Mean-field calculations with regularized pseudopotentials
(2- and 3-body)

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Effective field theories for nuclei and nuclear matter

Outline

Motivation (in a nutshell)

- Effective interactions (pseudopotentials) and/or functionals are the key ingredient for mean-field and beyond-mean-field calculations.

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- A two-body interaction (whatever it is) can not give a satisfying description of infinite nuclear matter (*e.g.* $m^*/m \sim 0.4$ ☹).

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- A two-body density dependent interaction is fine for mean-field calculations but leads to formal questions and calculation's problems which may (or may not?) be overcome.

  May:
  - M. Bender *et al.*, PRC 79, 044319 (2009)
  - T.R. Rodríguez, J.L. Egido, PRC 81, 064323 (2010)
  - G. Hupin *et al.*, PRC 84, 014309 (2011)
  - W. Satuła, J. Dobaczewski, PRC 90, 054303 (2014)

  May not:
  - T. Duguet *et al.*, PRC 79, 044320 (2009)
  - L. Robledo, JPG 37, 064020 (2010)

Choice for the effective interaction

Radical solution: no density dependent term

$$V = V_{2-\mathrm{body}} + V_{3-\mathrm{body}} \quad \text{and} \quad \begin{aligned} E &= \langle\Phi| \, (T + V) \, |\Phi\rangle \\ &= E_H + E_F + E_P \, . \end{aligned}$$

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- 2-body part: zero-range, finite-range ?
  ⇒ Finite-range (Coulomb has to be treated exactly anyway...)

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- 2-body part: zero-range, finite-range ?
  ⇒ Finite-range (Coulomb has to be treated exactly anyway...)
- 3-body part: zero-range, finite-range ?

Zero-range: not fully satisfying,
Finite-range: too much time-consuming,
⇒ something between.

Finite-range two-body pseudopotentials[1]

- General idea:

  take a Skyrme interaction and replace $\delta(\mathbf{r})$ with $g_a(\mathbf{r}) = \frac{e^{-\frac{r^2}{a^2}}}{(a\sqrt{\pi})^3}$

- Pseudopotential at "NLO"

$$\begin{aligned} v &= \tilde{v}_0(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4)\left(W_0 1_{\sigma q} + B_0 1_q \hat{P}^\sigma - H_0 1_\sigma \hat{P}^q - M_0 \hat{P}^\sigma \hat{P}^q\right) \\ &+ \tilde{v}_1(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4)\left(W_1 1_{\sigma q} + B_1 1_q \hat{P}^\sigma - H_1 1_\sigma \hat{P}^q - M_1 \hat{P}^\sigma \hat{P}^q\right) \\ &+ \tilde{v}_2(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4)\left(W_2 1_{\sigma q} + B_2 1_q \hat{P}^\sigma - H_2 1_\sigma \hat{P}^q - M_2 \hat{P}^\sigma \hat{P}^q\right) \end{aligned}$$

with

$$\begin{aligned} \tilde{v}_0(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) &= \delta(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_2-\mathbf{r}_4)g_a(\mathbf{r}_1-\mathbf{r}_2) \\ \tilde{v}_1(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) &= \delta(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_2-\mathbf{r}_4)g_a(\mathbf{r}_1-\mathbf{r}_2)\,\frac{1}{2}\left[\mathbf{k}_{12}^{*2} + \mathbf{k}_{34}^2\right] \\ \tilde{v}_2(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) &= \delta(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_2-\mathbf{r}_4)g_a(\mathbf{r}_1-\mathbf{r}_2)\,\mathbf{k}_{12}^{*}\cdot\mathbf{k}_{34} \end{aligned}$$

- Thanks to the finite range: $\hat{P}^\sigma \hat{P}^q \equiv -\hat{P}^x \not\equiv \pm 1$
- Can be generalized at N^2LO, N^3LO, ...

