Effective interactions for mean-field and beyond-mean-field calculations

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Workshop: "EDMs: complementary experiments and theory connections"
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Outline

Nuclear landscape and (main) methods in nuclear structure

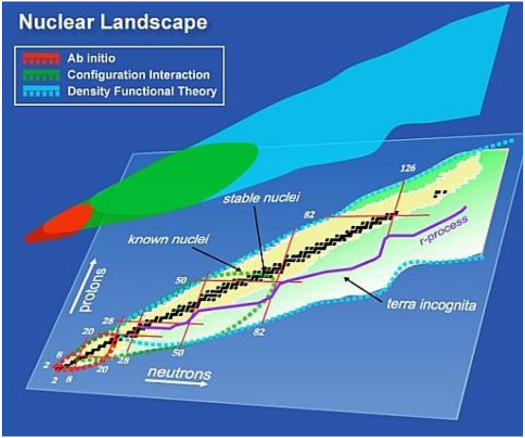

Fig. by W. Nazarewicz, UNEDF SciDAC Collaboration,
https://unedf.mps.ohio-state.edu/

Motivation (in a nutshell): effective interactions

- What they are

  Effective interactions and/or functionals model the strong interaction in the nuclear medium, *i.e.* with coupling constants which absorb effects which are not resolved and correlations not taken into account in the wave function

$$E_{\rm eff} = \left\langle \Phi \middle| \left(\hat{T} + \hat{V}_{\rm eff} \right) \middle| \Phi \right\rangle \, .$$

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- What they are supposed to be used for
  - Mean-field:

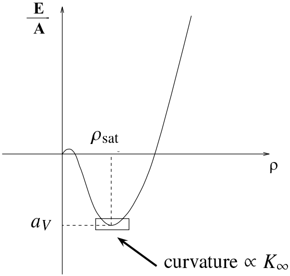
    $$|\Phi\rangle \in \mathcal{S}\ell_A \subset \mathcal{H}_A : \ \delta E_{\mathrm{eff}}[\rho] = 0 \ \Rightarrow \ \text{mean-field equations}$$

    with $\mathcal{S}\ell_A =$ (generalized-)Slater determinants for A nucleons. The energy $E_{\mathrm{eff}}[\rho]$ is a functional of the one-body density ρ (called the EDF).
  - Beyond-mean-field: many flavors

    (Q)RPA, (p)GCM, MPMH, etc.

    with $|\Phi\rangle \notin \mathcal{S}\ell_A$ (and possibly $|\Phi\rangle \notin \mathcal{H}_A$!)

Infinite nuclear matter properties (“known unknowns”)



- Saturation density:
  $$\rho_{\rm sat} \sim 0.16\ \mathrm{fm}^{-3};$$
- Binding energy per nucleon:
  $$\lim_{A\to+\infty} \frac{E(N,Z)}{A} = a_v \sim -16\ \mathrm{MeV};$$

curvature $\propto K_\infty = 9\rho_{\rm sat}^2 \frac{\mathrm{d}^2 E/A}{\mathrm{d}\rho^2} \sim 210$ MeV

(Compression modulus)

- Effective mass: $m^*/m \sim 0.7$ to 1;
- Compression modulus: $K_\infty \sim 210$ MeV.
- Symmetry energy J and its slope L: $J \simeq 30 - 32$ MeV, $L \simeq 40 - 50$ MeV.

Standard effective interactions (two-body part)[1]

$$\hat{V}_{\text{eff}} = \hat{V}_{\text{Coulomb}} + \begin{cases} \hat{V}_{\text{Skyrme}} \, , \\ \hat{V}_{\text{Gogny}} \, , \end{cases} \qquad \text{(or others) with}$$

- Coulomb (for $t_1 = t_2 \equiv \mathrm{p}$)

$$\hat{V}_{\text{Coulomb}} = \frac{e^2}{\|\mathbf{r}_2 - \mathbf{r}_1\|} \, \delta(\mathbf{r}_1 - \mathbf{r}_3) \delta(\mathbf{r}_2 - \mathbf{r}_4) \mathbb{1}^{\sigma} \mathbb{1}^{\tau} \, .$$

[1] Notations: $\mathbf{k}_{ij} = \mathbf{k}_j - \mathbf{k}_i$, $\mathbb{1}^{\sigma} \equiv \delta_{s_1 s_3} \delta_{s_2 s_4}$, $\hat{P}^{\sigma} \equiv \delta_{s_1 s_4} \delta_{s_2 s_3}$ and the same for isospin.

