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Nuclear EoS and dynamical fluctuations in the Constrained Molecular Dynamics

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Summary. — Many-body correlations characterizing the Constrained Molecular Dynamics (CoMD)are analysed in the case of finite and zero range effective microscopic interactions. This work illustrates the case of infinite nuclear matter at zero temperature. A comparison with the predictions in the mean-field (MF) limit corresponding to different effective masses, highlights non-negligible differences regarding the produced Equation of State (EoS).

1. – Introduction

The description of many-body systems is one of the most difficult problems in nuclear physics due to their complexity being quantum objects described by a large number of degrees of freedom. In particular, the heavy ion collisions (HIC) at energy well above the mutual Coulomb barriers are usually described through semi-classical approaches based on the mean-field (MF) approximation or quantum molecular dynamics approaches (QMD) [1]. These last describe the single particle wave functions by means of well localized wave-packets (WPs) with fixed widths. In this way many-body correlations are produced which lead to the spontaneous formation of clusters. In these semi-classical approaches the effective interaction plays obviously a key role, and in many cases it just represents the main subject of investigation. In several cases MF and molecular dynamics approaches [1] share the same microscopic effective interactions. From a general point of view, it can be expected that the typical and explicit two or many-body correlations of QMD like approaches could instead play a role in many-body quantities as for the total energy. In these cases, therefore, it would be desirable to investigate at what extent these specific correlations may affect the many-body functional (EDF) related to the total energy in the case of infinite nuclear matter(NM). In particular, by using the CoMD model [2],in this contribution it is illustrated a study performed for a finite range (FR) interaction trying to produce a ground state Equation of State (EoS) with common accepted behaviours at the saturation density.

2. – The microscopic effective interaction

In the following we will refer to an example of EoS characterized by some properties at zero temperature that we choose as reference. Equilibrium density $\rho_0 = 0.165\ fm^{-3}$, associated binding energy $E(\rho_0) = -16$ MeV, incompressibility $K(\rho_0) = 240$ MeV, symmetry energy $E_{sym} = 30$ MeV, an effective pairing energy (it include the spin dependent produced trough the exchange terms [3]) equal to -2 MeV per nucleon at the saturation density in finite systems (around mass 100). Moreover, the functional will correspond in the MF limit to a relative effective mass $m^*_r = 0.67$, and neutron-proton effective mass splitting $m^*_{rn} - m^*_{rp} = 0.4\beta$. Finally, different values of the slope parameter associated to the symmetry energy $L = 3\rho_0(\frac{dE_{sym}}{d\rho})_{\rho_0}$ have been considered changing in the range $55 \div 105$ MeV as suggested from different investigations (see as an example [4]).

We now proceed in fixing the structure of the effective microscopic interaction starting from which the energy functional of the density can be obtained according to the chosen models.

The microscopic effective interaction in the original formulation of the CoMD model [2] was a simple zero range interaction of the Skyrme type. We used a 2-body plus a 3-body interaction. A third term describes the iso-vectorial interaction. the effects related to the finite range interaction in MF and QMD-like approaches. The total microscopic interaction, inspired from the Gogny interaction, will be the sum of the following contributions ($\mathbf{dr} = \mathbf{r} - \mathbf{r'}$).

$$V(\mathbf{dr}) = [P_2 + 2P_3(\frac{\rho}{\rho_0})^{\sigma-1}]e^{-(\mathbf{dr})^2/\mu^2} \tag{1a}$$

$$V_0(\mathbf{dr}) = \frac{1}{\rho_0}[P_{20} + \frac{2P_{30}}{\sigma+1}(\frac{\rho}{\rho_0})^{(\sigma-1)}\delta(\mathbf{dr}) \tag{1b}$$

$$V^{sy}(\mathbf{dr}) = [P_4(\frac{\rho}{\rho_0})^{(\gamma-1)}(2\delta_{\tau-\tau'} - 1)]e^{-(\mathbf{dr})^2/\mu^2} \tag{1c}$$

$$V_0^{sy}(\mathbf{dr}) = \frac{1}{\rho_0}P_{40}(\frac{\rho}{\rho_0})^{(\gamma-1)}(2\delta_{\tau-\tau'} - 1)\delta(\mathbf{dr}) \tag{1d}$$

$$V_S(\mathbf{dr}) = \frac{1}{\rho_0}P_\pi(\frac{\rho}{\rho_0})^{(\gamma-1)}\delta_{s+s'}\delta_{\tau-\tau'}\delta(\mathbf{dr}) \tag{1e}$$

τ and s indicate the third components of the nucleon iso-spin and spin quantum numbers respectively. The contributions in eq. (1a) and eq. (1c) represent a generalization of the terms reported in [2] associated to the two, three-body and iso-vectorial interactions. In analogy with the Gogny interaction, we have substituted the delta functions in the spatial relative coordinates with a Gaussian whose width defines the only range $\mu = 1.1$ fm that is used in this representation.

