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Extensions of mean-field descriptions in dynamical processes of nucleonic degrees of freedom

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Summary. — We propose new theoretical approaches in order to introduce fluctuations in an Extended-TDHF description. On the one side, a prescription for estimating the dispersions in one-body observables related to small amplitude fluctuations of the statistical kind is proposed. On the other side, the characterization of large amplitude density fluctuations generated by multiparticle correlations is addressed through a stochastic extension yielding Langevin-type fluctuations. Applications to nuclear collisions at incident energies around the Fermi energy are presented.

1. – Motivation

The relevance of the contribution to nuclear physics of dynamical mean-field theories is well established. These models have been successful namely in the description of collective behavior in nuclei and in heavy-ion collisions (HIC) at low energies (less than 10 MeV/n). At higher energies this approximation turned to be insufficient to correctly describe the dissipative processes experimentally observed. Then extensions have been developed aiming at incorporating, at least partially, those residual interactions neglected in pure mean field descriptions. Semi-classical or quantal models have been advanced, by incorporating a Boltzmannian (or Uehling-Uhlenbeck) collision term. These models described efficiently the dissipative and irreversible evolution of nuclear systems toward equilibrium.

Nevertheless, these approaches also attained their limits when they failed to describe the dispersions of measured observables and the occurrence new phenomena evidenced in increasingly more accurate experimental investigations. Among these phenomena, intermediate mass fragment production, multifragmentation and vaporization are found.

The search of a convenient description of those processes has been a challenge for nuclear many body theories for many years but complex dissipative processes, where

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thresholds are present and where different types of instabilities compete, are still difficult to describe within a unified picture.

The purpose of this work is to contribute to this problematics proposing a new approach based on a model belonging to the class of extended mean field theories, the so-called Extended Time Dependent Hartree-Fock model (E-TDHF), which has been conditioned to generate the required fluctuation phenomenology.

2. – Extended Time Dependent Hartree-Fock description

The starting point is the quantal Boltzmann-like equation of motion for the one-body density matrix [1]:

(1*a*)
$$i\hbar\dot{\rho} = [\mathbf{h}, \rho] + i\mathcal{K}(\rho),$$

(1b) with
$$\mathbf{h} = \frac{\mathbf{p}^2}{2m} + \mathbf{V}^{HF}(\rho),$$

where $V^{HF} = Tr_2\{\mathbf{V}^A(1,2)\rho(2)\}$ is the self-consistent mean field. In this work we have implemented the so-called SKT5 force [2], which is an interaction of the Skyrme type:

$$V_{q}^{HF} = \frac{3}{4}t_{0}\rho + \frac{(\sigma+2)}{16}t_{3}\rho^{\sigma+1} - \frac{\sigma t_{3}}{24}\left(x_{3} + \frac{1}{2}\right)\rho^{\sigma-1}\xi^{2} - \tau_{(p,n)}\frac{t_{3}}{12}\left(x_{3} + \frac{1}{2}\right)\rho^{\sigma}\xi$$
$$- \tau_{(p,n)}\frac{1}{2}t_{0}\left(x_{0} + \frac{1}{2}\right)\xi - \frac{1}{8}\left[\frac{9}{4}t_{1} - t_{2}\left(x_{2} + \frac{5}{4}\right)\right]\Delta\rho$$
$$(2) \qquad + \tau_{(p,n)}\frac{1}{16}\left[3t_{1}\left(x_{1} + \frac{1}{2}\right) + t_{2}\left(x_{2} + \frac{1}{2}\right)\right]\Delta\xi.$$

The nuclear matter coefficients corresponding to (2) are listed in table I.

The \mathcal{K} term is the collision kernel, consisting in a master equation for the populations [1]:

(3)
$$\mathcal{K}_{\alpha}(\rho) = \sum_{\beta,\gamma,\delta} W_{\alpha\beta\gamma\delta}[\rho_{\gamma}\rho_{\delta}(1-\rho_{\alpha})(1-\rho_{\beta}) - \rho_{\alpha}\rho_{\beta}(1-\rho_{\gamma})(1-\rho_{\delta})],$$

where the terms $W_{\alpha\beta\gamma\delta}$ are transition probabilities usually obtained in the weakinteraction and Markovian limits. They go as the square of the two-body interaction and the matrix elements of the latter are modelized in terms of nucleon-nucleon cross-section σ_{nn} . In all calculations σ_{nn} is energy and isospin dependent, without any in-medium corrections. Equation (1*a*) is solved by expanding single particle wave functions and the one-body density matrix in a time-dependent coherent states (CS) basis $|\alpha_i^{\lambda}\rangle(t)$:

(4)
$$|\varphi_{\lambda}\rangle(t) = \sum_{i}^{m_{\lambda}} c_{i}^{\lambda} |\alpha_{i}^{\lambda}\rangle(t),$$

TABLE I. – Infinite nuclear matter properties.

