Iso-Vectorial interaction and many-body correlations in Nuclear Dynamics

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Abstract. Comparisons involving Nuclear Matter calculations based on the Constraint Molecular model CoMD and semi-classical Mean-Field approximation using an effective interactions of the Skyrme type are presented. The performed study shows that specific correlations induced by the iso-vectorial interaction investigated in the framework of the molecular dynamics approach strongly affect parameter values of the effective interaction to be used to reproduce the standard saturation properties of Nuclear Matter. Moreover an example showing consequences in the balance between reaction mechanisms in the $^{48}$Ca + $^{48}$Ca at 25 MeV/nucleon system is also discussed.

1. Introduction

The description of many-body systems is one of the most difficult problems in nuclear physics due to the complexity of this kind of systems which are quantum objects described by a large number of degrees of freedom. A large variety of theoretical models have been developed using mean-field based and beyond-mean field approaches. In these approaches which use the independent particle approximation as a starting point, phenomenological effective interaction like Skyrme and Gogny forces are widely used taking advantage of their simple form[1, 2, 3, 4].

At the Fermi energy and beyond semiclassical methods become necessary to describe the produced processes in which practically all the degrees of freedom are involved. Many-body correlations are responsible for the reorganization of the hot Nuclear Matter(NM) in to clusters. Two main classes of approaches have been developed to handle this complex scenario. The first one is based on the Boltzman transport equation including, at the higher energy, three body collisions term[5, 6, 7]and stochastic forces (typical of Langevin processes) [8, 9]. In this case the theoretical approach is able to describe the time evolution of the one-body distribution function in phase-space.

In these models the main ingredient concerning the interaction is the energy density which for a Skyrme type phenomenological interaction has a rather manageable form. The second line of development of theoretical semiclassical approaches to deal the nuclear many-body problem is represented by the so called Molecular Dynamics models. The point of view of these methods is some sense antithetic compared to the ones based on the mean-field concept. However also in these cases, due to their simplicity the same kind of phenomenological effective interactions Skyrme and Gogny are widely used. The starting point of all these models is a basic assumption on the wave function describing the single nucleon which is represented through a wave packet.
well localized in phase-space with uncertainty satisfying the uncertainty principle. The many-body wave function can be expressed through a direct product, leading to the so called Quantum Molecular Dynamics (QMD)-like models [10, 11, 12, 13] or an anti-symmetrized product like in FMD and AMD [14, 15].

Within their own approximation schemes these models treat the many-body problem without the usage of the mean-field approximation. Many-body correlations are spontaneously produced and in general are able to describe the main features concerning the multi-breakup processes [16] observed in heavy ion collisions at intermediate energy and beyond. Due to these deep conceptual differences between the mean-field based models and the molecular dynamics ones it becomes interesting, and necessary in our opinion, to investigate the differences between the energy-density functionals which are produced with these two classes of approaches when one uses, in both the cases, the same kind of effective elementary interaction between nucleons. Clearly strongly correlated to this aspect are the differences produced on the behavior of simple observables obtained in the study of heavy ion collisions.

The study presented in this work is performed by using the Constraint Molecular Dynamical Model CoMD-II [11, 12].

The quantitative results obviously will be related to some specificity of the model and to the used effective interaction, but as due to the common features which links most of the molecular dynamics models (semi classical wave packet dynamics), the obtained results could assume a more wide meaning at a qualitative level. The work is organized as follows: in Sec. II we illustrate the choice of the effective interaction and the related total energy functional are introduced. In Sec.III we describe the results obtained from NM simulations. In Sec.IV we describe how the discussed many-body correlation can affect the balance between different reaction mechanisms in the $^{48}Ca + ^{48}Ca$ collision at 25 Mev/nucelon. Sec.V contains the summary and the concluding remarks.