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- Skyrme (NLO in modern language)

$$\begin{aligned} \hat{V}_{\text{Skyrme}} = \Bigg\{ \Bigg[& t_0 \left(\mathbb{1}^\sigma + x_0 \, \hat{P}^\sigma \right) \\ & + \tfrac{1}{2} \, t_1 \left(\mathbb{1}^\sigma + x_1 \, \hat{P}^\sigma \right) \left(\mathbf{k}_{12}^{*2} + \mathbf{k}_{34}^2 \right) + t_2 \left(\mathbb{1}^\sigma + x_2 \, \hat{P}^\sigma \right) \mathbf{k}_{12}^{*} \cdot \mathbf{k}_{34} \\ & + \mathrm{i} \, W_{so} \left(\hat{\boldsymbol{\sigma}}_{s_1 s_3} \delta_{s_2 s_4} + \hat{\boldsymbol{\sigma}}_{s_2 s_4} \delta_{s_1 s_3} \right) \cdot \left(\mathbf{k}_{12}^{*} \times \mathbf{k}_{34} \right) \Bigg] \\ & \mathbf{1}^\tau \underbrace{\delta(\mathbf{r}_1 - \mathbf{r}_2)}_{\text{range}} \underbrace{\delta(\mathbf{r}_1 - \mathbf{r}_3) \delta(\mathbf{r}_2 - \mathbf{r}_4)}_{\text{locality}} \Bigg\} . \end{aligned}$$

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- Gogny (Brink & Boeker for the two-body part)

$$\hat{V}_{\text{Gogny}} = \Bigg\{ \Bigg[\sum_{i=1,2} \left(W_i \mathbb{1}^\sigma \mathbb{1}^\tau + B_i \hat{P}^\sigma \mathbb{1}^\tau - H_i \mathbb{1}^\sigma \hat{P}^\tau - M_i \hat{P}^\sigma \hat{P}^\tau \right) \underbrace{\mathrm{e}^{-\frac{(\mathbf{r}_1-\mathbf{r}_2)^2}{{a_i}^2}}}_{\text{range}}$$

$$+\mathrm{i}\, W_{so} \left(\hat{\boldsymbol{\sigma}}_{s_1 s_3} \delta_{s_2 s_4} + \hat{\boldsymbol{\sigma}}_{s_2 s_4} \delta_{s_1 s_3} \right) \cdot \left(\mathbf{k}_{12}^* \times \mathbf{k}_{34} \right) \underbrace{\delta(\mathbf{r}_1 - \mathbf{r}_2)}_{\text{range}} \Bigg]$$

$$\mathbb{1}^\tau \underbrace{\delta(\mathbf{r}_1 - \mathbf{r}_3)\delta(\mathbf{r}_2 - \mathbf{r}_4)}_{\text{locality}} \Bigg\} .$$

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Can we do mean-field calculations with a two-body interaction only?

- Infinite nuclear matter properties can be used as a filters:

$$\frac{E}{A}\,,\ \rho_{\rm sat}\,,\ K_\infty\,,\ \frac{m^*}{m}\,,\ J\,,\ L\,,\ \text{etc.}$$

- V.S. Weisskopf, Nucl. Phys. 3, 423 (1957): zero-range interaction at NLO

$$\frac{m^*}{m} \simeq 0.4 \neq \text{ anything reasonable.} \quad ☹$$

- Feature confirmed for zero- and finite-range interactions at any order...
  D. Davesne, J. Navarro, J. Meyer, K.B. and A. Pastore, Phys. Rev. C97, 044304 (2018).

⇒ Something "beyond" two-body is mandatory.

What about a (simple) three-body term?

