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

M. Papa

Istituto Nazionale di Fisica Nucleare – Sezione di Catania
V. S.Sofia 64 95123 Catania Italy

3° International Symposyum on Nuclear Symmetry Energy

NSCL/FRIB, East Lansing, Michigan July 22 - 26, 2013

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(Stocastic-Semiclassical Mean-Field)
•QMD(direct), CoMD(direct+constraint), ImQMD, FMD, AMD (anti-symmetric)

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

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

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A simple effective N-N Interaction

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

2-body Iso-Scalar

"3-body" Iso-Scalar
ρ 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 ρ dependence of the symmetry energy (calculation based on realistic Interaction)

γ- degree of stiness for the isovect. interaction

•A short remind of the Se-MF approximation

$D(\mathbf{r},\mathbf{r}',\mathbf{p},\mathbf{p}')$ ≡ 2-body density in phase-space

Se-MF means: $D = D_1(\mathbf{r},\mathbf{p}) \cdot D_1(\mathbf{r}',\mathbf{p}')$ $\int D_1(\mathbf{r},\mathbf{p})d\mathbf{p} = \rho$

Due the properties of the δ in the Skyrme interaction:

$W = \frac{1}{2}\int V^{(2)}\rho^2 d\mathbf{r}$ ≡ Total interaction energy

E_{pot}=Interaction energy per Nucleon

$$
\begin{aligned}
E_{pot} &= U_{twb} + U_{trb} + U_{asy} \\
&= \frac{1}{2}V^{(2)}\rho = \frac{1}{2}\frac{T_0\rho}{\rho_0} + \frac{T_3\rho^\sigma}{(\sigma+1)\rho_0^\sigma} + \frac{1}{2}T_4F(\rho)\beta^2
\end{aligned}
$$

The total energy E per nucleon is a rather simple functional of ρ

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

$$E_{sym} = e_{sym}\beta^2$$

$$e_{sym} = \frac{1}{2}\left(\frac{\partial^2 E}{\partial \beta^2}\right)/_{\rho=\rho_0}$$
$$= \frac{1}{6}\frac{\hbar^2}{m_0}\left(\frac{3\pi^2\rho}{2}\right)^{2/3} + \frac{1}{2}T_4 F(\rho)$$

$$\rho_0 = 0.165\ fm^{-3}$$

$$E(\rho_0) = -16\ \mathrm{MeV}$$

$$\frac{dE}{d\rho}/\rho_0 = 0$$

$$9\rho_0^2\frac{d^2E}{d^2E}/\rho_0 = 220\ \mathrm{MeV}$$

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

$e_{sym}(\rho_0) \approx 28\text{-}30$ MeV ; $E(\rho_0) \approx -16$ MeV; $K_0 \approx 220\text{-}270$ MeV
$\rho_0 \approx 0.15\text{-}0.16$ (fm^{-3})

•The case of the SWPD-CoMD

$$\phi_i = \frac{1}{(2\pi\sigma_r^2)^{\frac{3}{4}}} exp[-\frac{(\mathbf{r}-\mathbf{r}_i)^2}{2\sigma_r^2} - i\frac{\mathbf{r}\mathbf{p}_i}{\hbar}]$$

WP with fixed widths $\sigma_r\sigma_p=1/2\ \eta$

$$f_i = \frac{1}{(2\pi\sigma_r\sigma_p)^3} exp[-\frac{(\mathbf{r}-\mathbf{r}_i)^2}{2\sigma_r^2} - \frac{(\mathbf{p}-\mathbf{p}_i)^2}{2\sigma_p^2}]$$

Single particle phace-space distribution

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

$$D_1(\mathbf{r},\mathbf{p}) = \sum_1^A f_i(\mathbf{r},\mathbf{p})$$

1-body density distribution

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

2-body density distribution

$$\boxed{D \neq D_1(\mathbf{r},\mathbf{p}) D_1(\mathbf{r}',\mathbf{p}')}$$

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 ≈1/(A_i-1); never small !!!

$$W = \frac{1}{2}\int V^{(2)} D(\mathrm{r},\mathrm{p},\mathrm{r}',\mathrm{p}')\delta(\mathrm{r}-\mathrm{r}')d\mathrm{r}d\mathrm{r}'\,d\mathrm{p}d\mathrm{p}' =$$

$$\frac{1}{2}\sum_{i\neq j=1}^{A}\int V^{(2)} f_i(\mathrm{r},\mathrm{p})\, f_j(\mathrm{r},\mathrm{p}')d\mathrm{r}d\mathrm{p}d\mathrm{p}'$$

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

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

$$S_v^i = \sum_{j\neq i=1}^{A} \frac{1}{(4\pi\sigma_r^2)^{3/2}} exp[-\frac{(\mathbf{r}_i - \mathbf{r}_j)^2}{4\sigma_r^2}]$$

σ_r determine the 2-body effective potential responsible for the dynamics of the WP centers with a characteristic width 2 times larger

$$\boxed{\begin{aligned} W_{twb} &= \frac{T_0 A}{2\rho_0}\overline{S_v} \\ U_{twb} &= \frac{W_{twb}}{A} = \frac{T_0}{2\rho_0}\overline{S_v} \end{aligned}}$$