[1] *Cf* Jacek's presentation from yesterday

Finite-range two-body local pseudopotentials

- The conditions

$$W_1 = -W_2\,, \quad B_1 = -B_2\,, \quad H_1 = -H_2\,, \quad M_1 = -M_2$$

  (and same for higher order terms) make the pseudopotential local
- These are **severe** restrictions on the flexibility of the functional
- ... but this greatly simplifies the implementation in computer codes
- ... and limits the number of free parameters
- Use of a standard two-body zero-range spin-orbit interaction

Options for terms beyond two-body

- Contact LO 3- and 4-body terms: SLyMR0 interaction

  J. Sadoudi *et al.*, Phys. Scr. T154 (2013) 014013, B. Bally *et al.*, PRL 113, 162501 (2014)

- Contact LO and NLO 3-body terms: SLyMR1 interaction

  J. Sadoudi *et al.*, PRC 88 (2013) 064326, R. Jodon, Phys. PhD Thesis, tel-01158085

  See recent preprint arXiv:2301.02420 "The shape of gold", by B. Bally, G. Giacolone and M. Bender.
  Works pretty well in some limited regions of the nuclear chart (*e.g.* for gold[2]).

[2] If I was working for gold, I wouldn't be a physicist.

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  Works pretty well in some limited regions of the nuclear chart (*e.g.* for gold[2]).

- Finite-range 2-body + zero-range 3-body $\Rightarrow$ pathological pairing.
- Semi-regularized three-body interaction: symmetrized version of

$$V_3(x_1,x_2,x_3;x_4,x_5,x_6) = W_3 \overbrace{\delta(\mathbf{r}_{14})\delta(\mathbf{r}_{25})\delta(\mathbf{r}_{36})}^{\text{locality}} \delta_{q_1 q_4}\delta_{q_2 q_5}\delta_{q_3 q_6}$$
$$\times\, \delta_{s_1 s_4} \underbrace{(\delta_{s_2 s_5}\delta_{s_3 s_6} + \delta_{s_2 s_6}\delta_{s_3 s_5})}_{=\mathbb{1}^{\sigma}_{23}+P^{\sigma}_{23}} \underbrace{g_a(\mathbf{r}_{12})}_{\text{finite range}} \underbrace{\delta(\mathbf{r}_{23})}_{\text{zero range}}$$

with $x \equiv \mathbf{r}sq$ and $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$.

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EDF from the semi-regularized three-body term

- Normal part

$$E = \frac{W_3}{8}\int \mathrm{d}^3 r_1\,\mathrm{d}^3 r_2\, g_a(\mathbf{r}_{12})\Big\{\rho_0(\mathbf{r}_2)\rho_0^2(\mathbf{r}_1) - \rho_0(\mathbf{r}_1)\rho_1^2(\mathbf{r}_2) + \frac{1}{3}\,\rho_0(\mathbf{r}_2)\mathbf{s}_0^2(\mathbf{r}_1) - \frac{1}{3}\,\rho_0(\mathbf{r}_2)\mathbf{s}_1^2(\mathbf{r}_1)$$
$$- \frac{1}{4}\Big[\rho_0(\mathbf{r}_1) + \rho_0(\mathbf{r}_2)\Big]\Big[\rho_0(\mathbf{r}_2,\mathbf{r}_1)\rho_0(\mathbf{r}_1,\mathbf{r}_2) + \rho_1(\mathbf{r}_2,\mathbf{r}_1)\rho_1(\mathbf{r}_1,\mathbf{r}_2)$$
$$+ \mathbf{s}_0(\mathbf{r}_2,\mathbf{r}_1)\cdot\mathbf{s}_0(\mathbf{r}_1,\mathbf{r}_2) + \mathbf{s}_1(\mathbf{r}_2,\mathbf{r}_1)\cdot\mathbf{s}_1(\mathbf{r}_1,\mathbf{r}_2)\Big]$$
$$+ \frac{1}{2}\Big[\rho_1(\mathbf{r}_1) + \rho_1(\mathbf{r}_2)\Big]\Big[\rho_0(\mathbf{r}_2,\mathbf{r}_1)\rho_1(\mathbf{r}_1,\mathbf{r}_2) + \mathbf{s}_0(\mathbf{r}_2,\mathbf{r}_1)\cdot\mathbf{s}_1(\mathbf{r}_1,\mathbf{r}_2)\Big]$$
$$- \frac{1}{6}\Big[\mathbf{s}_0(\mathbf{r}_1) + \mathbf{s}_0(\mathbf{r}_2)\Big]\cdot\Big[\mathbf{s}_0(\mathbf{r}_2,\mathbf{r}_1)\rho_0(\mathbf{r}_1,\mathbf{r}_2) + \mathbf{s}_1(\mathbf{r}_2,\mathbf{r}_1)\rho_1(\mathbf{r}_1,\mathbf{r}_2)\Big]$$
$$+ \frac{1}{6}\Big[\mathbf{s}_1(\mathbf{r}_1) + \mathbf{s}_1(\mathbf{r}_2)\Big]\cdot\Big[\mathbf{s}_0(\mathbf{r}_2,\mathbf{r}_1)\rho_1(\mathbf{r}_1,\mathbf{r}_2) + \mathbf{s}_1(\mathbf{r}_2,\mathbf{r}_1)\rho_0(\mathbf{r}_1,\mathbf{r}_2)\Big]\Big\}\,.$$