2. The effective interaction and the total energy
In the present work the elementary interaction between two nucleons with spacial coordinates $r, r'$ and third isospin component $\tau, \tau'$ is of the Skyrme type and has the following form, around the saturation density:

$$V(r, r') = V^{(2)}(r - r') + \frac{T_0}{\rho_0} \delta(r - r') + \frac{2T_3\rho^{\sigma-1}}{(\sigma + 1)\rho_0^\gamma} \delta(r - r') + \frac{T_4}{\rho_0} \left( \frac{\rho}{\rho_0} \right)^{\gamma-1} (2\delta_{\tau,\tau'} - 1) \delta(r - r') \quad (1)$$

The first term of eq.(1) represents the iso-scalar contribution to the two-body interaction, the second one is the usual 3-body effective interaction. For this term the $\rho$ density dependence is modeled through the parameter $\sigma$.

The third term represents instead the Iso-Vectorial contribution. Also in this case the density dependence is introduced to reproduce the results of more complex microscopic calculations based on realistic interaction concerning the symmetry energy[18, 19, 20, 21, 22] and reflects effects beyond the two-body interaction.

2.1. The Semiclassical Mean Field Approximation
At a fixed time starting from eq.(1) (we are considering here a stationary problem), in a rather general way, we can obtain the expression for the total energy $W$ related to the potential interaction by folding the elementary interaction with the two-body density distribution in phase-space $D(r, r', p, p')$. By taking into account the usual truncation condition, $D$ can be expressed through the product of the one-body distributions and we obtain for the potential interaction
\[ E_{\text{pot}}: \]

\[ E_{\text{pot}} = U_{\text{turb}} + U_{\text{trb}} + U_{\text{asy}} = \frac{1}{2} V^{(2)} \rho = \frac{1}{2} \frac{T_{0} \rho}{\rho_{0}} + \frac{T_{\text{sym}} \rho_{\text{sym}}}{(\sigma + 1) \rho_{0}^{\sigma}} + \frac{1}{2} T_{4} F_{4}(\rho) \beta^{2} \tag{2} \]

\[ \beta = \frac{n_{\text{pro}} - n_{\text{neu}}}{} \]

represents the charge/mass asymmetry parameter evaluated from the neutron and proton density \( \rho_{n}, \rho_{p} \) respectively. The total binding energy \( E \) is obtained by adding the kinetic contribution coming from the Fermi motion

\[ E = E_{\text{pot}} + E_{\text{kin}}^{F} \tag{3} \]

\[ E_{\text{kin}}^{F} = \frac{3}{5} \frac{\hbar}{2m_{0}} \left( \frac{3 \pi^{2} \rho}{2} \right)^{2/3} \left[ 1 + \frac{5}{9} \beta^{2} \right] \tag{4} \]

In particular we see how the iso-vectorial vectorial forces with strength proportional to \( T_{4} \) contribute to the symmetry energy \( E_{\text{sym}} \) depending on the asymmetry parameter \( \beta \). For quadratic form in \( \beta \) we get:

\[ E_{\text{sym}}(\rho) = e_{\text{sym}} \beta^{2} \tag{5} \]

\[ e_{\text{sym}} = \frac{1}{2} \left( \frac{\rho^{2} E}{\partial \rho^{2}} \right) = \frac{1}{6} \frac{\hbar^{2}}{m_{0}} \left( \frac{3 \pi^{2} \rho}{2} \right)^{2/3} + \frac{1}{2} T_{4} F(\rho) \tag{6} \]

The common accepted bulk value of \( e_{\text{sym}} \) at the saturation density is about 30 MeV even if relativistic Hartree-Fock models can predict higher values up to about 40 MeV [24, 25]. However, still under study is the density dependence of this quantity which is able to affect neutron-skin thickness in nuclei and the Giant Monopole Resonances [24, 25, 26]. Finally we note that the structure of the obtained energy-density functional in Se-MFA makes independent the choice of the parameter describing the main properties of the symmetry energy from the other ones which instead are fixed from the saturation properties of the symmetric nuclear matter. We will show that this is no longer true in the CoMD approach.