$< S_v > \equiv$ Average overlap per nucleon

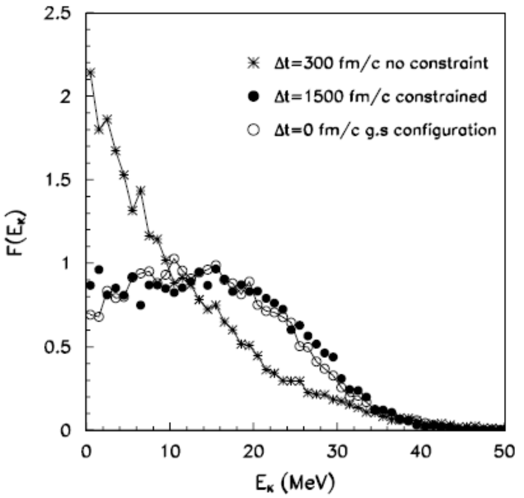
We have an analogy, unfortunately only formal, between $< S_v >$ and ρ

$$U_{trb} = = \frac{T_3}{(\sigma+1)\rho_0^\sigma}\overline{S_v}^\sigma$$

$$\tilde{\rho}^{nn} = \frac{1}{(4\pi\sigma_r^2)^{3/2}N^2}\sum_{i\neq j\in\mathbb{N}} exp[-\frac{(\mathbf{r}_i-\mathbf{r}_j)^2}{4\sigma_r^2}]$$

$$\tilde{\rho}^{pp} = \frac{1}{(4\pi\sigma_r^2)^{3/2}Z^2}\sum_{i\neq j\in\mathbb{Z}} exp[-\frac{(\mathbf{r}_i-\mathbf{r}_j)^2}{4\sigma_r^2}]$$

$$\tilde{\rho}^{np} = \frac{1}{(4\pi\sigma_r^2)^{3/2}2NZ}\sum_{i\neq j\in\mathbb{NZ}} exp[-\frac{(\mathbf{r}_i-\mathbf{r}_j)^2}{4\sigma_r^2}]$$



$$\overline{f_i} \leq 1 \quad (\text{for all } i),$$

$$\tilde{\rho} = \frac{N^2\widetilde{\rho^{nn}} + Z^2\widetilde{\rho^{pp}}}{N^2+Z^2}$$

$$\alpha = \frac{\widetilde{\rho^{np}} - \tilde{\rho}}{\tilde{\rho}}$$

α gives the enhancement of the np overlap

$$\overline{f_i} \equiv \sum_j \delta_{\tau_i,\tau_j}\delta_{s_i,s_j}\int_{h^3} f_j(\mathbf{r},\mathbf{p})d^3r d^3p.$$

The constraint based on Pauli principle determine the kinetic energy controbution

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

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

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

$$F'(\frac{\rho}{\rho_0}) \rightarrow F'(\frac{\bar{S}_v}{\bar{S}_{v0}})$$

$$U_{tot} = U_{tot}(\overline{S}_v, \tilde{\rho}, \alpha, \beta)$$

•Overlap integrals, ρ and spatial correlations

v(r)≡Spatial correlation function

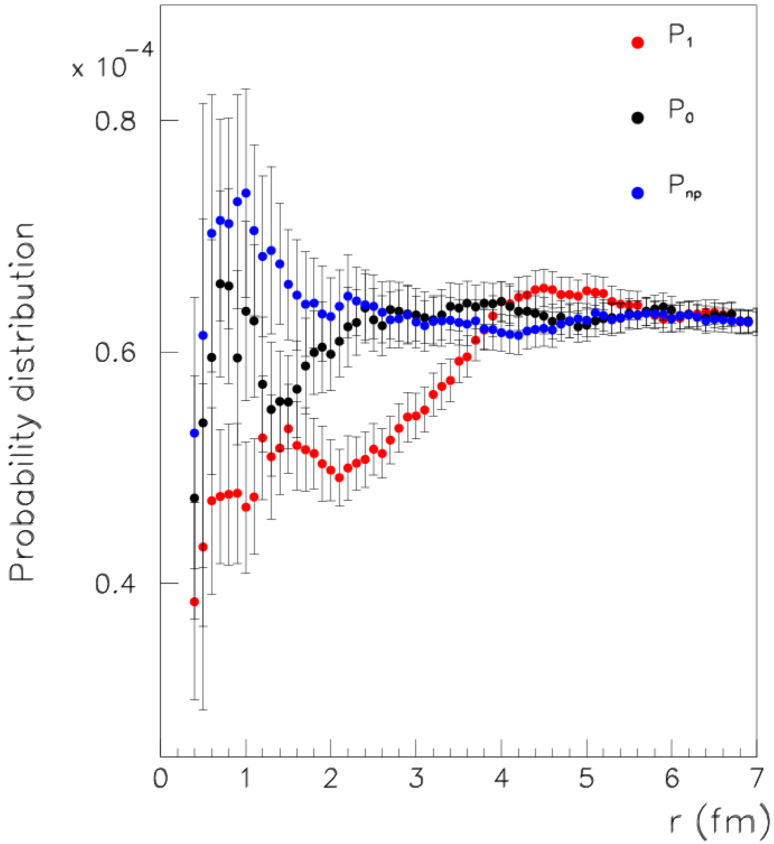
$$p = 1 \pm k_0 \nu(r) \qquad \nu(0) = 1 \qquad k_0 \geq 0$$

$$\lim_{r\to\infty} \nu(r) = 0$$

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

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

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



$$\overline{S_v} = \frac{\overline{S_v^T}}{A} = \frac{1}{(4\pi\sigma_r^2)^{3/2}} \int P(r) exp[-\frac{r^2}{4\sigma_r^2}] dV$$
$$= \rho(1 \pm I)$$

