

Nuclear structure with regularized EDF generators

Why one more effective interaction ?!

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Outline

Mean-field and effective interactions

Constraints on the effective interactions

Finite-range pseudopotentials

Conclusion and outlooks

Open questions

Mean-field methods and nuclear structure

- ▶ Time-independent Schrödinger equation for A particles

$$\hat{H}\Psi = (\hat{T} + \hat{V}_2 + \hat{V}_3 + \dots)\Psi = E_0\Psi$$

- ▶ Mean-field approximation, Hartree-Fock(-Bogolyubov) equations

$$E = \langle \Phi | \hat{H}_{\text{eff}} | \Phi \rangle \simeq E_0 = \langle \Psi | \hat{H} | \Psi \rangle$$

- ▶ Effective interaction $\hat{H}_{\text{eff}} = \hat{T} + \hat{V}_{\text{eff}}$

$$\hat{V}_{\text{eff}} = \hat{V}_{\text{eff}}(\mathbf{p}), \quad \mathbf{p} \in \mathbb{R}^n, \quad n \lesssim 10$$

Standard form of the Skyrme interaction $\hat{V}_{\text{eff}} = \hat{V}_2 + \hat{V}_3$

- Two-body term (with $x \equiv \mathbf{r}, s, q$) \simeq SV interaction

$$\begin{aligned} \hat{V}_2(x_1, x_2; x_3, x_4) = & \left[t_0 (\delta^s + x_0 \mathbf{P}^s) \right. \\ & + \frac{1}{2} t_1 (\delta^s + x_1 \mathbf{P}^s) (\hat{\mathbf{k}}_{12}^{*2} + \hat{\mathbf{k}}_{34}^2) \\ & + t_2 (\delta^s + x_2 \mathbf{P}^s) \hat{\mathbf{k}}_{12}^* \cdot \hat{\mathbf{k}}_{34} \\ & \left. + i W_0 \delta^s (\hat{\boldsymbol{\sigma}}_{13} + \hat{\boldsymbol{\sigma}}_{24}) \cdot (\hat{\mathbf{k}}_{12}^* \times \hat{\mathbf{k}}_{34}) \right] \\ & \times \delta(\mathbf{r}_1 - \mathbf{r}_3) \delta(\mathbf{r}_2 - \mathbf{r}_4) \delta(\mathbf{r}_1 - \mathbf{r}_2) \end{aligned}$$

$$\text{☺ } \rho_{\text{sat}}, \quad \text{☺ } E/A, \quad \text{☹ } m^*/m, \quad \text{☹ } K_\infty$$

- Three-body term

$$\hat{V}_3(x_1, x_2, x_3; x_4, x_5, x_6) = t_3 \delta_{x_1 x_4} \delta_{x_2 x_5} \delta_{x_3 x_6} \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}_3)$$

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$$\text{☺ } \rho_{\text{sat}}, \quad \text{☺ } E/A, \quad \text{☹ } m^*/m, \quad \text{☹ } K_\infty$$

- Two-body density dependent term \simeq SIII interaction

$$\hat{V}_3(x_1, x_2; x_3, x_4) = \frac{1}{6} t_3 (\delta^s + x_3 \mathbf{P}^s) \rho_0(\mathbf{r}_1) \delta(\mathbf{r}_1 - \mathbf{r}_3) \delta(\mathbf{r}_2 - \mathbf{r}_4) \delta(\mathbf{r}_1 - \mathbf{r}_2)$$

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$$\text{☺ } \rho_{\text{sat}}, \quad \text{☺ } E/A, \quad \text{☹ } m^*/m, \quad \text{☹ } K_\infty$$

- Two-body term depending on a fractional power of the density \simeq SLy

$$\hat{V}_3(x_1, x_2; x_3, x_4) = \frac{1}{6} t_3 (\delta^s + x_3 \mathbf{P}^s) \rho_0^\alpha(\mathbf{r}_1) \delta(\mathbf{r}_1 - \mathbf{r}_3) \delta(\mathbf{r}_2 - \mathbf{r}_4) \delta(\mathbf{r}_1 - \mathbf{r}_2)$$

$$\text{☺ } \rho_{\text{sat}}, \quad \text{☺ } E/A, \quad \text{☺ } m^*/m, \quad \text{☺ } K_\infty$$

Gogny effective interaction

J. Dechargé and D. Gogny, Phys. Rev. C 21 (1980) 1568

- ▶ Two-body finite-range term

$$\hat{V}_2(x_1, x_2; x_3, x_4) = \left[\sum_{i=1,2} (W_i \delta^s \delta^q + B_i \mathbf{P}^s \delta^q - H_i \delta^q \mathbf{P}^q - M_i \mathbf{P}^s \mathbf{P}^q) e^{-\frac{(r_1-r_2)^2}{\mu_i^2}} \right. \\ \left. + i W_0 \delta^s (\hat{\sigma}_{13} + \hat{\sigma}_{24}) \cdot (\hat{\mathbf{k}}_{12}^* \times \hat{\mathbf{k}}_{34}) \delta(\mathbf{r}_1 - \mathbf{r}_2) \right] \\ \times \delta(\mathbf{r}_1 - \mathbf{r}_3) \delta(\mathbf{r}_2 - \mathbf{r}_4)$$

