Calculations for Asymmetric Nuclear matter and many-body correlations in Semi-classical Molecular Dynamics

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Introduction

• Skyrme (and Gogny) effective interactions due to their simplicity have been widely used to study the Nuclear Many-Body problem (MBP) including the related EOS.

• Different theoretical approaches have been developed using Mean-Field (MF) based approaches and beyond. SHF, RMF, HFB have been used in nuclear structure modeling and EOS calculation.

• For Nucleus-Nucleus collision at the Fermi energies complexity becomes higher. Really all the nucleonic degree of freedom participate to produce fluctuations of the most simple observables and re-organization processes of Nuclear Matter in to Clusters.

• We can use only semi-classical approaches. We need to go beyond MF approaches.

• BUU+cluster, BNV, BNV+white noise, SSMF(Stochastic-Semicalssical Mean-Field)
• QMD(direct), CoMD(direct+constraint), ImQMD, FMD, AMD (anti-symmetric)

• “Quantum Molecular Dynamics Approaches –Semi-classical Wave-Packets Dynamics (SWPD).

How the necessary correlations introduced in these last models (SWPD CoMD) affect the parameter values of the Skyrme interaction and the symmetry energy properties?

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A simple effective N-N Interaction

\[ V(r, r') = V^{(2)} \delta(r - r') = \]
\[ \frac{T_0}{\rho_0} \delta(r - r') + \]
\[ \frac{2T_3 \rho^{\sigma - 1}}{(\sigma + 1) \rho_0^\sigma} \delta(r' - r') \]
\[ + \frac{T_4}{\rho_0} F'_k (2\delta_{T,T'} - 1) \delta(r - r') \]

2-body Iso-Scalar
“3-body” Iso-Scalar
\( \rho \) dependence
2-body Iso-Vectorial

\[ F_k = (\rho/\rho_0) F'_k \]
\[ F'_1 = \frac{2(\rho/\rho_0)}{1 + \rho/\rho_0} \]
\[ F'_2 = 1 \]
\[ F'_3 = (\rho/\rho_0)^{-1/2} \]
\[ F'_4 = (\rho/\rho_0)^{\gamma - 1} \]

Common suggested form factors to model the \( \rho \) dependence of the symmetry energy
( calculation based on realistic Interaction)
\( \gamma \)- degree of stiness for the iso vect. interaction

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A short remind of the Se-MF approximation

\[ D(r, r', p, p') \equiv 2\text{-body density in phase-space} \]

Se-MF means:

\[ D = D_1(r, p) \cdot D_1(r', p') \int D_1(r, p) dp = \rho \]

Due the properties of the \( \delta \) in the Skyrme interaction:

\[ W = \frac{1}{2} \int V^{(2)} \rho^2 dr \equiv \text{Total interaction energy} \]

\[ E_{\text{pot}} = \text{Interaction energy per Nucleon} \]

\[ E_{\text{pot}} = U_{twb} + U_{trb} + U_{asy} \]

\[ = \frac{1}{2} V^{(2)} \rho = \frac{1}{2} \frac{T_0 \rho}{\rho_0} + \frac{T_3 \rho^\sigma}{(\sigma + 1) \rho_0^\sigma} + \frac{1}{2} T_4 F(\rho) \beta^2 \]

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The total energy \( E \) per nucleon is a rather simple functional of \( \rho \)

\[
E = E_{\text{pot}} + E_{\text{kin}}
\]

\[
E_{\text{kin}} = \frac{3}{5} \frac{\hbar^2}{2m_0} \left( \frac{3\pi^2 \rho}{2} \right)^{2/3} [1 + \frac{20}{36} \beta^2]
\]

\[
E_{\text{sym}} = e_{\text{sym}} \beta^2
\]

\[
e_{\text{sym}} = \frac{1}{2} \left( \frac{\partial^2 E}{\partial \beta^2} \right)_{\rho=\rho_0}
\]

\[
= \frac{1}{6} \frac{\hbar^2}{m_0} \left( \frac{3\pi^2 \rho}{2} \right)^{2/3} + \frac{1}{2} T_4 F(\rho)
\]

Commonly accepted values of fundamental quantities related to the EOS saturation properties

\[
e_{\text{sym}}(\rho_0) \approx 28-30 \text{ MeV} ; \quad E(\rho_0) \approx -16 \text{ MeV} ; \quad K_0 \approx 220-270 \text{ MeV}
\]

\[
\rho_0 = 0.165 \text{ fm}^{-3}
\]

\[
E(\rho_0) = -16 \text{ MeV}
\]

\[
\frac{dE}{d\rho}/\rho_0 = 0
\]

\[
9\rho_0^2 \frac{d^2E}{d^2\rho}/\rho_0 = 220 \text{ MeV}
\]