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

L≡characteristic length of ν

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

Se-MF limit

σ_r~1.15 fm mainly fixed to describe surface and radii of nuclei

Generalization to asymmetric systems

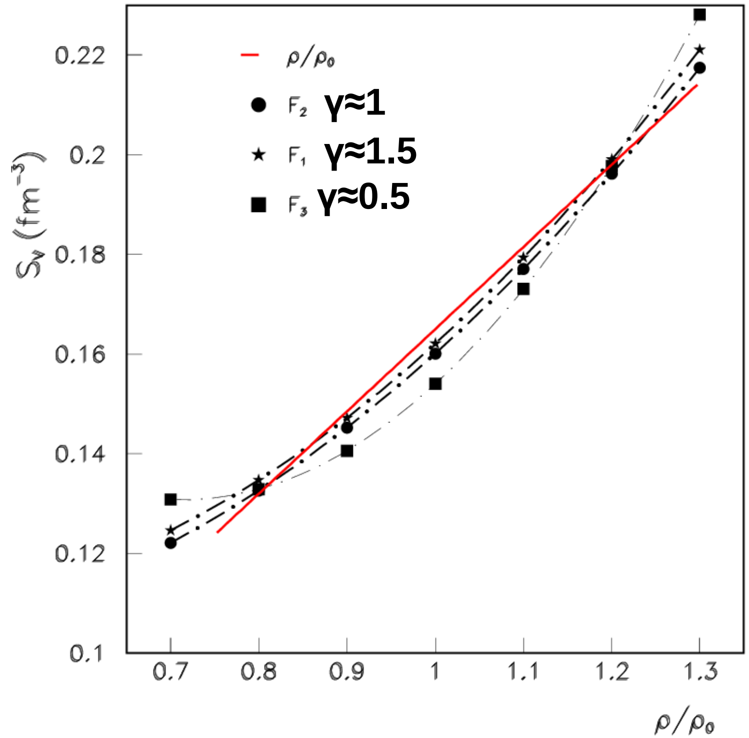
$$\overline{S_v} = \frac{\rho}{8}[8 + (1+\beta)^2(I_{0,-1} - I_{1,-1}) + (1-\beta)^2(I_{0,1} - I_{1,1}) + 4(1-\beta^2)I^0]$$

with analogous procedure for the other main quant: we get:

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

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

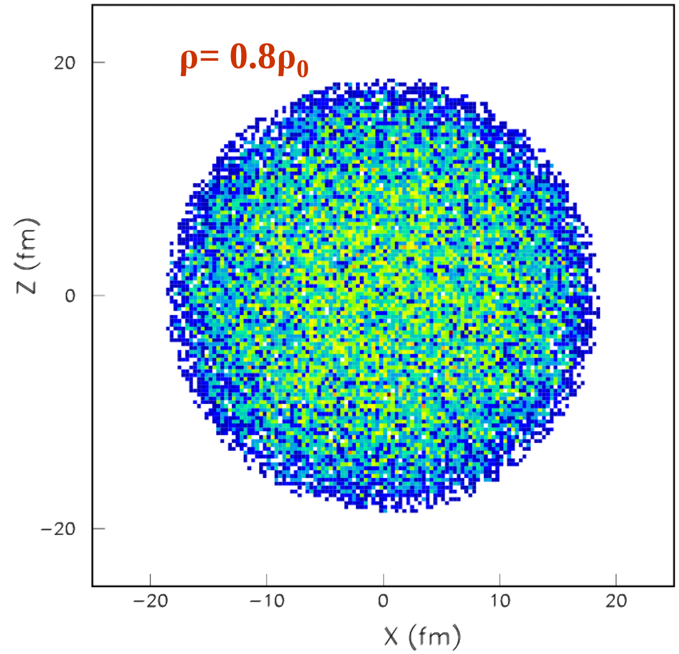
Corrected for surface effects



All these expressions keep the symmetry under the β→-β transformation

Both I^0,$I_{s,t}$ can have a dependence on ρ and β

In the explored range also a non linear behavior is observed well fitted with a 2th-order polynomial of ρ



