharing the same centroid:

$$
\varphi_j = g_j(\vec{r}) \cdot \sum_I \frac{C_I}{C_{\mathrm{norm}}} H_I\Big(\frac{x-x_j}{\sqrt{(2\chi_{x_j})}}, \frac{y-y_j}{\sqrt{(2\chi_{y_j})}}, \frac{z-z_j}{\sqrt{(2\chi_{z_j})}}\Big),
\tag{3}
$$

where g_j is the Gaussian function defined in eq. (2), here used as a weighting function, C_I weights the Hermite modes, C_{norm} ensures normalisation, and the superindex I accounts for all possible configurations of Hermite modes that could be accommodated up to a given maximum level N_{max}. While a given wave function propagates, all the corresponding Hermite modes explore different evolutions while keeping orthogonality with the rest of the system. As shown in fig. 1, the orthogonal wave function dynamics (OWFD) approach could be considered intermediate between the mean-field and the molecular-dynamics branches.

Since the purpose is to address heavy-ion collisions up to Fermi and intermediate energies, in addition to the mean-field evolution $[h, \rho]$, the model should also handle a dissipative contribution $I_{\mathrm{coll.fluct.}}(\rho)$ related to particle emission, two-body dissipation, and the associated large-amplitude fluctuations, so that the density evolves as $i\hbar\dot{\rho} = [h, \rho] + I_{\mathrm{coll.fluct.}}(\rho)$. In particular, an excited wave function feeds higher Hermite modes which are the most delocalized so that, while progressively loosing binding, its variance expands faster than the width evolution of the corresponding nuclear potential. Such behaviour may affect only one or few distinct wave functions, typically the most external ones. As in TDHF, excited wave functions tend to carry on expanding around their source, even when they are favoured candidates to reach separation from the system. In this case, an emission probability is estimated from overlap conditions and

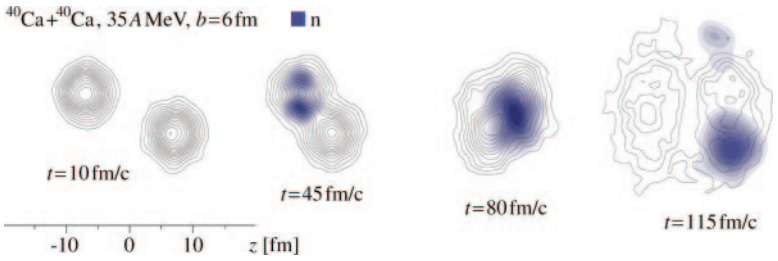

Fig. 3. – Simulation of the system $^{40}\mathrm{Ca} + {}^{40}\mathrm{Ca}$ at 35 AMeV and $b = 6$ fm at different times (the nuclei are spaced of 20 fm at $t = 0$). The contribution of one single wave function (one neutron, blue shades) is shown on top of the density distribution of the full system (contour lines).

treated as a random effective emission term. The emission is achieved by redefining the properties of the escaping wave function together with the surrounding ones, by means of a re-orthogonalisation technique and by imposing conservation laws. Within the inherent TDHF scheme, the two-body nucleon-nucleon collision contribution is conceptually problematic because no decoherence approximation has been applied and because one-body density is not sufficient to build up nucleon-nucleon correlations. Thus, both the collision probability and the scattering geometry of colliding wave functions are obtained from schematic classical concepts similar to the BLOB approach [10, 15], with the difference that in the present model the nucleonic wave functions can be tracked (even if delocalised) and they should not be reconstructed at each time step. The collision rate is evaluated from the mean-free path, calculated from collapsing the two wave functions to phase-space points randomly chosen from the corresponding density distribution. The occupancy criterion used to satisfy the Pauli principle in the Uheling-Uhlenbeck treatment, is replaced by an orthogonality criterion, *i.e.*, the existence of an orthogonal solution for the scattered states which also respects all conservation conditions. The final states are assigned to the scattered wave functions after re-evaluating widths, amplitudes and number of the corresponding Hermite modes.

After introducing a Skyrme parameterisation as in ref. [23] (Skt5), we performed a few instructive simulations. The system $^{40}\mathrm{Ca} + {}^{40}\mathrm{Ca}$ at 35 AMeV and $b = 6$ fm is studied in fig. 3. The evolution of one single nucleonic wave function toward an excited state is tracked: its wide and complex shape manifests the contribution of high-number Hermite modes.

In fig. 4 the system $^{16}\mathrm{O} + {}^{20}\mathrm{Ne}$ at 25 AMeV and $b = 1$ fm exhibits a typical dissipative behaviour, where some nucleons are exchanged between the projectile and the target nuclei and a cluster is formed and separates from the system as a third nucleus. It may be noted that, differently from a typical mean-field approach, each nucleonic wave function selects one single nucleus, without splitting between projectile, target and fragment nuclei. For the same system, fig. 5 shows the evolution of the average widths $\bar{\chi}$ and $\bar{\phi}$ of the weighting function g_j of each nucleonic wave function and the corresponding relation, which reflects the Heisenberg uncertainty principle. Jumps in the trajectories correspond to nucleon-nucleon collisions followed by level rearrangement, while trajectories moving away from the bunch signal emission processes and splits.