Always in analogy to the Gogny interaction and after different attempts to satisfy the different requests of the reference energy density functional, it has been necessary to add residual ZR terms associated to the two, three-body and iso-vectorial contributions as shown in eq. (1b) and eq. (1d). Finally eq. (1e) represents a zero range spin-spin interaction. This contribution is necessary to reproduce an effective "pairing" energy of about -2 MeV at the ground state for finite system with mass around 100. At the same time, this further contribution is able to locally produce in box calculations (see next section) small value of average total spin at the stationary conditions. The introduction of this term produce a further contribution to the symmetry energy.

3. – The effective interaction

Starting from the above expressions concerning the microscopic interaction the expression of the effective interaction as a function of the density can be obtained in the MF approximation by evaluating the associated matrix elements using 2-body wave functions constructed with plane-waves in a large volume V. $\Phi = \frac{1}{\sqrt{V}} e^{i\mathbf{kr}}$. The zero range interactions will give arise to the usual terms proportional to powers of the density. The finite range interaction will give arise to a momentum dependent part because of the underlying Slater determinant structure of the 2-body wave function for the identical particles. Details on the obtained complete expression can be found in ref. [3]. In the following as an example we write the two-body exchange contribution

$$\Delta E_2^{ex}(\mathbf{k}_i, \mathbf{k}_j) = -\frac{P_2}{V}(\sqrt{\pi}\mu)^3 e^{-\mu^2(\mathbf{k}_i - \mathbf{k}_j)^2/4} \tag{2a}$$

The non-locality of the effective interactions produces corrective factors to the in medium nucleon kinetic energy formally represented through a density dependent nucleon effective mass m^*.

In the case of the CoMD model the first step is just to substitute the plane-waves convolution with the wave packets $\Phi = \frac{1}{(2\pi\sigma_r^2)^{3/4}} e^{-\frac{(\mathbf{r}-\mathbf{r}_{0,i})^2}{4\sigma_r^2} + i\mathbf{k}_{0,i}\mathbf{r}}$. As an example, the momentum dependent (MDI) 2-body contribution corresponding to eq. (2a) will be:

$$E_2^{i,j,MDI} = -\frac{P_2}{8\sigma_r^3}\xi^3 \times e^{-\frac{1}{4}[\frac{(\mathbf{r}_{0,i}-\mathbf{r}_{0,j})^2}{\sigma_r^2} + \xi^2(\mathbf{k}_1 - \mathbf{k}_1)^2]}(\delta_{\tau_i-\tau_j}\delta_{s_i-s_j}) \tag{3a}$$

With a modified width : $\frac{1}{\xi^2} = \frac{1}{4\sigma_r^2} + \frac{1}{\mu^2}$. While the gausssian width of the related direct contribution will be: $\lambda^2 = 4\sigma_r^2 + \mu^2$.

In the framework of the MF approximation, all the quantities characterizing the reference functional can be obtained in a relatively simple way by solving a linear system with the strength parameters as unknown quantities. For the example chosen here, the values of these quantities and the obtained interaction parameters are reported in the first row of table 1. Finally, in the upper panels of fig. 1(a) it is shown for the reference case the total energy as a function of the relative density $\rho_r = \frac{\rho}{\rho_0}$ and in the bottom panels the related symmetry energies. The results are plotted by means of a blue line.

To highlight the correlations produced by the CoMD model it will be instead necessary to simulate the NM by performing box calculations. In this work we adopt periodic boundary conditions. Results of this calculations will be shown in sect. 5.