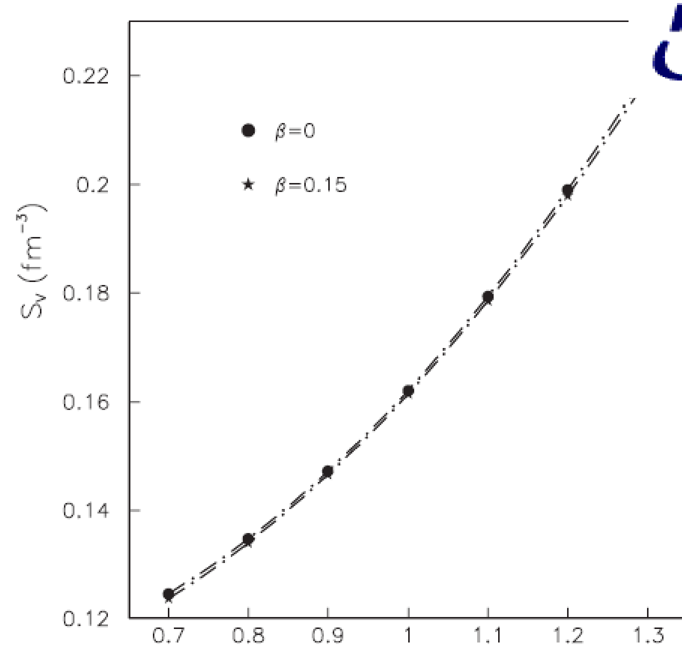


FIG. 3. Typical result for the total overlap per nucleon $\overline{S_v}$ as a function of the reduced density computed for two different values of the asymmetry parameter β as shown in the figure.

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 β values explored and within the precision of our calcolations we can assume no explicity dependence of S_v from β

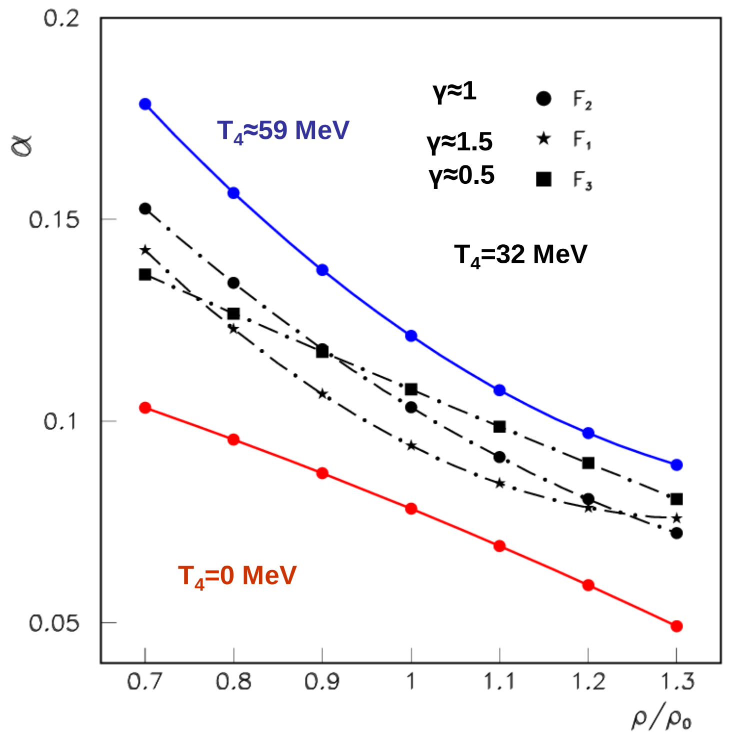
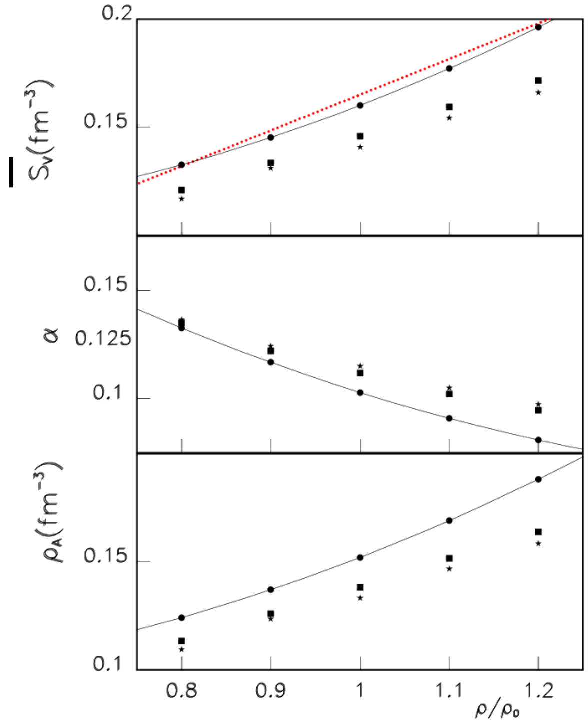


FIG. 6. (Color online) Final values of the α correlation coefficient for $\beta = 0$ as a function of reduced density and for different form factors F_k as indicated in the legend. The asterisk and full dot symbols (red and blue online) joined with continuous lines are associated to T_4 values 0 and 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.

•Surface effects



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

Microscopic simulations have been performed for two large spheres containing1600 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 then 5% .