In molecular dynamics approaches a strong assumption is done on the wave functions describing the nucleonic degree of freedom. It is commonly assumed that the wave function is a gaussian wave packet with width \( \sigma_{r} \) in coordinate space.

The widths in momentum and space satisfy the minimum uncertainty principle condition \( \sigma_{p} \sigma_{r} = \frac{1}{2} \hbar \). Another assumption concerns the N-body Wigner distribution that in CoMD model [11] (like in QMD approach [10]) is a direct product of the single particle distributions. In this case therefore for a system formed by \( A \) nucleons the one-body and 2-body distributions above introduced have a multi-component structure that is:

\[ D_{1}(r,p) = \sum_{i}^{A} f_{i}(r,p) \tag{7} \]

\[ D(r,p,r',p') = \sum_{i \neq j=1}^{A} f_{i}(r,p)f_{j}(r',p') \tag{8} \]

\( f_{i} \) represents the Gaussian Wigner transform of the wave packet associated to the generic nucleon \( i \). From the above relations we can see that in general \( D \neq D_{1}(r,p)D_{1}(r',p') \). In particular, for the case in which these distributions are expressed as a sum of different localized components inside a volume \( V_{g} \), we can indicate with \( a_{g} \) the number of components which give non negligible contributions in \( V_{g} \). The relative difference \( 1 - \frac{D_{1}(r,p)D_{1}(r',p')}{D} \) can be estimated to be of the order of \( 1/a_{g} \) which corresponds to the ratio between diagonal \( (i = j) \) and off-diagonal elements \( (i \neq j) \) within the ensemble of \( a_{g}(a_{g} - 1) \) terms. In semiclassical mean-field models \( a_{g} \) can be enough
high to make the difference negligible, in fact the single particle distribution usually spreads over the whole system (test particles methods) and therefore the truncation condition can be retained valid [5, 6, 7]. On the contrary this is not surely the case for the molecular dynamics approaches for which the typical spreading volume is of the order of 2-10 fm$^3$. Localization and therefore coherence of the wave-packed used to describe the single-particle wave-functions allows to keep memory of the two-body nature of the inter-particles interaction, and at same time, allows for the spontaneous appearance of the clustering phenomena in simulations concerning low-density and excited portion of nuclear matter [27].

With these assumptions on the 2-body phase-space distribution, taking in to account the properties of the $\delta$ function, we can obtain the explicity expression for the different terms concerning the total energy; for the two-body isoscalar contribution $W_{twb}$ we get:

$$ W_{twb} = \frac{T_0}{2\rho_0} \sum_{i=1}^{A} S^i_v $$

$$ S^i_v = \sum_{j \neq i=1}^{A} \frac{1}{(4\pi\sigma^2)^{3/2}} \exp\left(-\frac{(r_i - r_j)^2}{4\sigma^2}\right) $$

In the above expression $S^i_v$ is the normalized sum of the Gaussian terms and it represents just a measure of the overlap between the nucleonic wave-packets. Its two body character is quite explicit. In the calculations concerning the NM simulation that we will illustrate in the next sections, the large number of particles $A$ involved in the system allows us to write the above quantity in a simpler way by introducing the average overlap per nucleon $\bar{S}_v^i = \overline{S}_v$ whose dependence on the particle index in the ideal case can be omitted:

$$ E_{twb}^C = \frac{W_{twb}}{A} = \frac{T_0}{2\rho_0} \overline{S}_v $$

Concerning the three-body term, taking in to account the previous obervations we get:

$$ E_{trb}^C = \frac{T_3}{(\sigma + 1)\rho_0} \overline{S}_v^\sigma $$

For the term related to the iso-vectorial interaction in the limit $A, N, Z >> 1$ ($N$ and $Z$ represent the number of neutron and protons) we obtain:

$$ E_{isv}^C = \frac{T_4}{2\rho_0} \tilde{\rho}_A \left(\frac{\overline{S}_v}{\overline{S}_{v_0}}\right)^{\gamma - 1} \left(1 + \frac{\alpha}{2}\right)\beta^2 - \frac{\alpha}{2} $$

$$ E_{bias} = -\frac{T_4}{4\rho_0} F_k^i(\overline{S}_v) \tilde{\rho}_A \alpha $$

where $\tilde{\rho}_A \equiv A\tilde{\rho}$ is related ot the average overlap for couples of homonym nucleons. From eq.(13) we obtain that for $\alpha \neq 0$ ($\alpha \sim 0.15$ as CoMD calculations predicts) the iso-vectorial force produces a term which we name $E_{bias}$. It has no explicit dependence on $\beta$ (likewise iso-scalara term) but depends on the same parameter and density form factor which characterize the symmetry energy (first term in eq.(13)) The related effect is not-negligible if compared to the balance of the different terms appearing in the expression of the total energy. The correlation coefficient $\alpha$ responsible for the appearance of the $E_{bias}$ term represents the difference in percentage of the overlap between the neutron-proton couples (n-p) from the one related to the couples formed by homonym nucleons. It is positive because n-p pairs experience a larger overlap with respect the other ones due to the more attractive interaction. $\alpha$ also increases with the strength of the iso-vectorial forces ($T_4$ parameter).
Finally, the kinetic contribution $E_{\text{kin}}$ is obtained in a self-consistent way for ground state configurations by applying the cooling-warming procedure coupled with the constraint on the occupation numbers (see Ref.[12]) given by the Pauli principle. The total energy per nucleon is therefore obtained by adding all the contributions discussed in this section and it will be indicated as $E^C = E^C_{\text{pot}}(\bar{\rho}_s, \alpha, \rho_A) + E_{\text{kin}}(\rho)$. In particular we note that, at this level, it depends on the new defined primary quantity $\bar{\rho}_s$, $\alpha$, $\bar{\rho}_A$. It can be shown that these quantity are strictly related to the spatial correlation function between nucleon pairs and to the density. However a complete and explicit expression for the density dependence of these quantities cannot be obtained in an analytical way due to the problem complexity. Therefore in the following we will briefly illustrate the obtained results which are based on the dynamical simulation of very large slabs of nuclear matter.

3. The nuclear matter simulation

As mentioned in the introduction the main goal of the present work is to understand also at a quantitative level and for a given simple form of the effective interaction, what are the consequences produced by the correlations above discussed by taking as a reference point the results obtainable in the framework of the Se-MFA approach. The study will be performed in a narrow region of density around the saturation density $\rho_0$. To this aim in the following we will try to find the set of parameters for the effective interaction which reproduce in both the cases some of the commonly accepted saturation properties of symmetric nuclear matter. In particular we will refer to $\rho_0=0.165$ fm$^{-3}$, binding energy $E(\rho_0) = -16$ MeV, compressibility modulus for symmetric nuclear mater $K_{\text{NM}}(\rho_0) = 220$ MeV. The strength of the iso-vectorial interaction $T_4$ will be chosen in such way to produce a symmetry energy value $e_{\text{sym}}(\rho_0) \approx 28.6$ MeV in the case of the Se-MFA, i.e. $T_4 = 32$ MeV. From the functional $E$ reported in eqs.(3-4) we can find easily the parameter values satisfying the above conditions by solving the system formed by the following set of equations for symmetric NM:

$$\rho_0 = 0.165; \quad E(\rho_0) = -16\text{MeV}; \quad \frac{dE}{d\rho}/\rho_0 = 0; \quad 9\rho_0^2 \frac{d^2E}{d\rho^2}/\rho_0 = K_{\text{NM}}(\rho_0) = 220\text{MeV} \quad (15)$$