$\overline{K_0 \ ({ m MeV})}$	K_{sym} (MeV)	$J \ ({ m MeV})$	$L \ (MeV)$
201.69	-24.76	36.30	96.52

where m_{λ} is the number of CS per single-particle (SP) level and does not need to be the same for all levels, and where the coefficients c_i^{λ} are constant and fixed at t = 0. The evolution of the moving basis is given through the equations of motion of the corresponding α 's parameters, *i.e.*, centroids and widths [1]. This description provides all the available information about the (irreversible) mean behavior of the system.

3. – Untangling fluctuations in E-TDHF approximations

In order to describe the dispersion of observables around their mean values we searched a prescription to untangle fluctuations around the average density from our E-TDHF description. It can be postulated that statistical fluctuations are generated by a manifold of microscopic configurations each one described by a convenient many-body state. A unique Slater determinant (SD) cannot be a solution of the many-body problem, the description must allow the possibility for the system to perform transitions from one SD to another as a result of nucleon interactions. For this reason instead of associating the one-body density matrix to a single SD, we can associate it to a set of SD $|\Psi_k\rangle$, all compatible with the initial conditions [3].

(5)
$$|\Psi\rangle = \sum_{k} a_k(t) |\Psi_k\rangle \text{ with } |\Psi_k\rangle = \mathcal{A} |\varphi_{\lambda_1}\rangle |\varphi_{\lambda_2}\rangle ... |\varphi_{\lambda_N}\rangle,$$

where \mathcal{A} is an antisymetrization operator. The evolution of the coefficients $a_k(t)$ can formally be extracted from the Schrödinger equation and then density matrices, from the *N*-body one $\rho^{(N)}$ to all reduced density matrices, can be obtained. In practical grounds, due to the use of finite sets of SD and to the lack of information about the initial state, this description turns to be anyways incomplete and the idea of solving the equations of motion for the coefficients a(t) must be abandoned.

A statistical point of view may then be adopted proposing that at any time the state of the system is a statistical admixture of SD $\{\Psi_k\}$ with probabilities $\{p_k\}$. These SD actually evolve in a modified mean field, different from a pure mean field since it has been updated as a consequence of residual interactions. In this way the most general (or least biased) solution to the N-body problem compatible with the one and two-body information contained in the E-TDHF description is an incoherent superposition of the corresponding single particle SD:

(6)
$$\rho^{(N)} = \sum_{k} p_k \{ |\Psi_k\rangle \langle \Psi_k | \}.$$

One-particle states are spanned in a time-dependent CS basis and after some mathematical handling it is possible to write the N-body density matrix in terms of CS slater determinants (CSSD):

(7)
$$\rho^{(N)} \sim \sum_{I} \omega_{I} |\Pi_{I}\rangle \langle \Pi_{I}| \quad \text{with} \quad |\Pi_{q}^{(k)}\rangle = \mathcal{A} |\alpha_{i_{1}}\alpha_{i_{2}}...\alpha_{i_{N}}\rangle,$$

where a supplementary decoherence assumption of vanishing non-diagonal contributions has been made.

With the purpose of illustrating this procedure the, ⁵⁸Ni+⁵⁸Ni reaction at 50 MeV/n incident energy and b = 3 fm impact parameter has been considered. The isotropy ratio $R_E = \langle E_{\perp} \rangle / 2 \langle E_{\parallel} \rangle$, where E_{\perp} and E_{\parallel} are perpendicular and parallel kinetic energy



Fig. 1. – (Color online) Mean isotropy ratio (triangles) and dispersions (squares) as a function of time. Full lines correspond to data from ref. [4] (upper line) and [5] (lower line).

contributions, respectively, was calculated and represented in fig. 1 as a function of time. The interest of this observable lies in that kinetic energy transfer, which is related to microscopic collisional processes, can serve to constrain theoretical models and to obtain informations about the nucleon-nucleon cross-section. The theoretical values of R_E , obtained for 10⁴ CSSD, are represented in blue tones squares and the corresponding average value in black triangles. They are compared with experimental data from refs. [4] (red) and [5] (yellow) straight lines. The above references correspond to different event selections: Z = 1 in [4] and all fragments in [5]. For the simulation there is neither particular selection nor experimental bias corrections. It can be noticed that after a strong enhancement, taking place during the interpenetration stage, $\langle R_E \rangle$ values reflect some resilience effect from the mean field and are then confined between both experimental results.

Another exemple is depicted in fig. 2 where transverse kinetic energy distributions in the ${}^{36}\text{Ar}+{}^{58}\text{Ni}$ reaction at 95 AMeV are shown. Experimental data are extracted form ref. [6] and represented on the right. The calculated values are obtained for a sample of 10⁴ CSSD and for an impact parameter spectrum from 1 to 10 fm. The most central collisions are depicted in orange tones while the more peripheral ones are in green.



Fig. 2. – (Color online) Left: transverse energy distribution for different impact parameters b. Right: data extracted from ref. [6].