- Zero-range three-body term (LO): easy to implement and not too time-consuming

$$u_0 \, \delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_2 - \mathbf{r}_3)\mathbb{1}^{\sigma}\mathbb{1}^{\tau} \, .$$

  Improves the effective mass ☺, but K_∞ is too high ☹ and polarized matter collapses ☹☹ (therefore unusable for time-odd nuclei) .

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A possible solution is to use a two-body density dependent interaction instead of the three-body

$$\frac{1}{6} \, t_3 \, \rho_0(\mathbf{r}_1) \, \delta(\mathbf{r}_1 - \mathbf{r}_2)\mathbb{1}^\sigma \mathbb{1}^\tau \, .$$

Equivalent to a three-body interaction in symmetric matter.

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Equivalent to a three-body interaction in symmetric matter.

Changed to $\frac{1}{6}\,t_3\left(\mathbb{1}^\sigma+x_3\hat{P}^\sigma\right)\rho_0(\mathbf{r}_1)\,\delta(\mathbf{r}_1-\mathbf{r}_2)\mathbb{1}^\tau$ for a better flexibility in spin/isospin channels,

and then to $\frac{1}{6}\,t_3\left(\mathbb{1}^\sigma+x_3\hat{P}^\sigma\right)\rho_0^\alpha(\mathbf{r}_1)\,\delta(\mathbf{r}_1-\mathbf{r}_2)\mathbb{1}^\tau$ to improve K_∞ .

This is not an interaction, it does not respect the Pauli principle, but this may be acceptable in an effective approach.

Last (but not least) mistreatment of the EDF

Once you have chosen your favorite flavor of interaction, mean-fields equations are obtained from

$$\delta E_{\mathrm{eff}} = 0 \quad \text{with} \quad E_{\mathrm{eff}} = \left\langle \Phi \left| \left(\hat{T} + \hat{V}_{\mathrm{eff}} \right) \right| \Phi \right\rangle = T + E_H + E_F + E_P$$

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but, often, E_H, E_F and E_P are not strictly derived from the same interaction $\hat{V}_{\text{eff}}$ or some parts are note derived from an interaction at all:

- some terms can be dropped (*e.g.* "J^2" terms);
- other can be modified (*e.g.* Coulomb exchange);
- E_P can be derived from a simpler interaction;
- ...

And this works pretty well for mean-field calculations,

see *e.g.* W. Ryssen *et al.*, EPJA 59, 96 (2023).

... This is, more or less, where we are now.

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- To be usable in beyond-mean-field calculations, a functional must be strictly derived from an effective interaction.

M. Anguiano *et al.*, NPA 696 (2001)
J. Dobaczewski *et al.*, PRC 76, 054315 (2007)
D. Lacroix *et al.*, PRC 79, 044318 (2009)

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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)

Hill-Wheeler-Griffin equations

- Configuration mixing along a given collective coordinate q

$$|\tilde{\Phi}\rangle = \int \mathrm{d}q \; f(q)\, |\Phi(q)\rangle$$

- Energy

$$E = \frac{\langle \tilde{\Phi} | \hat{H}_{\mathrm{eff}} | \tilde{\Phi} \rangle}{\langle \tilde{\Phi} | \tilde{\Phi} \rangle}$$

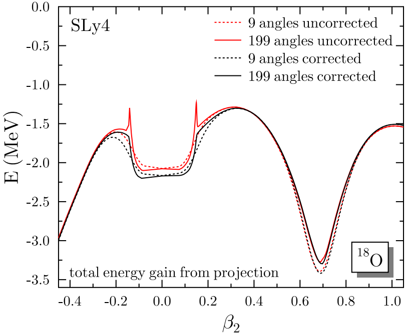
- Hill-Wheeler-Griffin equations:

$$\delta E = 0 \quad \Rightarrow \quad \int \left[\mathcal{H}(q, q') - E_k \, \mathcal{I}(q, q') \right] f_k(q') \, \mathrm{d}q' = 0$$