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

•The iterative procedure **Step 0**

$\boxed{\text{E in Se-MF } \beta=0}$

a) $E(\rho_0) = -16 MeV$

b) $\left.\dfrac{dE}{d\rho}\right|_{\rho_0} = 0$

c) $9\rho_0{}^2 \left.\dfrac{d^2E}{d^2\rho}\right|_{\rho_0} = K_0 = 220 MeV$

d) $\rho_0 = 0.16\, fm^{-3}$

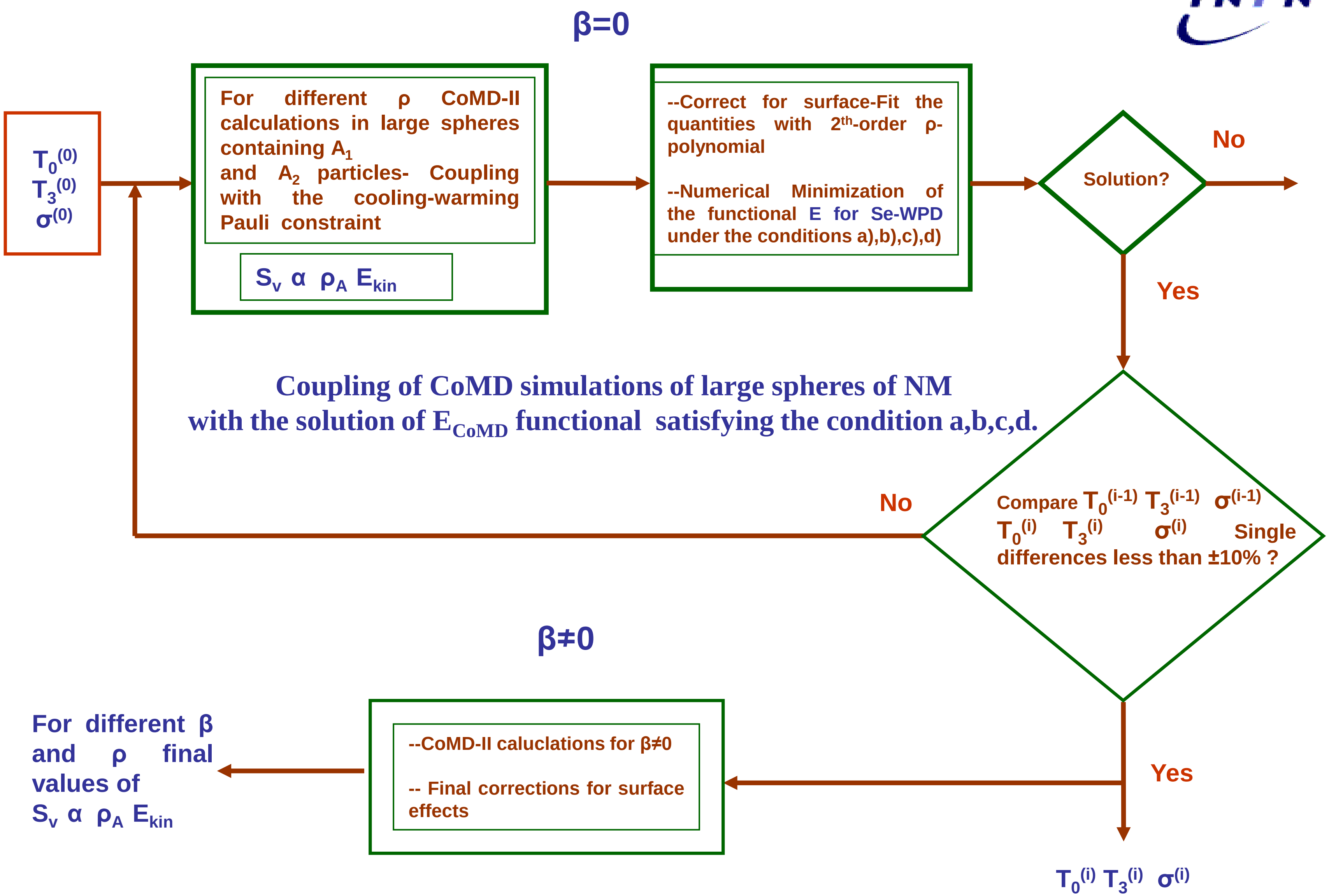
$\longleftrightarrow$

$T_0^{(0)}$ = -263 MeV

$T_3^{(0)}$ = 210.7 MeV

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

E in CoMD T_4=32 MeV



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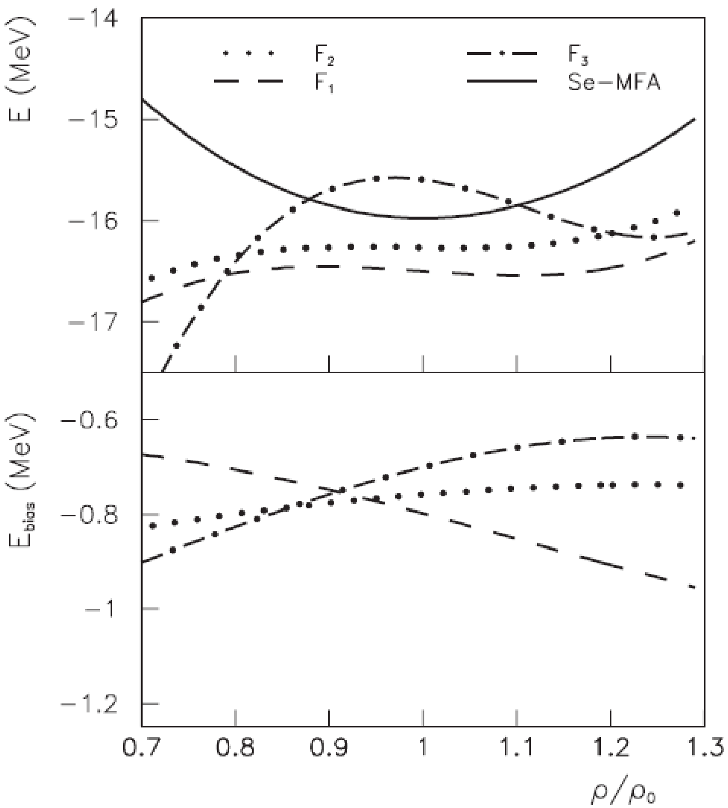
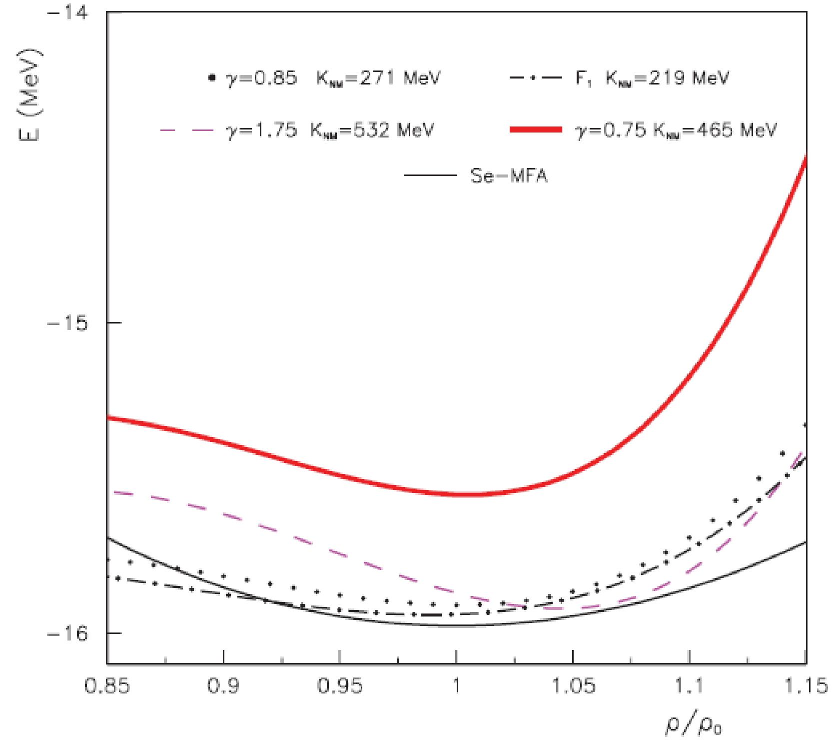
• Results