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• The case of the SWPD-CoMD

\[
\phi_i = \frac{1}{(2\pi\sigma_r^2)^{3/4}} \exp\left[-\frac{(r - r_i)^2}{2\sigma_r^2} - i\frac{rp_i}{\hbar}\right]
\]

WP with fixed widths \(\sigma_r\sigma_p = 1/2\)

\[
f_i = \frac{1}{(2\pi\sigma_r\sigma_p)^3} \exp\left[-\frac{(r - r_i)^2}{2\sigma_r^2} - \frac{(p - p_i)^2}{2\sigma_p^2}\right]
\]

Single particle phase-space distribution

The Many-body wave function is a direct product + constraint

\[
D_1(r, p) = \sum_{i=1}^{A} f_i(r, p)
\]

1-body density distribution

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

2-body density distribution

\[
D \neq D_1(r, p)D_1(r', p')
\]

I=J terms can not be included

Given a particle \(i\), define \(A_i\) nr of particles which gives non negligible value to \(D\) diagonal/ off-diagona \(\approx 1/(A_i-1)\); never small !!!

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\[ W = \frac{1}{2} \int V^{(2)}D(r, p, r', p')\delta(r - r')drdr'dpdp' = \]
\[ \frac{1}{2} \sum_{i \neq j=1}^{A} \int V^{(2)}f_i(r, p)f_j(r, p')drdpdp' \]

\[ W_{twb} = \frac{T_0}{2\rho_0(4\pi\sigma_r^2)^{3/2}} \sum_{i \neq j=1}^{A} \exp[-\frac{(r_i - r_j)^2}{4\sigma_r^2}] \]

\[ W_{twb} = \frac{T_0}{2\rho_0} \sum_{i=1}^{A} S_v^i \]

\[ S_v^i = \sum_{j \neq i=1}^{A} \frac{1}{(4\pi\sigma_r^2)^{3/2}} \exp[-\frac{(r_i - r_j)^2}{4\sigma_r^2}] \]

\[ \sigma_r \text{ determine the 2-body effective potential responsible for the dynamics of the WP centers with a characteristic width 2 times larger} \]

\[ <S_v> \equiv \text{Average overlap per nucleon} \]

We have an analogy, unfortunately only formal, between \(<S_v>\) and \(\rho\)

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\[ U_{trb} = \frac{T_3}{(\sigma + 1)\rho_0^\sigma} \]

\[ \tilde{\rho}^{nn} = \frac{1}{(4\pi\sigma^2)^{3/2}N^2} \sum_{i \neq j \in \mathbb{N}} \exp[-\frac{(r_i - r_j)^2}{4\sigma^2}] \]

\[ \tilde{\rho}^{pp} = \frac{1}{(4\pi\sigma^2)^{3/2}Z^2} \sum_{i \neq j \in \mathbb{Z}} \exp[-\frac{(r_i - r_j)^2}{4\sigma^2}] \]

\[ \tilde{\rho}^{np} = \frac{1}{(4\pi\sigma^2)^{3/2}2NZ} \sum_{i \neq j \in \mathbb{NZ}} \exp[-\frac{(r_i - r_j)^2}{4\sigma^2}] \]

\[ \tilde{\rho} = \frac{N^2\tilde{\rho}^{nn} + Z^2\tilde{\rho}^{pp}}{N^2 + Z^2} \]

\[ \alpha = \frac{\tilde{\rho}^{np} - \tilde{\rho}}{\tilde{\rho}} \]

\[ \alpha \text{ gives the enhancement of the np overlap} \]

\[ U_{Se-MF}^{Se-MF} = \frac{1}{2} \frac{T_4}{\rho_0} F(\rho) \beta^2 \]

\[ U_{isv} = \frac{T_4}{2\rho_0} F'(\bar{S}_v) \tilde{\rho}_A [(1 + \alpha)\beta^2 - \frac{\alpha}{2}] \]

\[ F'(\frac{\rho}{\rho_0}) \rightarrow F'(\frac{\bar{S}_v}{\bar{S}_v\rho_0}) \]

\[ U_{tot} = U_{tot}(\bar{S}_v, \tilde{\rho}, \alpha, \beta) \]

α gives the enhancement of the np overlap

The isov. Energy term gives 2 contributions
One is analogous to \( e_{sym} \) in Se-MF
the other one looks like e Bias term

\[ \bar{f}_i \leq 1 \text{ (for all } i) \]

\[ \bar{f}_i = \sum_j \delta_{\tau_i, \tau_j} \delta_{\delta_i, \delta_j} \int d^3r f_j(r, \rho) d^3r d^3p. \]