$\mathcal{H}(q, q') = \langle \Phi(q) | \hat{H}_{\mathrm{eff}} | \Phi(q') \rangle$ *energy kernels* (what if $\hat{H}_{\mathrm{eff}}$ depends on ρ?),
$\mathcal{I}(q, q') = \langle \Phi(q) | \Phi(q') \rangle$ *overlaps kernels.*

Density dependent terms (with fractional power of the density[2])

- The energy kermel $\mathcal{E}[q, q']$ must be extented in $\mathbb{C}$
- $\rho_0^\alpha \;\Rightarrow\; \mathcal{E}[q, q']$ is a multivalued function in the complexe plane



Problem analyzed by J. Dobaczewski *et al.*, PRC 76, 054315:

... with solutions that might not be usable with all symmetry restorations

[2] T. Duguet, M. Bender, K.B., D. Lacroix, T. Lesinski, PRC 79, 044320

Choice for the effective interaction

Radical solution: no density dependent term

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

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- 2-body part: zero-range, finite-range ?
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- 3-body part: zero-range, finite-range ?

Zero-range: not fully satisfying,
Finite-range: too much time-consuming,
$\Rightarrow$ 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"

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

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: $\hat{P}^\sigma \hat{P}^\tau \equiv -\hat{P}^x \not\equiv \pm 1$
- Can be generalized at N^{2}LO, N^{3}LO, ...

[1] *Cf:* J. Phys. G: Nucl. Part. Phys. 44 (2017) 045106.

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 the recent article "The shape of gold",

  B. Bally, G. Giacolone and M. Bender, EPJA 59 (2023) 58.

  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.

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- Semi-regularized three-body interaction: symmetrized version of

$$V_3(x_1,x_2,x_3;x_4,x_5,x_6) = W_3\,\overbrace{\delta(\mathbf{r}_{14})\delta(\mathbf{r}_{25})\delta(\mathbf{r}_{36})}^{\text{locality}}\,\delta_{q_1q_4}\delta_{q_2q_5}\delta_{q_3q_6}$$
$$\times\,\delta_{s_1s_4}\underbrace{\left(\delta_{s_2s_5}\delta_{s_3s_6}+\delta_{s_2s_6}\delta_{s_3s_5}\right)}_{=\mathbf{1}^{\sigma}_{23}+P^{\sigma}_{23}}\,\underbrace{g_a(\mathbf{r}_{12})}_{\text{finite range}}\,\underbrace{\delta(\mathbf{r}_{23})}_{\text{zero range}}$$

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

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Comparison with finite-range Gogny pseudopotentials

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

$$V_{D1S}(x_1, x_2; x_3, x_4) = \Bigg[\sum_{j=1,2} \mathrm{e}^{-\frac{\mathbf{r}_{12}^2}{\mu_j^2}} \left(W_j \mathbb{1}^\sigma \mathbb{1}^\tau + B_j P^\sigma \mathbb{1}^\tau - H_j \mathbb{1}^\sigma P^\tau - M_j P^\sigma P^\tau \right)$$

$$+ t_3 \left(\mathbb{1}^\sigma + P^\sigma \right) \mathbb{1}^\tau \rho_0^\alpha(\mathbf{r}_1) \delta(\mathbf{r}_{12})$$

$$+ \mathrm{i}\, W_0\, \mathbf{1}^\tau \left(\delta_{\sigma_1\sigma_3} \boldsymbol{\sigma}_{\sigma_2\sigma_4} + \boldsymbol{\sigma}_{\sigma_1\sigma_3} \delta_{\sigma_2\sigma_4} \right) \cdot \left(\mathbf{k}_{12}^* \times \mathbf{k}_{34} \right) \Bigg]$$

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

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

$$V_{D2}(x_1, x_2; x_3, x_4) = \Bigg[\sum_{j=1,2} \mathrm{e}^{-\frac{\mathbf{r}_{12}^2}{\mu_j^2}} \left(W_j \mathbb{1}^\sigma \mathbb{1}^\tau + B_j P^\sigma \mathbb{1}^\tau - H_j \mathbb{1}^\sigma P^\tau - M_j P^\sigma P^\tau \right)$$