5. – Conclusions

While we can still progress in further refining semiclassical approaches, ranked among either mean-field or molecular-dynamics models, a suggestive alternative is to move back

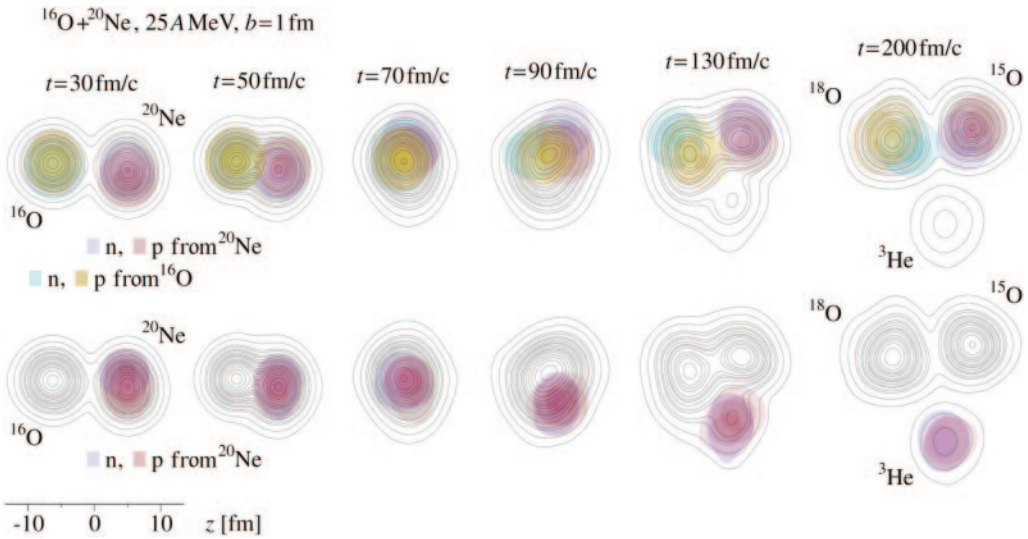

Fig. 4. – Simulation of the system ^{16}O + ^{20}Ne at 25 AMeV and $b = 1$ fm at different times (the nuclei are spaced of 20 fm at $t = 0$). On top of the density distribution of the full system (contour lines), the contributions of seven wave functions which are exchanged between the target and the projectile are shown in the upper sequence (colour shades, two protons and two neutrons transferred from the initial ^{16}O to the final ^{18}O; two protons and one neutron transferred from the initial ^{20}Ne to the final ^{15}O). The lower sequence displays the contributions of three wave functions which separate into a ^{3}He cluster (colour shades).

in the sequence of approximations. As discussed, a set of orthogonal wave functions, each one composed of several modes, allows to preserve some quantum features, like non-locality, and to achieve a more general scheme where both mean-field and molecular-dynamics features are inherent in the model.

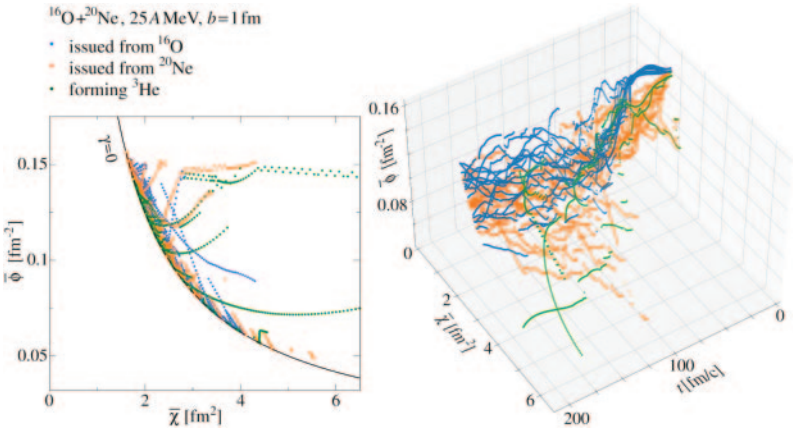

Fig. 5. – Evolution of the average width of the weighting function of each wave function in the system ^{16}O+^{20}Ne at 25 AMeV and $b = 1$ fm. Left panel: $\bar{\chi}$ *vs.* $\bar{\phi}$ projection compared to the condition $\chi\phi - \sigma = 1/4$, for $\gamma = \sigma/(2\chi) = 0$. Right panel: $\bar{\chi}$ *vs.* $\bar{\phi}$ relation as a function of time. The trajectories track the wave functions initially belonging to ^{16}O and ^{20}Ne (blue and orange, respectively) or the wave functions which separate into a ^{3}He cluster (green). See text.

In a simulation of dissipative nuclear collisions, we could track how nucleonic wave functions rearrange in the system. Some wave functions are exchanged between the projectile and target nuclei, while few others can even leave the system to form a separate nucleus.

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