We get the following values for the parameters: $T_0 = -263 \pm 1.3$ MeV, $T_3 = 208 \pm 1$ MeV and $\sigma = 1.25 \pm 0.02$. The evaluation of the total energy per nucleon $E^C$ related to the CoMD calculations requires the solution of the many-body problem using the equation of motion regulating the wave-packet dynamics in large portion of nuclear matter and also correction for surface effects. Details on the self-consistent and the iterative procedure used can be found in ref.[27]. In particular these calculation shows that as expected $\bar{\rho}_s(\rho)$ increases with the density, while $\alpha(\rho)$ decreases. The density dependence of this quantities is not linear. In particular, quadratic corrections with the density are not negligible around the saturation density and are enough to well represent the global behavior.

In the left-panel of Fig.1 we show the final values of the interaction parameters which are able within 10-20% to reproduce the above mentioned EOS properties. To satisfy these condition the $\gamma$ parameter describing the degree of stiffness of the iso-vectorial interaction has to change in a rather restricted range of values, approximately 0.85-1.5.

We also note that as due to the coupling effects generated by the many-body correlations (including also the one derived from the Pauli principle) the new set of parameters which describes the iso-scalar interaction show a dependence on $\gamma$. Furthermore, the magnitude of the new parameter values is about a factor two smaller than the one obtained in the limit of the semiclassical approximation. Calculations have been performed also for asymmetric nuclear matter. The obtained value of the symmetry energy at the saturation density is about 1-1.6 MeV lower than the value obtained in the case of the mean-field approximation. Larger differences are instead observed for the density dependence of the symmetry energy. In particular it can
be shown that the larger values (about a factor 3) [27] of $K_{sym}$ (proportional to the second derivative of the symmetry energy at $\rho_0$) are strongly related to the Gaussian shape of the wave function used in molecular dynamics approaches. This result surely will affect the predicted the incompressibility modulus for asymmetric NM and an evaluation of this effect is in progress.

4. Effects on the nuclear dynamics

Up to now we have discussed the EOS limit, it is however very interesting to illustrate the effect of the correlation discussed also at a more qualitative level on the nuclear dynamics.

As an example in the right panel of Fig.1 we show experimental results on the $^{48}\text{Ca} + ^{48}\text{Ca}$ at 25 Mev/A. Data have been collected with the Multi-detector CHIMERA [28]. In the figure we report the relative yields of well reconstructed events ordered through the parameter $\Delta M_{nor} = \frac{m_1 - m_2}{m_{tot}}$, where $m_1$ and $m_2$ represent the mass of the biggest and the second biggest fragments produced. The yield of essentially binary processes including IMF production therefore can be located at small values of $\Delta M_{nor}$ while complete and incomplete fusion events are located at the larger $\Delta M_{nor}$ values. The continues line represents CoMD-II calculations which well fit the data using a $\gamma$ value about 1. Consistently, same results are obtained when studying the similar systems $^{40}\text{Ca} + ^{40}\text{Ca}$, $^{40}\text{Ca} + ^{48}\text{Ca}$ and $^{48}\text{Ca} + ^{46}\text{Ti}$ [29]. In particular the collected data for all these systems show that incomplete fusion processes are more suppressed for systems with the highest $N/Z$ asymmetry. In the left panel of Fig.2 we show with different lines CoMD-II calculations performed by using different $\gamma$ values and same set of parameter values concerning the iso-scalar interaction. The different curves indicate that the increasing of the stiffness associated to the iso-vectorial interaction (increasing values of the $\gamma$ parameter) produce an increasing attractive effect with a correlated enhance of the incomplete fusion process. In the right upper panel of Fig.2 as an example we show a corresponding estimation of the coupling term $E_{bias}$ in the EOS limit (see eq. 14) as function of the density for two extremal values of the