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

$$+ \mathrm{i}\, W_0\, \mathbf{1}^\tau \left(\delta_{\sigma_1\sigma_3} \boldsymbol{\sigma}_{\sigma_2\sigma_4} + \boldsymbol{\sigma}_{\sigma_1\sigma_3} \delta_{\sigma_2\sigma_4} \right) \cdot \left(\mathbf{k}_{12}^* \times \mathbf{k}_{34} \right) \Bigg]$$

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

Overview of the fits of the parameters

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

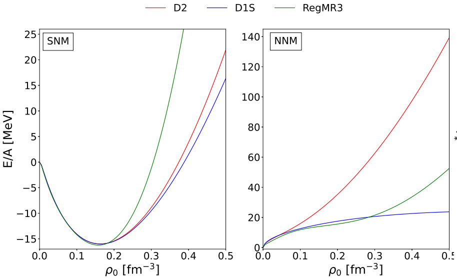
Minimization of a penalty function built from:

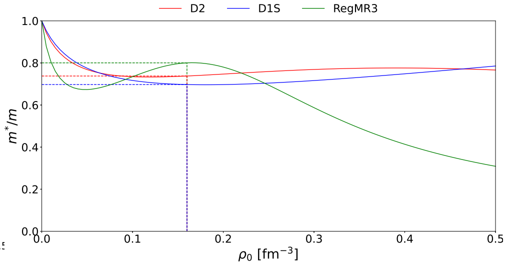
- Infinite nuclear matter properties (ρ_{sat}, E/A, K_∞, m^*/m, J, L)
- Neutron matter equation of state
- Simple constraints on pairing strengths (strong enough scalar pairing and weak enough vector pairing)
- Binding energies of spherical nuclei
- Single particle energies in ^{208}Pb
- Charge radii
- Charge density profiles[3]
- Salt and pepper.

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.

[3] which helps to prevent finite-size instabilities, this is a very interesting topic but I don't have time to talk about it.

Properties of infinite nuclear matter

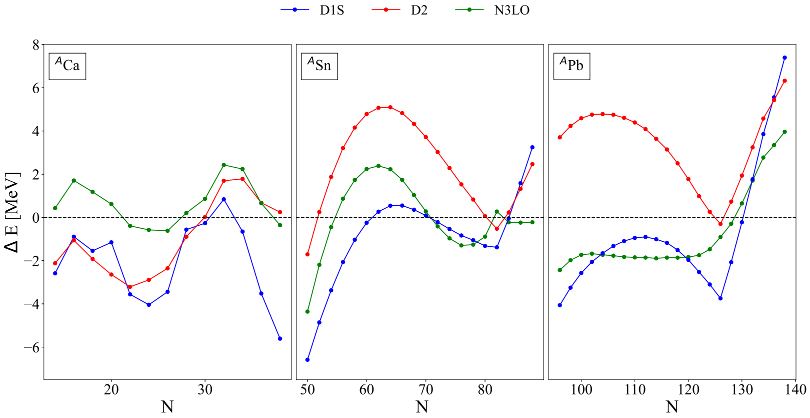




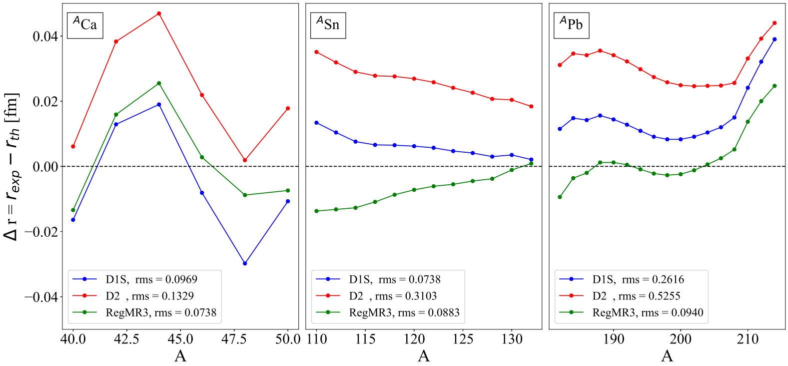
	ρ_{sat} [fm^{-3}]	E/A [MeV]	K_∞ [MeV]	J [MeV]	L [MeV]	m^*/m
D2	0.163	-16.000	209.251	31.110	44.831	0.738
D1S	0.163	-16.007	202.840	31.125	22.441	0.697
RegMR3	0.158 ☺	-16.237 ☺	285.654 ☹	31.954 ☺	12.798 ☹	0.800 ☺