- ▶ Two-body zero-range term depending on $\rho_0^{1/3}$

$$\hat{V}_3(x_1, x_2; x_3, x_4) = t_3 (\delta^s + \mathbf{P}^s) \rho_0^{1/3}(\mathbf{r}_1) \delta(\mathbf{r}_1 - \mathbf{r}_3) \delta(\mathbf{r}_2 - \mathbf{r}_4) \delta(\mathbf{r}_1 - \mathbf{r}_2)$$

$$\text{☺ } \rho_{\text{sat}}, \quad \text{☺ } E/A, \quad \text{☺ } m^*/m, \quad \text{☺ } K_\infty$$

Functional derived from an *effective* (Skyrme) interaction

For a spherical nucleus at the HF approximation

$$E = \langle \hat{T} + \hat{V}_{\text{eff}} \rangle = \int \frac{\hbar^2}{2m} \tau_0 d^3r + \sum_{t=0,1} \int \mathcal{E}_t d^3r$$

with

$$\mathcal{E}_t = C_t^\rho[\rho_0] \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^{\Delta\rho} \rho_t \Delta\rho_t + C_t^{\nabla J} \rho_t \nabla \cdot \mathbf{J}_t + \frac{1}{2} C_t^J \mathbf{J}_t^2$$

The coupling constants of the functional $C_t^\rho[\rho_0]$, C_t^τ , etc., are entirely determined by the parameters \mathbf{p} of the interaction

Skyrme interaction and Skyrme functional: $E \neq \langle \hat{T} + \hat{V}_{\text{eff}} \rangle$

▸ Interaction:

- All the terms of the functional determined by the parameters of the interaction
- Tricky to obtain satisfactory properties in all channels
- Some terms of the functional are difficult to constrain

▸ Functional: more versatile

- Complicated, poorly determined or “dangerous” terms, *i.e.* \mathbb{J}^2 , $\rho_1 \Delta \rho_1$, $\mathbf{s}_0 \Delta \mathbf{s}_0$, $\mathbf{s}_1 \Delta \mathbf{s}_1$, ... omitted or separately adjusted
- A different interaction can be used in the pairing channel
- Slater approximation can be used for the Coulomb exchange term

⇒ Very efficient at the mean-field level

- SLyn ($n = 4, 5, 6, 7$),
Nucl. Phys. **A 627** (1997) 710 et **A 635** (1998) 231
- UNEDFn' ($n' = 0, 1, 2$)
Phys. Rev. **C 82**, 024313, **C 85**, 024304 et **C 89**, 054314

Constraints on the effective interactions

- ▶ Mean-field approximation
 - ▶ sometimes inadequate to describe the ground states of nuclei
 - ▶ does not provide excited states energies and good quantum numbers

- ▶ Beyond mean-field approaches
 - ▶ Use of symmetry breaking / symmetry restoration mechanisms
 - ▶ Configuration mixing along collective coordinates (GCM)
 - ▶ Need to calculate energy $\mathcal{E}[q, q']$ and overlap $\mathcal{N}[q, q']$ kernels to evaluate E with correlations
 - ▶ For example

$$E^N = \int_0^{2\pi} d\varphi \mathcal{E}[0, \varphi] \mathcal{N}[0, \varphi]$$

depends on transition densities between an HFB state $|\Phi_0\rangle$ and a *rotated* state $|\Phi_\varphi\rangle$: $\rho^{0\varphi}$, $\kappa^{0\varphi}$ et $\kappa^{\varphi 0*}$

Pitfalls with functionals not derived from an interaction

- ▶ Skyrme functionals are (most of the time) not strictly derived from an interaction
- ▶ E^N will show divergences each time a single particle state goes through the Fermi energy

Cf. M. Anguiano et al., NPA 696, 467

J. Dobaczewski et al., PRC 76, 054315

D. Lacroix et al., PRC 79, 044318

- ▶ Even if the functional is derived from an interaction, the density dependent term ρ_0^α requires a particular treatment
 - ▶ transition (or mixed) density: $\rho^{0\varphi} = \langle \Phi_0 | \hat{\rho} | \Phi_\varphi \rangle$
 - ▶ average density: $\bar{\rho}^\alpha = \frac{1}{2} (\langle \Phi_0 | \hat{\rho} | \Phi_0 \rangle^\alpha + \langle \Phi_\varphi | \hat{\rho} | \Phi_\varphi \rangle^\alpha)$
 - ▶ correlated density: $\rho^N = \int d\varphi \rho^{0\varphi} \mathcal{N}[0, \varphi]$

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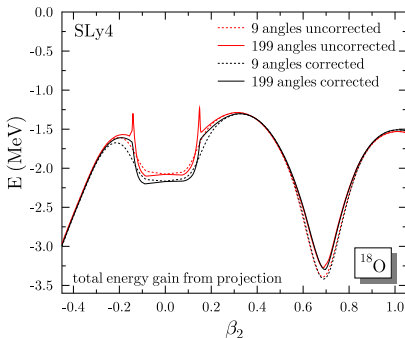
J. Dobaczewski *et al.*, PRC 76, 054315