4. – Source of many-body correlations in phase-space

With reference to the MDI interaction, it can be shown [3] that contrary to the CoMD case, the usage of plane waves in the MF approaches produces an internal averaging on the spatial part of the interaction. This gives arise to a correction with respect to the CoMD energy per nucleon ΔE_b that can be expressed as ([3]):

$$E_{MD} = E_{MF} + \Delta E_b \tag{4a}$$

$$\Delta E_b = -\frac{P_2 A}{2}(\overline{\overline{\delta A_{i,j}} * \overline{B^{MF,2}}} + \overline{\overline{\delta B_{i,j}} * \overline{A^{MF,2}}} + \overline{\overline{\delta A_{i,j}\delta B_{i,j}}}) \tag{4b}$$

TABLE I. – *For the chosen example, in the first row we report the parameters values characterizing the adopted effective interaction in the MF approximation. The units of the P and L parameters are MeV. The set corresponds to relative effective masses m^*_r and $m^*_{nr} - m^*_{pr}$ equal to 0.67 and 0.4β. The second row show the new set of parameter values(see the text)*

P_2	P_3	P_{20}	P_{30}	P_π	P_{40}	P_4	L	σ	γ
1042.8	-434.1	-870.0	169.9	-213.4	478.1	-300.0	63.3	0.9	0.7
1776.8	-1279.6	-1503.1	920.8	-171.4	551.1	-425.6	67.5	0.7	0.9

with: $\delta A^{MD,2}_{i,j} = A^{MD,2}_{i,j} - \overline{\overline{A^{MF,2}}}$; $\delta B^{MD,2}_{i,j} = B^{MD,2}_{i,j} - \overline{\overline{B^{MF,2}}}$; The $A_{i,j}$ and $B_{i,j}$ are the 2-body matrix elements of functional associated to the spatial and phase-space coordinates respectively (see eqs. (1a)-(3a)). The double overline symbols indicate the average per pairs of nucleons. Beyond the effects due to the many-body dynamics the first two contributions in eq. (4b) can be largely affected by the convolution operation with the Gaussian associated to the WPs (differences in the widths of the overlap integrals with respect to the MF case). The last term contains the dynamical correlation between the "fluctuations" in phase-space associated to the functional $A_{i,j}(\mathbf{r}, \mathbf{r'})$ and $B_{i,j}(\mathbf{k}, \mathbf{k'})$ with respect to the mean value related to the MF approache.

Furthermore, more generally, we have to observe that another source of correlations able to produce a ΔE_b different from zero is obtained whenever a microscopic interaction (also for zero range) acts in a different way, for example with opposite signs, on two different subsets of nucleon pairs. In this case the interaction can affect on average the overlap integrals related to the two subsets (*i.e.*, can affect the relative distances between the nucleons belonging to the different kinds of pairs) modifying the related energies. This pure two-body effect, cannot be achieved in the MF case just due to the one-body internal average generated by the use of plane-wave. An example of these correlations was studied in [2]. This was the case of the iso-vectorial interaction coupled with the Pauli constraint affecting in different way *nn* and *pp* pairs with respect to the *np* ones. This kind of short range correlations can be interpreted as a tendency to form deuteron-like particles (or more generally clusters) also at density around the saturation one.

5. – Box calculations with CoMD model

The CoMD effective interaction that is a functional of the wave-packed centroids has been evaluated in box calculations with periodic boundary conditions to simulate the "ground state" NM. In this stage the set of MF strength parameters reported on the first row of table 1 was used. The calculations have been performed for different densities (number of particles in the unitary volume) and β values using 2000 WPs . The evolution of the WP's centroids was applied for each configuration following the CoMD approach [2]. For density lower than $0.8\rho_0$ the WPs coordinates were not evolved in time. Because the increasing of fluctuations destroy the homogeneity-uniformity conditions, which are reflected in the static MF expression. The results obtained for the total energy is the average on the four independent microscopic configurations. The small spread around the average determine the error. In the upper panel of fig. 1(a), for the charge/mass symmetric NM, are shown with open symbols the obtained results from