- Pairing part

$$E_P = \frac{W_3}{8}\int \mathrm{d}^3 r_1\,\mathrm{d}^3 r_2\, g_a(\mathbf{r}_{12})\sum_q\Big\{\Big[\rho_q(\mathbf{r}_1) + \rho_q(\mathbf{r}_2)\Big]\Big[\tilde{\rho}_{\bar{q}}^*(\mathbf{r}_1,\mathbf{r}_2)\tilde{\rho}_{\bar{q}}(\mathbf{r}_1,\mathbf{r}_2) + \tilde{\mathbf{s}}_{\bar{q}}^*(\mathbf{r}_1,\mathbf{r}_2)\cdot\tilde{\mathbf{s}}_{\bar{q}}(\mathbf{r}_1,\mathbf{r}_2)\Big]$$
$$+\frac{1}{3}\Big[\mathbf{s}_q(\mathbf{r}_1) - \mathbf{s}_q(\mathbf{r}_2)\Big]\cdot\Big[\tilde{\rho}_{\bar{q}}^*(\mathbf{r}_1,\mathbf{r}_2)\tilde{\mathbf{s}}_{\bar{q}}(\mathbf{r}_1,\mathbf{r}_2) + \tilde{\mathbf{s}}_{\bar{q}}^*(\mathbf{r}_1,\mathbf{r}_2)\tilde{\rho}_{\bar{q}}(\mathbf{r}_1,\mathbf{r}_2)\Big]\Big\}\,.$$

EDF from the semi-regularized three-body term

- Pairing part

$$E_P = \frac{W_3}{8} \int \mathrm{d}^3 r_1 \, \mathrm{d}^3 r_2 \, g_a(\mathbf{r}_{12}) \times \sum_q \Big\{ \Big[\rho_q(\mathbf{r}_1) + \rho_q(\mathbf{r}_2) \Big] \Big[\tilde{\rho}^*_{\bar{q}}(\mathbf{r}_1, \mathbf{r}_2) \tilde{\rho}_{\bar{q}}(\mathbf{r}_1, \mathbf{r}_2) + \tilde{\mathbf{s}}^*_{\bar{q}}(\mathbf{r}_1, \mathbf{r}_2) \cdot \tilde{\mathbf{s}}_{\bar{q}}(\mathbf{r}_1, \mathbf{r}_2) \Big] + \frac{1}{3} \Big[\mathbf{s}_q(\mathbf{r}_1) - \mathbf{s}_q(\mathbf{r}_2) \Big] \cdot \Big[\tilde{\rho}^*_{\bar{q}}(\mathbf{r}_1, \mathbf{r}_2) \tilde{\mathbf{s}}_{\bar{q}}(\mathbf{r}_1, \mathbf{r}_2) + \tilde{\mathbf{s}}^*_{\bar{q}}(\mathbf{r}_1, \mathbf{r}_2) \tilde{\rho}_{\bar{q}}(\mathbf{r}_1, \mathbf{r}_2) \Big] \Big\} .$$

Does not depend on the local pairing densities ! No cut-off needed !

(as long as we don't mix protons and neutrons.)

Finite-range Gogny pseudopotentials

- Gaussian form factors + zero-range DD term = D1S

$$V_{D1S}(x_1,x_2;x_3,x_4) = \Bigg[\sum_{j=1,2} \mathrm{e}^{-\frac{\mathbf{r}_{12}^2}{\mu_j^2}} \left(W_j \mathbb{1}^\sigma \mathbb{1}^q + B_j P^\sigma \mathbb{1}^q - H_j \mathbb{1}^\sigma P^q - M_j P^\sigma P^q\right)$$
$$+ t_3 \left(\mathbb{1}^\sigma + P^\sigma\right) \mathbb{1}^q \rho_0^\alpha(\mathbf{r}_1)\delta(\mathbf{r}_{12})$$
$$+ \mathrm{i}\, W_0\, \mathbb{1}^q \left(\delta_{\sigma_1\sigma_3}\boldsymbol{\sigma}_{\sigma_2\sigma_4} + \boldsymbol{\sigma}_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\right) \cdot \left(\mathbf{k}_{12}^* \times \mathbf{k}_{34}\right)\Bigg]$$