Semi-magic nuclei: binding energy residuals

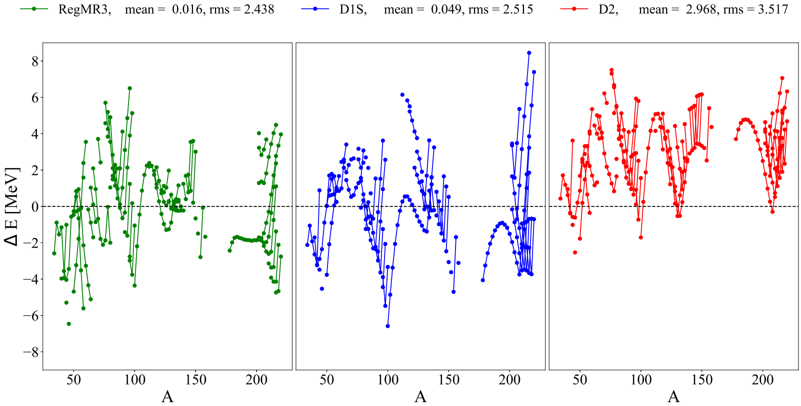
Comparison with Gogny interactions is not a beauty pageant



Semi-magic nuclei: charge radii



Spherical nuclei: binding energy residuals

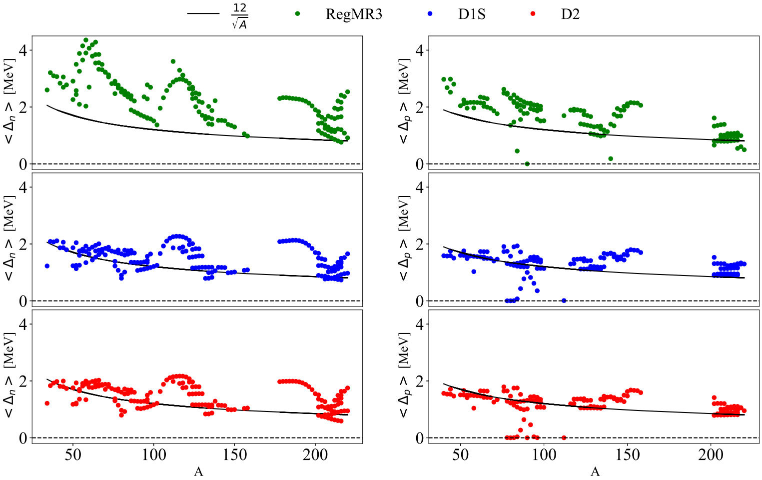


Set of 214 nuclei with $Z \geqslant 20$ predicted as (quasi-)spherical by D1S

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

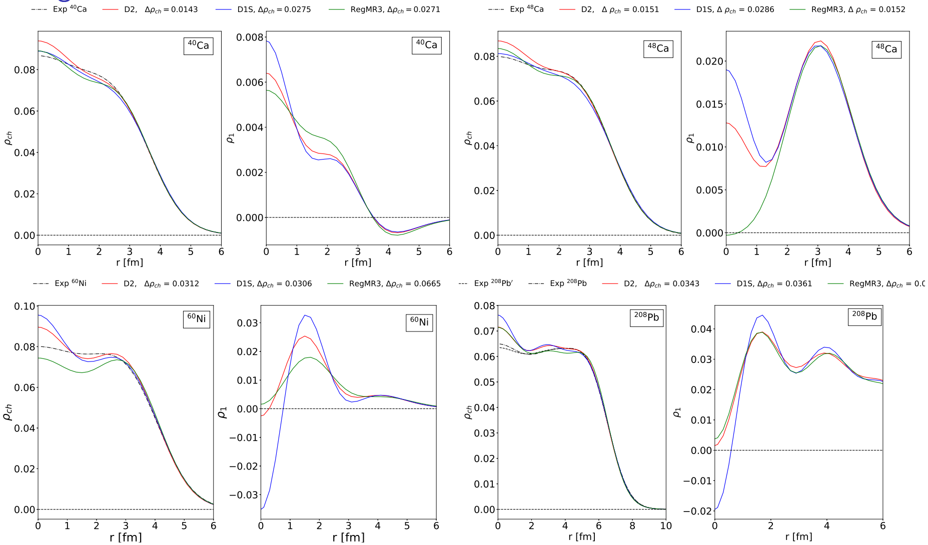
or google it...