Figure 1. (Left-panel) The values of the parameters $T_0$, $T_3$, and $\sigma$ (panel a,b,c respectively) obtained through the iterative procedure applied to CoMD calculations are shown as a function of the stiffness parameter $\gamma$. The bar errors represent the global uncertainty on the parameter values related to the numerical procedures-(Right-panel) Experimental $\Delta_{nor}$ yield distribution for the $^{48}\text{Ca} + ^{48}\text{Ca}$ collision at 25 MeV/nucleon is shown with marked points. The red line represents CoMD-II calculations with $\gamma = 1$ (Stiff2 option)
Figure 2. (Left panel) $\Delta M_{\text{nor}}$ (see the text) distribution evaluated through CoMD-II calculations for the $^{48}\text{Ca}^{+}\text{^{48}Ca}$ collision at 25 Mev/nucleon and corresponding to different $\gamma$ values. Stiff1 label indicates $\gamma \approx 1.5$ while Soft $\gamma \approx 0.5$ The Stiff2 option which fit well the experimental data (see Left panel of Fig.1) corresponds to $\gamma = 1$. (Right-upper panel) Estimated value of the $E_{\text{bias}}$ term in NM limit corresponding to the above mentioned colliding system for two different extremal values of $\gamma$. (Right-bottom) Symmetry potential evaluated in the NM limit in the framework of the Se-MF approximation. We note that in this approximation $E_{\text{sym}}$ is the only term related to the Iso-vectorial interaction

$\gamma$ parameter. In the right-bottom panel, the symmetry potential $E_{\text{sym}}$ (see last term in eq.2) is shown in the semiclassical Mean-Field limit. As can be seen from a comparison between the panels the repulsive/actractive behavior of the iso-vectorial interaction, (magnitude of the slope as function of the density) and the one related to the $\Delta_{\text{nor}}$ in the nuclear dynamics obtained by decreasing/increasing the values of the $\gamma$ parameter is strongly correlated with the behavior of the $E_{\text{bias}}$ correlation term rather than with the symmetry energy itself which shows instead an opposite trend. This comparison therefore shows that the many-body correlations discussed in this work concerning the iso-vectorial interaction strongly influence the behavior of observable related to the nuclear dynamics and surely they can strongly affect the results obtained from the fit procedure of experimental data with model based on the semiclassical wave packets dynamics.

5. Summary and Concluding Remarks

Many-body correlations produced in Molecular Dynamics approach based on the CoMD model have been discussed and their connection with the used effective interaction have been analyzed in the case of nuclear matter simulations. This study has been performed by comparing the results obtained for the total energy functional and the nuclear matter (NM) main saturation properties with the ones obtainable in the case of a semiclassical mean field approximations (Se-MFA). This comparison has been performed by using the same kind of simple effective Skyrme interaction. While we can expect the two approaches to produce large differences at low density due to the cluster formation process, the following study shows that noticeable differences are obtained also in a narrow range of densities around the saturation one where no cluster production has been observed. For asymmetric NM, in the range of the investigated asymmetry parameters ($\beta = 0. - 0.2$), the values of the obtained symmetry energies around the
saturation density are only slightly different, but rather large differences are instead obtained for the slope $L$ and especially for the $K_{sym}$ curvature parameter. In CoMD calculations $K_{sym}$ assume in fact rather higher and positive values. This result can be attributed to the shape of the single particle wave-packets which determines the behavior of the average overlap per nucleon as a function of the density. An example showing the effects of these correlations on a simple observable related to the balance between different reaction mechanisms in the $^{48}\text{Ca} + {^{48}\text{Ca}}$ at 25 MeV/nucleon collision has been also discussed. Finally we conclude by observing that even if from a numerical point of view the obtained results are strictly valid for the CoMD model, the performed study shows that the observed differences in the parameter values describing the effective interaction can have a more wide meaning. In fact, they are strictly linked to some rather general properties of the semiclassical wave packets dynamics.

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