J.F. Berger *et al.*, CPC 63 (1991) 365

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$$
\begin{aligned}
V_{D1S}(x_1,x_2;x_3,x_4) = \Bigg[& \sum_{j=1,2} \mathrm{e}^{-\frac{\mathbf{r}_{12}^2}{\mu_j^2}} \left(W_j \mathbb{1}^\sigma \mathbb{1}^q + B_j P^\sigma \mathbb{1}^q - H_j \mathbb{1}^\sigma P^q - M_j P^\sigma P^q\right) \\
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& + \mathrm{i}\, W_0\, \mathbb{1}^q \left(\delta_{\sigma_1\sigma_3}\boldsymbol{\sigma}_{\sigma_2\sigma_4} + \boldsymbol{\sigma}_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\right) \cdot \left(\mathbf{k}_{12}^* \times \mathbf{k}_{34}\right) \Bigg]
\end{aligned}
$$

J.F. Berger *et al.*, CPC 63 (1991) 365

- Gaussian form factors + finite-range DD term = D2

$$
\begin{aligned}
V_{D2}(x_1,x_2;x_3,x_4) = \Bigg[& \sum_{j=1,2} \mathrm{e}^{-\frac{\mathbf{r}_{12}^2}{\mu_j^2}} \left(W_j \mathbb{1}^\sigma \mathbb{1}^q + B_j P^\sigma \mathbb{1}^q - H_j \mathbb{1}^\sigma P^q - M_j P^\sigma P^q\right) \\
& + \frac{\mathrm{e}^{-\frac{\mathbf{r}_{12}^2}{\mu_3^2}}}{\left(\mu_3\sqrt{\pi}\right)^3} \frac{\rho_0^\alpha(\mathbf{r}_1) + \rho_0^\alpha(\mathbf{r}_2)}{2} \left(W_3 \mathbb{1}^\sigma \mathbb{1}^q + B_3 P^\sigma \mathbb{1}^q - H_3 \mathbb{1}^\sigma P^q - M_3 P^\sigma P^q\right) \\
& + \mathrm{i}\, W_0\, \mathbb{1}^q \left(\delta_{\sigma_1\sigma_3}\boldsymbol{\sigma}_{\sigma_2\sigma_4} + \boldsymbol{\sigma}_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\right) \cdot \left(\mathbf{k}_{12}^* \times \mathbf{k}_{34}\right) \Bigg]
\end{aligned}
$$

F. Chappert *et al.*, PRC 91, 034312 (2015)

Finite-range Gogny pseudopotentials

Density dependent part of D2 effective interaction

$$\frac{e^{-\frac{\mathbf{r}_{12}^2}{\mu_3^2}}}{\left(\mu_3\sqrt{\pi}\right)^3} \frac{\rho_0^\alpha(\mathbf{r}_1) + \rho_0^\alpha(\mathbf{r}_2)}{2} \left(W_3 \mathbb{1}^\sigma \mathbb{1}^q + B_3 P^\sigma \mathbb{1}^q - H_3 \mathbb{1}^\sigma P^q - M_3 P^\sigma P^q\right)$$

and three-body semi-regularized pseudopotential

$$W_3\, \delta(\mathbf{r}_{14})\delta(\mathbf{r}_{25})\delta(\mathbf{r}_{36})\delta_{q_1 q_4}\delta_{q_2 q_5}\delta_{q_3 q_6}\delta_{s_1 s_4}\left(\delta_{s_2 s_5}\delta_{s_3 s_6} + \delta_{s_2 s_6}\delta_{s_3 s_5}\right)\, g_a(\mathbf{r}_{12})\, \delta(\mathbf{r}_{23})$$

lead to similar terms in the functional *i.e.*

$$\rho^\alpha(\mathbf{r}_1)\rho(\mathbf{r}_1,\mathbf{r}_2)\rho(\mathbf{r}_2,\mathbf{r}_1) \quad \text{and} \quad \rho^\alpha(\mathbf{r}_1)\tilde{\rho}(\mathbf{r}_1,\mathbf{r}_2)\tilde{\rho}(\mathbf{r}_2,\mathbf{r}_1)$$

with $\alpha = \frac{1}{3}$ (Gogny D2) or $\alpha = 1$ (semi-regularized).