Average neutron and proton gaps



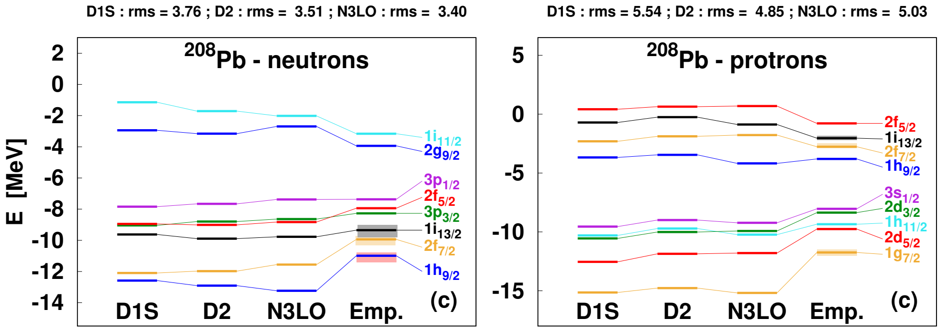
(Coulomb interaction included in the pairing channel)

Charge and isovector densities



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

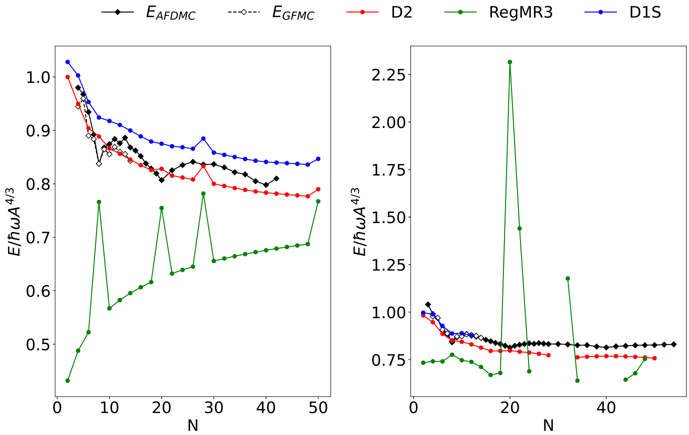
Single particle energies in ^{208}Pb



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:

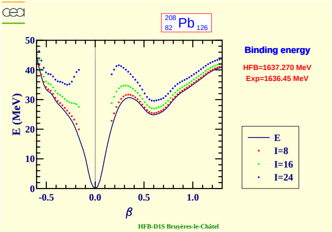
- Implementation in 3D codes for SR and MR calculations;
- Minor improvements for the effective mass, slope of the symmetry energy and incompressibility;
- Average gaps in neutron matter too strong...
  BUT: easy to correct using a slightly modified NLO 3-body term.

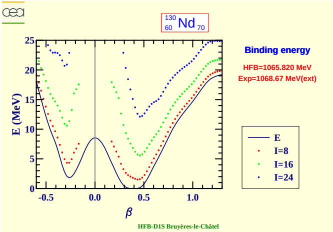
Thanks

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.

Examples of shapes of nuclei





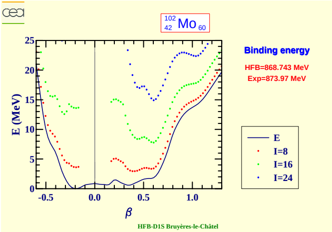


Fig. from CEA Bruyères-le-Châtel, `https://www-phynu.cea.fr/`

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.)