It can be noticed that the energy corresponding to the theoretical bell-shaped distribution maxima agree with the experimental values for the estimated impact parameter indicated by vertical lines (on the right). In this sense we can state that the calculated correlation E-b is consistent with the data.

4. – Beyond E-TDHF

One way to extend our description in order to describe large density fluctuations is by taking advantage of the significant work already done around the Botzmann-Langevin (BL) approach [7] which has been proven to be well suited for treating the fluctuations of the one-body distribution function f generated by multi-particle correlations in semiclassical transport approaches:

(8)
$$\frac{\partial f}{\partial t} = \{h[f], f\} + \bar{\mathcal{K}}[f] + \delta \mathcal{K}[f].$$

In this work we adopted the philosophy of the Bolzmann-Langevin One-Body (BLOB) model [8] which is a particular realization of the BL equation and adapted it to our formalism. A stochastic E-TDHF (S-E-TDHF) approach is then proposed taking advantage of the microscopic information in terms of SD which is available at any time during the collision. The model samples a given CSSD at each time step so as to define possible locations of nucleonic wave packets. Those latter are built around the sampled CS, taken as a reference, and incremented by other coherent states which are as close as possible to the reference CS in phase-space. The collisions proceed involving agglomerates of CS which are rearranged each time step into new nucleonic wave packets. Finally, the scattered nucleonic wave packets should be adapted to the final state in terms of momentum widths and occupancies, ensuring that Pauli blocking is not violated.

In order to inspect the consistency between both models the initial stages of the central ${}^{36}\text{Ar}+{}^{58}\text{Ni}$ reaction at 74 AMeV incident energy has been computed. Simulations were parameterized to use a comparable number of test particles and average coherent states per nucleon in BLOB and in S-E-TDHF models, respectively, and fixed to 64. The nucleon-nucleon cross-section is set in both simulations equal to the free isospin and energy dependent form. The respective effective forces are in both cases analogous adaptations of the Skyrme force. On the left panel of fig. 3 the spatial distribution on the reaction plane is depicted for some sorted coordinates points (yellow) as well as the projection onto the longitudinal direction (blue dashed-line) for the S-E-TDHF approach.



Fig. 3. – (Color online) On the left the spatial density projected on the reaction plane XZ (dots) and on the beam axis z for BLOB (in dashed line) and for E-TDHF (in solid line) models is shown. On the right the momentum distribution with the same conventions for both models is shown.



Fig. 4. - (Color online) Collision rates and variance as a function of time. On the left the number attempted collisions, on the right the effective ones. For more details see the text.

The projected spatial density for BLOB is depicted in red solid line. On the right panel are represented the corresponding projections onto the longitudinal direction of both momentum distributions with the same color convention as in the left panel. From these figures it can be noticed the good correspondence between both descriptions.

Another probe of the consistency of the description is the analysis of collision rates. In fig. 4 the attempted number of collisions (on the left) and the effective ones after Pauli blocking (on the right) are represented as a function of time for E-TDHF, BLOB and S-E-TDHF descriptions. The number of collisions increases during the initial compression stage and a dilute stage follows in which it drops and then slightly increases for both stochastic models. The corresponding minimum values should sign the onset of fragment formation or separation in a binary event. The similarity between S-E-TDHF mean collision number and the variance ensures that the fluctuations stand out with the correct Langevin amplitude [8].

Finally, let us consider again the head-on collision ${}^{36}\text{Ar}+{}^{58}\text{Ni}$ reaction at 74 AMeV. In fig. 5 the density profiles for the E-TDHF (top) and S-E-TDHF (bottom) descriptions are depicted. In the first case, the evolution remains essentially binary, while in the other the projectile completely breaks up after going through the target, producing a forward jet-like configuration [9] and leaving behind a massive target-like residue. The



Fig. 5. – (Color online) Density profiles at different times for E-TDHF model (top) and for its stochastic extension (bottom).

transition towards vaporisation on the system Ar+Ni has been measured experimentally [10]. Such phenomenology is consistently described both in the present approach and in it semiclassical analogue BLOB [9].

5. – Conclusions

The purpose of this work was to propose a new procedure for the description of density fluctuations on the basis of the extended TDHF. After recalling the bases of the model we discussed a prescription to untangle statistical, small-amplitude, fluctuations in terms of a manifold of incoherent mixing of coherent states Slater determinants as the least biased many-body state, compatible with the E-TDHF description. This prescription is shown to be compatible with the experimental trends in some exemples. On the other side, the treatment of large density fluctuations have been undertaken in the spirit of the Boltzmann-Langevin approach, in order to describe the occurrence of the variety of exit channel mechanisms observed in HIC experiments and their relative probabilities. Preliminary results exhibit, on the one side, the coherence of the description and, on the other, the significant improvement on the collision dynamics of the stochastic extension when compared with the standard ETDHF approximation. These results are promising, inciting us to move forward on the refinement of the model, in particular concerning the treatment of nucleon-nucleon correlations and intermediate-mass clusters formation in order to properly depict the onset and evolution of fragments.

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