$\Rightarrow$ doable in deformed (axial) calculations.

Overview of the fits of the parameters

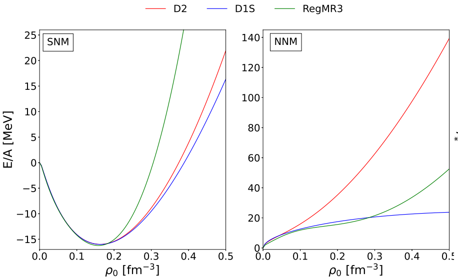
Many parameters to fit... Two-body up to N^3LO, spin-orbit, three-body.

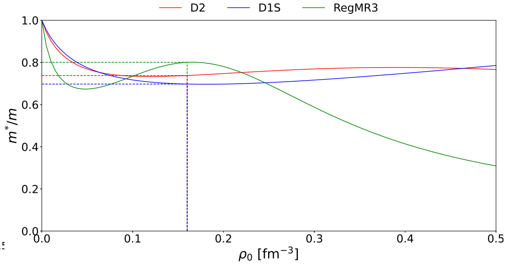
Minimization of a penalty function built from:

- Infinite nuclear matter properties ($\rho_{\rm sat}$, E/A, K_∞, m^*/m, J, L)
- Neutron matter equation of state
- Simple constraints on pairing strengths (strong enough scalar pairing and weak enough vector pairing)
- Binding energies of spherical nuclei
- Single particle energies in ^{208}Pb
- Charge radii
- Finite-size instabilities taken care using constraints on charge density profiles

The result is not a final set of parameters but a **proof of principle** that such an interaction can give a reasonable description of nuclei.

Properties of infinite nuclear matter

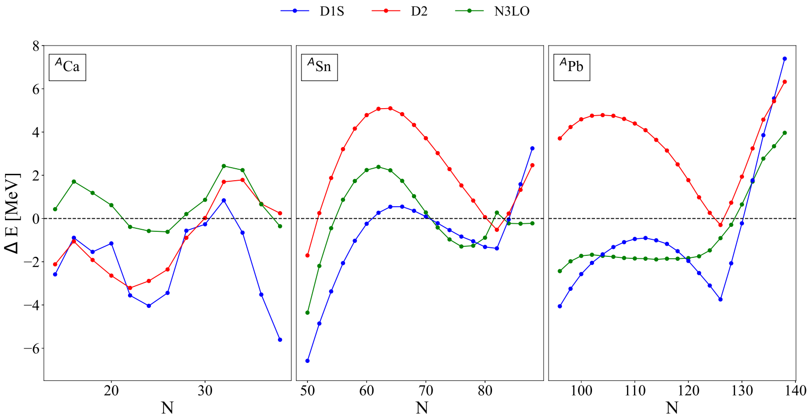




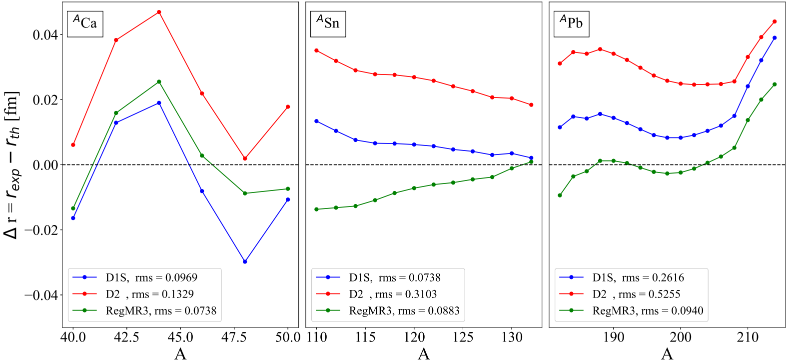
	ρ_{sat} [fm^{-3}]	E/A [MeV]	K_∞ [MeV]	J [MeV]	L [MeV]	m^*/m
D2	0.163	-16.000	209.251	31.110	44.831	0.738
D1S	0.163	-16.007	202.840	31.125	22.441	0.697
RegMR3	0.158 ☺	-16.237 ☺	285.654 ☹	31.954 ☺	12.798 ☹	0.800 ☺