Step - 0

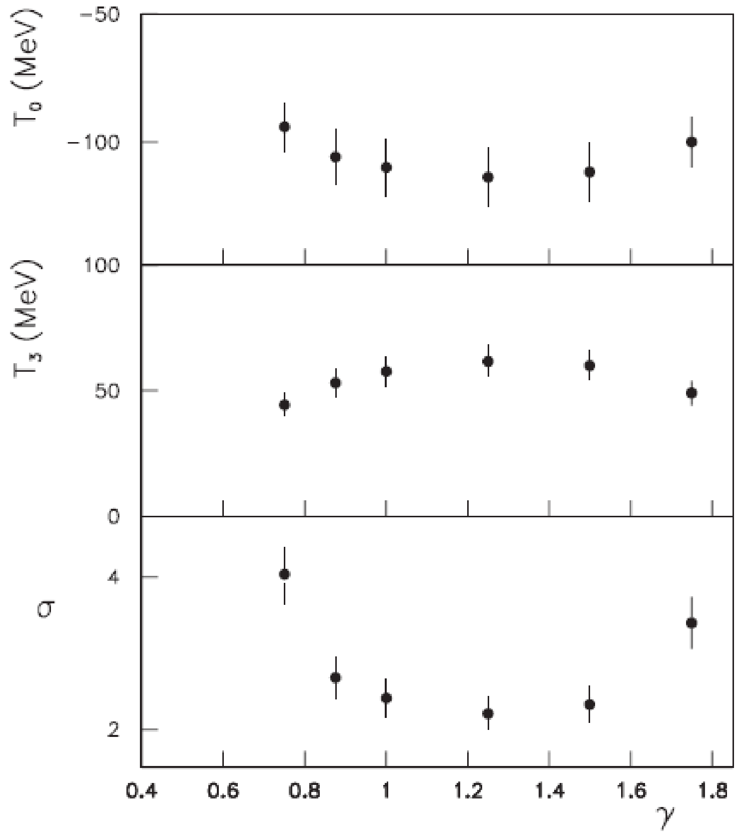


After the iterative procedure

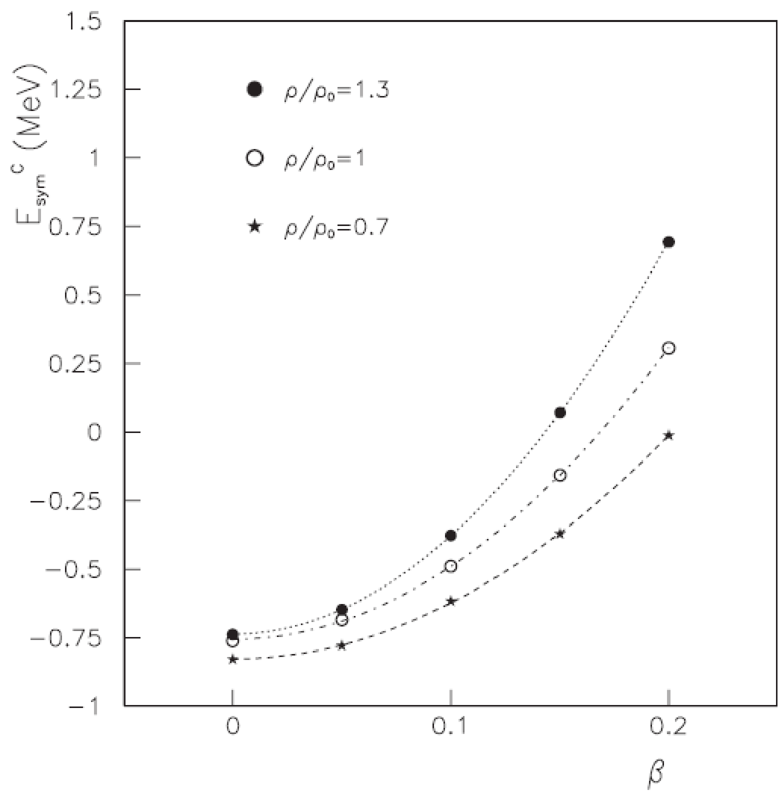
$$0.85 \leq \gamma \leq 1.5$$

Acceptable EOS Sat. properties

$$
\begin{aligned}
E^C_{\rm sym}(\rho,\beta) &= E^C(\rho,\beta) - E^C(\rho,0) \\
&= E^C_{\rm isv}(\rho,\beta) - E^C_{\rm isv}(\rho,0) \\
&\quad + E_{\rm kin}(\rho,\beta) - E_{\rm kin}(\rho,0)
\end{aligned}
$$



d



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$$\boxed{E^C_{\rm sym}(\rho,\beta) = e^C_{\rm sym}\beta^2.}$$

$$e_{sym}^{c} = \frac{T_4}{2\rho_0} F'_{\gamma}(\bar{S}_v)\tilde{\rho}_A(1+\alpha) + E_{kin}$$