The constraint based on Pauli principle determine the kinetic energy contribution

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• Overlap integrals, $\rho$ and spatial correlations

$$\nu(r) \equiv \text{Spatial correlation function}$$

$$p = 1 \pm k_0 \nu(r) \quad \nu(0) = 1 \quad k_0 \geq 0$$

$$\int_V PdV = 4\pi c \int_0^r p(r)r^2dr = A \quad \rightarrow c = \frac{A}{V - Vc}$$

$$\lim_{r \to \infty} c = \rho$$

$$P(r) = \rho(1 \pm k_0 \nu(r))$$

$$\overline{S_\nu} = \frac{\overline{S^T_\nu}}{A} = \frac{1}{(4\pi \sigma_r^2)^{3/2}} \int P(r) \exp[-\frac{r^2}{4\sigma_r^2}]dV$$

$$= \rho(1 \pm I)$$

$$I = \frac{1}{\sqrt{4\pi \sigma_r^3}} \int_0^\infty r^2 k_0 \exp[-\frac{r^2}{4\sigma_r^2}]\nu(r)dr$$

$L \equiv \text{characteristic length of } \nu$

$$\lim_{\sigma_r / L \to \infty} I = 0$$

$\sigma_r \sim 1.15 \text{ fm} \quad \text{mainly fixed to describe surface and radii of nuclei}$

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Generalization to asymmetric systems

\[
\overline{S_v} = \frac{\rho}{8} \left[ 8 + (1 + \beta^2)(I_{0,-1} - I_{1,-1}) + (1 - \beta^2)(I_{0,1} - I_{1,1}) + 4(1 - \beta^2)I^0 \right]
\]

with analogous procedure for the other main quantities we get:

\[
\rho_A = \frac{\rho}{4} \left[ 4 + (1 + 2\beta - 2\beta^3)(I_{0,-1} - I_{1,-1}) + (1 - 2\beta + 2\beta^3)(I_{0,1} - I_{1,1}) \right]
\]

\[
\alpha = \frac{(1 + I^0)}{\left[ (1 + \frac{(1+\beta)^2}{1+\beta^2})(I_{0,-1} - I_{1,-1}) + \frac{(1 - \beta)^2}{1+\beta^2}(I_{0,1} - I_{1,1}) \right]}
\]

All these expressions keep the symmetry under the \( \beta \rightarrow -\beta \) transformation

Both \( I^0, I_{s,t} \) can have a dependence on \( \rho \) and \( \beta \)

Corrected for surface effects

In the explored range also a non-linear behavior is observed well fitted with a 2\textsuperscript{nd}-order polynomial of \( \rho \)
In the explored density range no cluster production is observed. Only for the lower limit some light particles and a big agglomerate is observed but is not stable in time.

For the range of $\beta$ values explored and within the precision of our calculations we can assume no explicit dependence of $S_v$ from $\beta$.

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FIG. 6. (Color online) Final values of the $\alpha$ correlation coefficient for $\beta = 0$ as a function of reduced density and for different form factors $F_k$ as indicated in the legend. The asterisk and full dot symbols (red and blue online) joined with continuous lines are associated to $T_4$ values 0 and 59 MeV, respectively. The other ones are associated to $T_4 = 32$ MeV. The lines represent fit results with a second-order polynomial of the density.
Microscopic simulations have been performed for two large spheres containing 1600 and about 3500 particles. This allows for corrections due to surface effects on the above quantities $Q_i$. Curvature effects for such large systems are less than 5%.

Correction for the surface effects allows to evaluate the bulk values $Q_v$.

### Surface effects

\[
Q_i = Q_v + Q_s A^{-\frac{1}{3}} + 0.45Q_s A^{-\frac{2}{3}}
\]

### The iterative procedure

**Step 0**

- \( E(\rho_0) = -16\text{MeV} \)
- \( \left. \frac{dE}{d\rho} \right|_{\rho_0} = 0 \)
- \( 9\rho_0^2 \left. \frac{d^2E}{d^2\rho} \right|_{\rho_0} = K_0 = 220\text{MeV} \)
- \( \rho_0 = 0.16\text{fm}^{-3} \)

\( T_0^{(0)} = -263 \text{ MeV} \)

\( T_3^{(0)} = 210.7 \text{ MeV} \)

\( \sigma^{(0)} = 1.25 \)

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$E$ in CoMD $T_4=32$ MeV

For different $\rho$ CoMD-II calculations in large spheres containing $A_1$ and $A_2$ particles- Coupling with the cooling-warming Pauli constraint

$S_v \propto \rho_A E_{kin}$

--Correct for surface-Fit the quantities with 2nd-order $\rho$-polynomial

--Numerical Minimization of the functional $E$ for Se-WPD under the conditions a),b),c),d)

Solution? 