Semi-magic nuclei: binding energy residuals

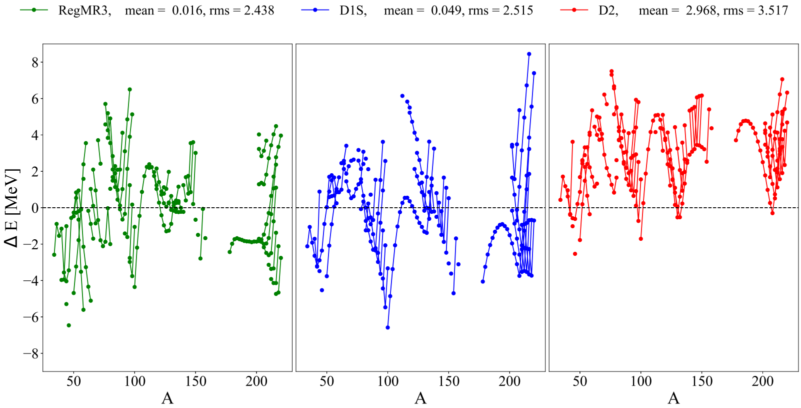
Comparison with Gogny interactions is not a beauty pageant



Semi-magic nuclei: charge radii



Spherical nuclei: binding energy residuals

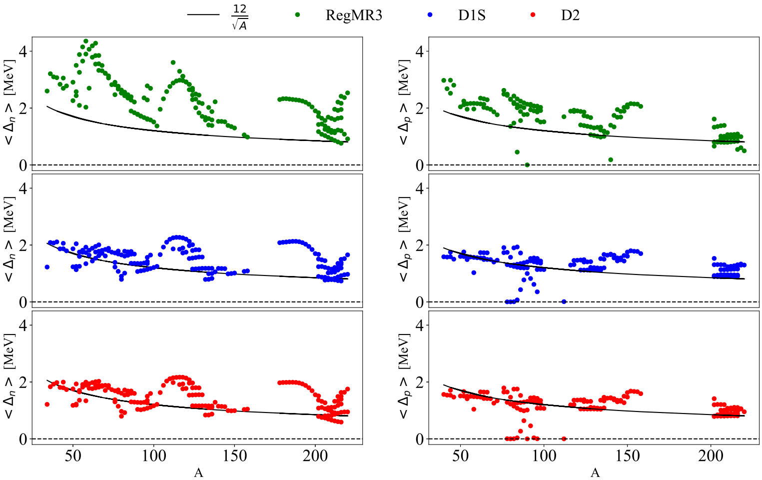


Set of 214 nuclei with $Z \geqslant 20$ predicted as (quasi-)spherical by D1S

www-phynu.cea.fr/science_en_ligne/carte_potentiels_microscopiques/carte_potentiel_nucleaire_eng.htm

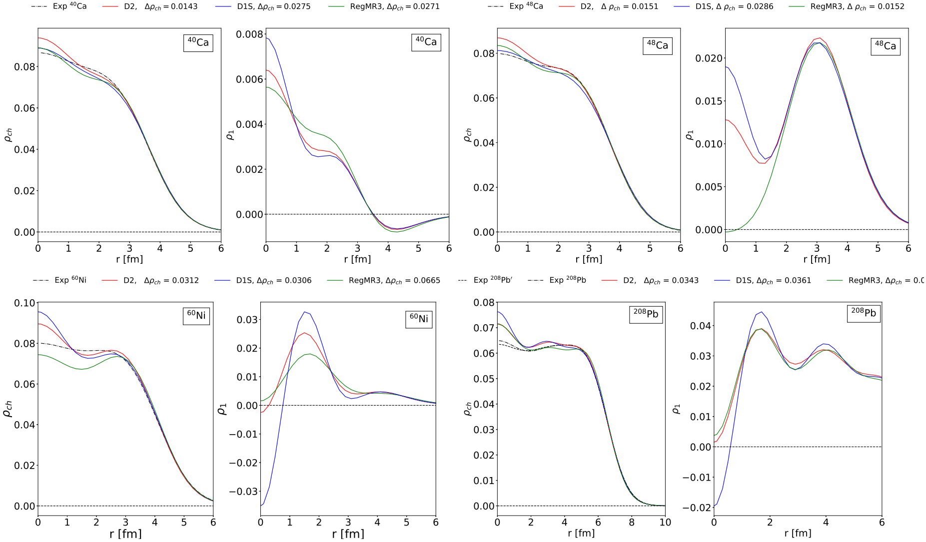
or google it...