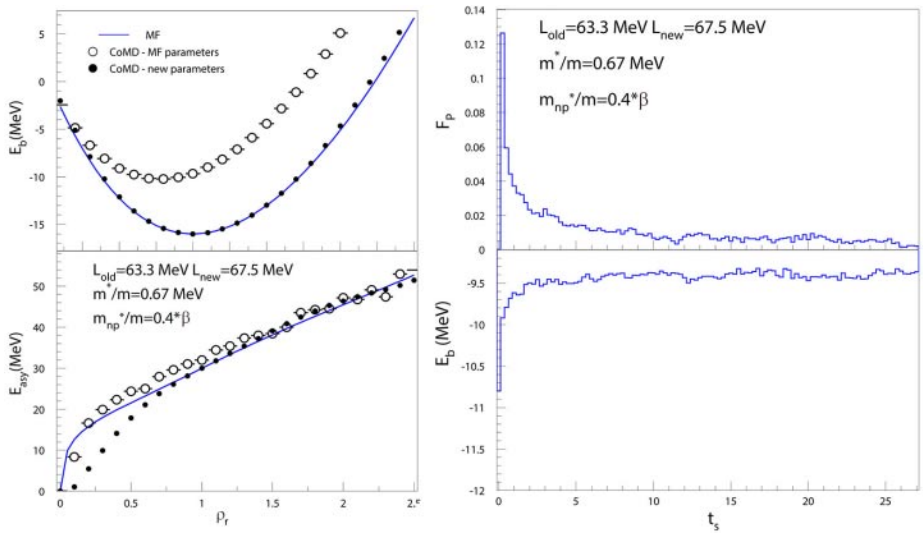

Fig. 1. – (a) According to the legend and to the text, upper panel: The total energy E_b as a function of the density evaluated for the different cases, bottom panel: same as the upper one but referring to the symmetry energy E_{asy}. (b) In the upper panel the Pauli-over-blocking F_P is plotted as a function of the time step t_s(see text). The box calculations are performed at the saturation density with an effective interaction corresponding to the parameters reported in the first row of table I. In the bottom panel the corresponding E_b per nucleon is plotted.

CoMD calculations concerning the total energy as a function of the relative density ρ_r for the chosen case. The error for each determination is within the symbol size. The blue solid lines represent instead the values obtained from the MF prediction which accurately reproduce the chosen characterizing EDF reference properties reported at the beginning of sect. 2.

6. – Discussion of the obtained results

For the case already reported in fig. (1a), in fig. (1b) (upper panel) we plot at the saturation density ρ_0, the average Pauli over-blocking $F_P = \overline{f} - f_m$ as function of the number of steps N_s that define the variable $t_s = 0.25 * N_s$. In this stage the coordinates are not evolved in time but only the numerical procedure related to the constraint is applied. $f_m \simeq 1.03$ is a bias related the occupation numbers produced by the finite efficiency e numerical of the Pauli constraint procedure. In the bottom panel the corresponding value of the total energy is plotted. We see that already for $t_s = 0$ the energy is larger than the expected value of -16 MeV as already shown in fig. 1(a). This is due to the convolution with the WPs in the evaluation of the effective interaction. Moreover as a function of t_s, the energy still increases up to a level of about 1.5 MeV in a correlated way with the reduction of F_P. This further increment of the total energy may be considered as a configuration energy associated to the correlation in phase space induced by the Pauli constraint. In fact, in the analyzed case, the total potential energy arising from the finite range interaction is negative, and the CoMD constraint tends to minimize the number of pairs of identical nucleons which are near in phase space where this negative MDI term is more effective.

The illustrated calculations have been performed for different densities and charge-mass asymmetries. The average overlaps integral related to the local and non-local interactions have been fitted with sixth order polynomials of the density and for each density with fourth order polynomials of the charge asymmetry parameter β. It's worth noting that the average overlap integrals, as evaluated from the described procedure in the previous section contain all the main correlations effects associated to the CoMD phase-space constraints related to the "ground state" configurations.

With this new functional of the density, it has been possible to define a linear system in the new parameters by imposing the usual condition already expressed in sect. 2 concerning symmetric and asymmetric NM ground state properties. The second row of table 1 contains the new set of obtained parameter values for the case evaluated in this work. Their uncertainty is of the order on $\pm 3\%$. The value of the total energy is plotted in fig. 1(a) with black circles for the $\gamma = 0.7$ case. The overall agreement wiht the reference case is satisfactory for density around an beyond the saturation one. To improve the agreement at lower density other free parameters should be introduced.

7. – Summary and final remarks

Many-body correlations developed in the constrained Molecular Dynamics, have been described in the present work. The analysis proceeded by taking as reference a nuclear matter density functional at zero temperature having commonly accepted properties around the saturation density.

This correlations are evidenced by performing a comparison between the results obtained through the CoMD model using the same effective interaction as the one deduced in the MF approximation.

In the case of a finite range interaction or a MDI the comparison highlights large differences between the reference density functional and the CoMD one. The latter in fact produces different saturation density, binding energy, etc. The sources of the correlations producing such differences have been discussed. They arise from the wave-packed dynamics and from the constraint associated to the Pauli principle. A procedure has been described to modify the values of the strength parameters in such a way to obtain the reference EoS properties also in the CoMD case. It's also worth noting that the rather general feature of the discussed correlations could give a wider meaning to the relative changes obtained in the comparisons between the different studied cases. An example of the effects of these correlations on observables commonly studied in HIC is presented in [3]

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