Coupling of CoMD simulations of large spheres of NM with the solution of $E_{CoMD}$ functional satisfying the condition a,b,c,d.

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Results

Step - 0

0.85 ≤ γ ≤ 1.5
Acceptable EOS Sat. properties

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\[ E_{\text{sym}}^C(\rho, \beta) = E^C(\rho, \beta) - E^C(\rho, 0) \]
\[ = E_{\text{isv}}^C(\rho, \beta) - E_{\text{isv}}^C(\rho, 0) \]
\[ + E_{\text{kin}}(\rho, \beta) - E_{\text{kin}}(\rho, 0) \]

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\[ E_{\text{sym}}^C(\rho, \beta) = e_{\text{sym}}^C \beta^2. \]
In the correlated case the symmetry energy (with $T_4=32$ MeV) is slightly lower, about 1 MeV, compared to the Se-MF approximation.

\[ e_{\text{sym}}^c = \frac{T_4}{2\rho_0} F'(\gamma \overline{S}) \tilde{\rho}_A (1 + \alpha) + E_{\text{kin}} \]

**FIG. 11.** (Color online) (a) $e_{\text{sym}}^c$ as a function of the density is plotted for the indicated form factors. (b) $e_{\text{sym}}$ in the case of the Se-MFA.
Pressure and compressibility related to the symmetry energy

\[ e_{\text{sym}}(\rho) = e_{\text{sym}}(\rho_0) + \frac{L}{3} \left( \frac{\rho - \rho_0}{\rho_0} \right) + \frac{K_{\text{sym}}}{18} \left( \frac{\rho - \rho_0}{\rho_0} \right)^2 \]

Largest differences in \( K_{\text{sym}} \) as function of \( \gamma \) and \( L \)

\[ L = 3 \rho_0 \left. \frac{\partial e_{\text{sym}}}{\partial \rho} \right|_{\rho_0} \]

\[ K_{\text{sym}} = 18 \rho_0^2 \left. \frac{\partial^2 e_{\text{sym}}}{\partial^2 \rho} \right|_{\rho_0} \]

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• Experiment – Exochim collaboration

FIG. 3. (Color online) Comparison of experimental $\Delta M_{\text{nor}}$ distributions for selected semi-central events of $^{40}\text{Ca}+^{40}\text{Ca}$ (black dots), $^{40}\text{Ca}+^{48}\text{Ca}$ (red dashes) and $^{48}\text{Ca}+^{40}\text{Ca}$ (blue solid line) reactions. In the insert, we show the probability of populating the $\Delta M_{\text{nor}} \geq 0.4$ region (typical of HR events) as a function of the N/Z of the total system. Solid stars are experimental data, while lines are predictions of CoMD-II model calculations performed by using different options for the stiffness of the symmetry potential: Stiff1 (red dotted line), Stiff2 (blue dashed line) and Soft (green dash-dotted line).

FIG. 3 (color online). CoMD-II + GEMINI calculations (shaded area histogram) and experimental results (dotted histograms) for the $^{48}\text{Ca}$ case for (a),(b) Stiff1 parametrization; (c),(d) Soft parametrization; (e),(f) Stiff2 parametrization, dashed line CoMD-II calculations, without the GEMINI stage.
• Summary and Outlooks

• Parameters of a simple Skyrme interaction have been found able to describe, with the CoMD model, the main saturation proprieties of symmetric and asymmetric Nuclear Matter
• The obtained values show marked differences compared to the values which can be obtained in the corresponding Se-MF approximation.
• In particular, the parameter values describing the Iso-Scalar forces are correlated with the ones describing the Iso-Vectorial interaction
• The observed differences have been explained in term of the 2-body spatial correlation between nucleons generated through the usage of wave-packets to describe the single-particle wave functions. In this sense, the obtained results, strictly valid for the CoMD model, could acquire a more general meaning.
• The performed study suggests that the changes in the parameter values of the effective interaction and the related changes of behavior should be checked by the community involved in Molecular Dynamics calculations.

The obtained values of $K_{sym}$ are larger than the values produced in Se-MF approximation:
1) Larger value of $K_{asy}$ are obtained – comparison with experimental values
2) To check eventually for another family of $F(\vec{S}_v[p])$ functional to describe Iso-Vectorial interaction in SWPD.

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