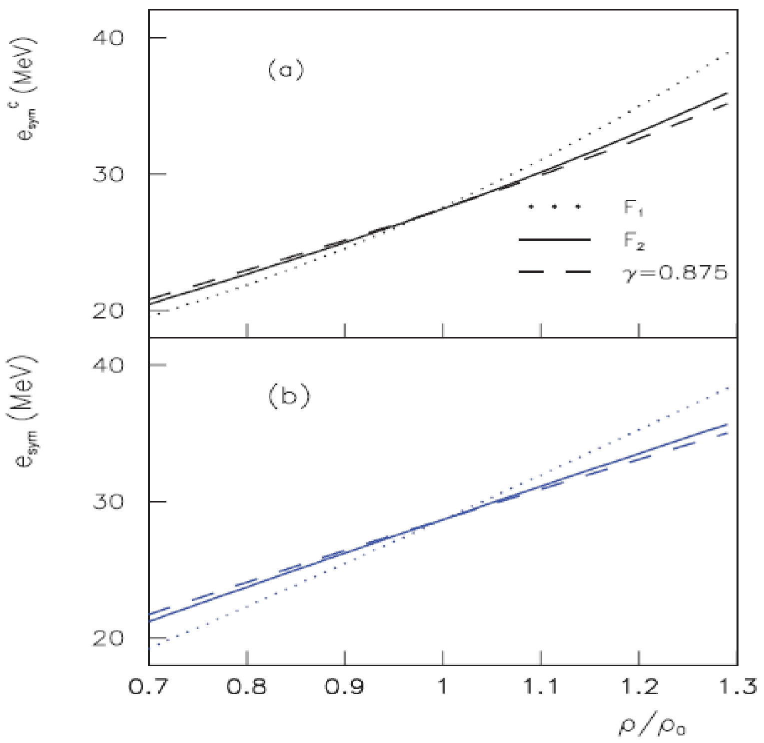


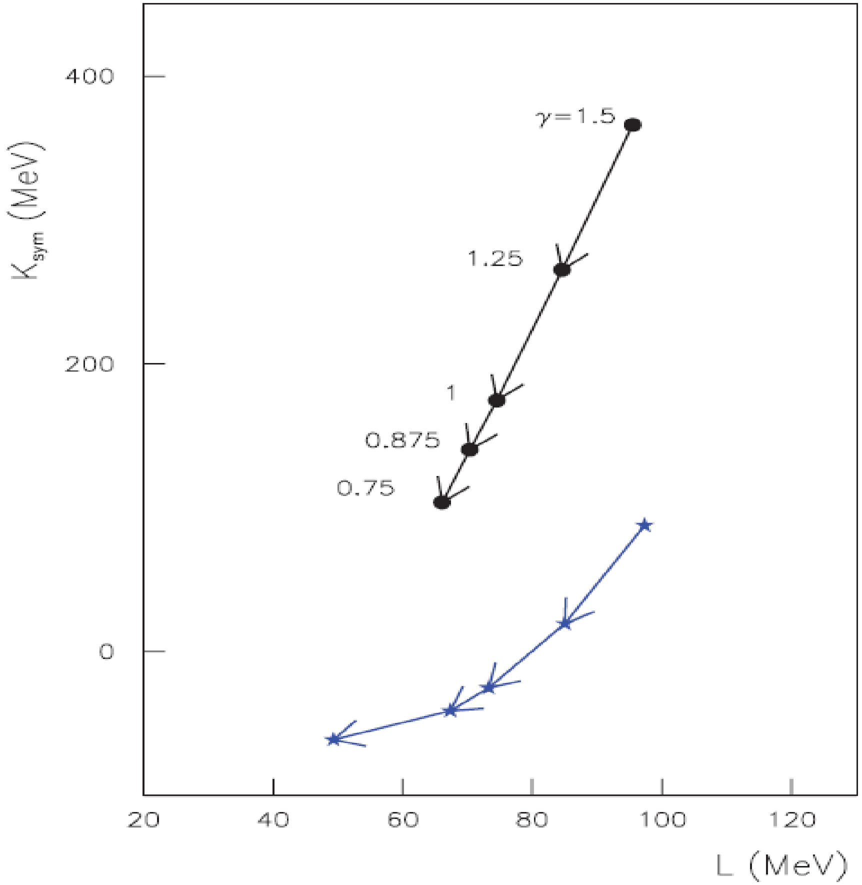
FIG. 11. (Color online) (a) $e^{C}_{\rm sym}$ as a function of the density is plotted for the indicated form factors. (b) $e_{\rm sym}$ in the case of the Se-MFA.

In the correlated case the symmetry energy (with T_4=32 MeV) is slightly lower, about 1 MeV, compared to the Se-MF approximation

$$e_{sym} = \frac{T_4}{2\rho_0} F_{\gamma}(\rho) + E_{kin}$$

Pressure and compressibility related to the symmetry energy

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



Largest differences in K_{sym} as function of γ and L

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

$$K_{sym} = 18\rho_0^{\,2} \left.\frac{\partial^2 e_{sym}}{\partial^2 \rho}\right|_{\rho_0}$$

• Experiment – Exochim collaboration

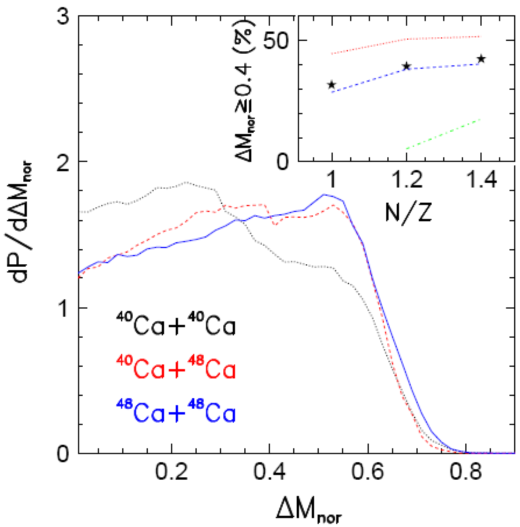


FIG. 3. (Color online) Comparison of experimental ΔM_{nor} distributions for selected semi-central events of ^{40}Ca+^{40}Ca (black dots), ^{40}Ca+^{48}Ca (red dashes) and ^{48}Ca+^{40}Ca (blue solid line) reactions. In the insert, we show the probability of populating the $\Delta M_{nor} \geq 0.4$ region (typical of HR events) as a function of the N/Z of the total system. Solid stars are experimental data, while lines are the 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).

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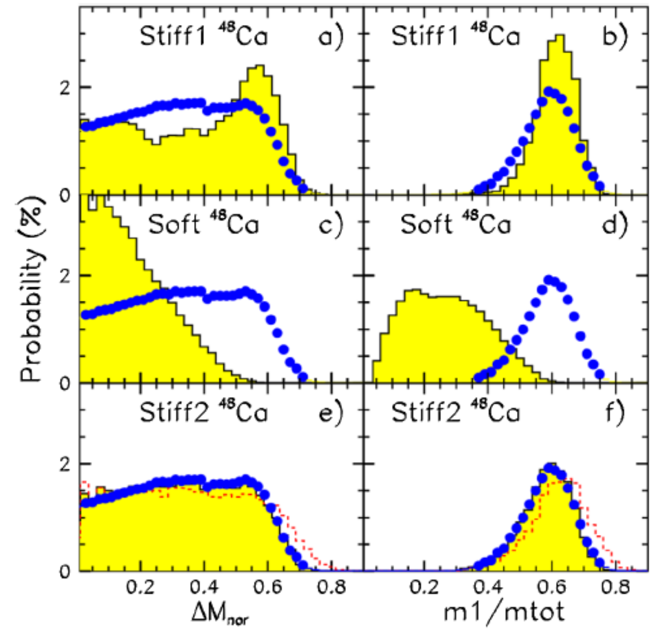

FIG. 3 (color online). CoMD-II + GEMINI calculations (shaded area histogram) and experimental results (dotted histograms) for the ^{48}Ca case for (a),(b) Stiff1 parametrization; (c),(d) Soft parametrization; (e),(f) Stiff2 parametrization, dashed line CoMD-II calculations, without the GEMINI stage.

• 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 cecked 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 $F(\overline{S}_v[\rho])$ functional to describe Iso-Vectorial interaction in SWPD.

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