Average neutron and proton gaps



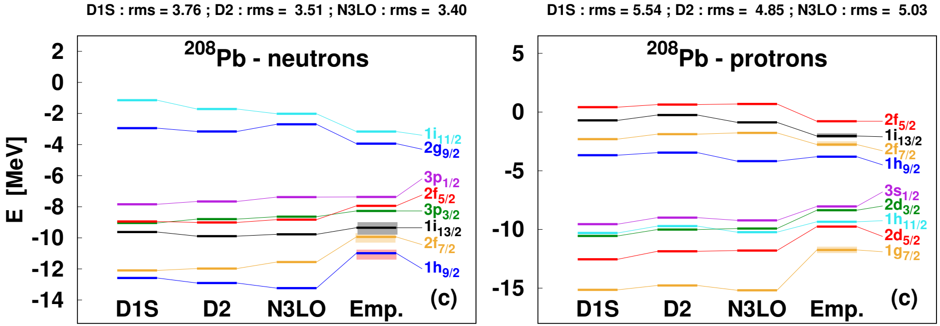
(Coulomb interaction included in the pairing channel)

Charge and isovector densities



Exp: H. de Vries *et al.*, ADNDT 36 (1987)

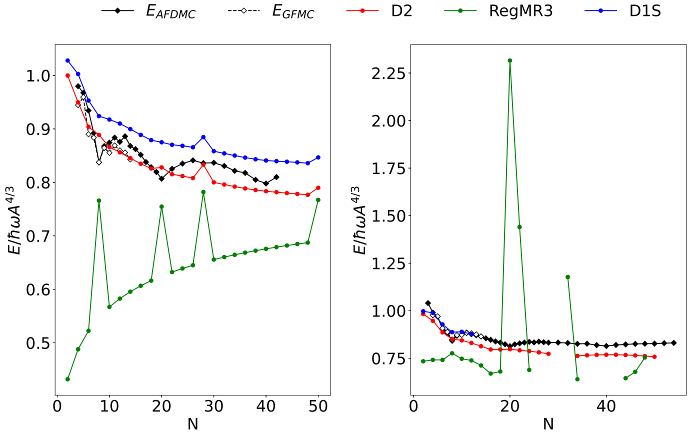
Single particle energies in ^{208}Pb



Effective mass probably to low near the nucleus surface...

Neutron droplets

S. Gandolfi *et al.* PRL 106, 012501 (2011)



Impressively catastrophic !

Pairing in symmetric and neutron matter

- Symmetric matter

	Gogny D1S	Gogny D2	RegMR3
2-body	$\sum_q \tilde{\rho}_q \tilde{\rho}_q$ attractive	$\sum_q \tilde{\rho}_q \tilde{\rho}_q$ attractive	$\sum_q \tilde{\rho}_q \tilde{\rho}_q$ attractive
3-body or d.d.	– –	$\rho_0^\alpha \sum_q \tilde{\rho}_q \tilde{\rho}_q$ repulsive	$\sum_q \rho_{\bar{q}} \tilde{\rho}_q \tilde{\rho}_q$ repulsive

- Neutron matter

	Gogny D1S	Gogny D2	RegMR3
2-body	$\tilde{\rho}_n \tilde{\rho}_n$ attractive	$\tilde{\rho}_n \tilde{\rho}_n$ attractive	$\tilde{\rho}_n \tilde{\rho}_n$ attractive
3-body or d.d.	– –	$\rho_n^\alpha \tilde{\rho}_n \tilde{\rho}_n$ repulsive	– –

Conclusion and outlooks

First density independent effective interaction which gives

- reasonable results at the SR approximation;
- no finite-size instabilities in the $T = 1$ channel;
- strong enough pairing in nuclei;
- possibility to do MR calculations without ambiguity.

Outlooks:

- Implementation in 3D codes for SR and MR calculations;
- Minor improvements for the effective mass, slope of the symmetry energy and incompressibility;
- Average gaps in neutron matter too strong...
  Might be corrected (?) using a slightly modified NLO 3-body term.

Thanks

Thank you for your attention

- Main collaborators on this project:
  Ph. da Costa, J. Dobaczewski, M. Kortelainen.
- Other colleagues involved:
  Y. Gao, T. Haverinen, A. Idini, D. Lacroix, M. Martini, A. de Pace, F. Raimondi.