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 - ▶ transition (or mixed) density: $\rho^{0\varphi} = \langle \Phi_0 | \hat{\rho} | \Phi_\varphi \rangle \in \mathbb{C}$
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 - ▶ correlated density: ~~$\rho^N = \int d\varphi \rho^{0\varphi} \mathcal{N}[0, \varphi]$~~

Fractional power of the density¹

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



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

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

¹T. Duguet, M. Bender, K.B., D. Lacroix, T. Lesinski, PRC 79, 044320

Functional for beyond mean-field calculations

- ▶ Functional not derived from an effective interaction
 - Divergences of the energie
 - ▶ The considered regularization methods might be difficult to implement, seem to be *ad hoc* and are not proven to be usable in all circumstances
- ▶ Effective interaction with density dependent term ρ_0^α
 - Steps in the energy
 - ▶ No solution proven to be usable in all situations (yet)

Drastic solution

The functional has to be strictly derived from an interaction with no density dependent term
(what we call a *pseudopotential*)

Finite-range two-body pseudopotentials²

- ▶ In a nutshell:

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”

$$\begin{aligned}
 v = & \tilde{v}_0(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_3, \mathbf{r}_4) t_0 (1_{\sigma q} + x_0 1_q \hat{P}^\sigma - y_0 1_\sigma \hat{P}^q - z_0 \hat{P}^\sigma \hat{P}^q) \\
 & + \tilde{v}_1(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_3, \mathbf{r}_4) t_1 (1_{\sigma q} + x_1 1_q \hat{P}^\sigma - y_1 1_\sigma \hat{P}^q - z_1 \hat{P}^\sigma \hat{P}^q) \\
 & + \tilde{v}_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_3, \mathbf{r}_4) t_2 (1_{\sigma q} + x_2 1_q \hat{P}^\sigma - y_2 1_\sigma \hat{P}^q - z_2 \hat{P}^\sigma \hat{P}^q)
 \end{aligned}$$

with $\tilde{v}_0(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_3, \mathbf{r}_4) = \delta(\mathbf{r}_1 - \mathbf{r}_3) \delta(\mathbf{r}_2 - \mathbf{r}_4) g_a(\mathbf{r}_1 - \mathbf{r}_2)$

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

$$\tilde{v}_2(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_3, \mathbf{r}_4) = \delta(\mathbf{r}_1 - \mathbf{r}_3) \delta(\mathbf{r}_2 - \mathbf{r}_4) g_a(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k}_{12}^* \cdot \mathbf{k}_{34}$$

- ▶ Thanks to the finite range: $\hat{P}^\sigma \hat{P}^q \equiv -\hat{P}^x \neq \pm 1$
- ▶ Can be generalized at N²LO, N³LO, ...

²F. Raimondi, K.B., J. Dobaczewski, J. Phys. G 41, 055112

Finite-range two-body local pseudopotentials

- ▶ The conditions

$$t_1 = -t_2, \quad x_1 = x_2, \quad y_1 = y_2, \quad z_1 = z_2$$

(and same for higher order terms) make the pseudopotential local

- ▶ This is a **severe** restriction on the flexibility of the functional
- ▶ ... but it greatly simplifies the implementation in computer codes
- ▶ and it limits the number of free parameters
(and that's all we have so far anyway...)
- ▶ Use of a standard two-body zero-range spin-orbit interaction

Preliminary fits of the parameters

- Two-body finite-range local pseudopotentials at NLO and N²LO

Details on the fits:

K.B., A. Idini, J. Dobaczewski, P. Dobaczewski, M. Kortelainen, F. Raimondi, J. Phys. G 44, 045106 (2017)

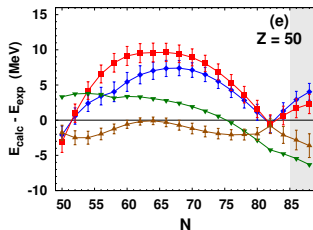
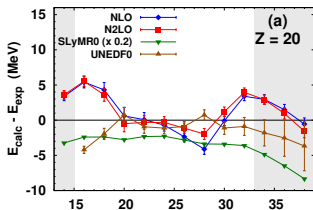
A. Idini, K.B., J. Dobaczewski, J. Phys. G 44, 064004 (2017)

K.B., J. Dobaczewski, Y. Gao, arXiv:1701.08062

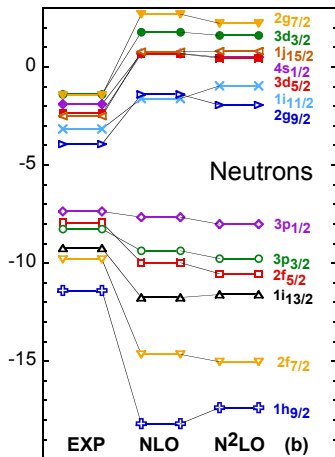
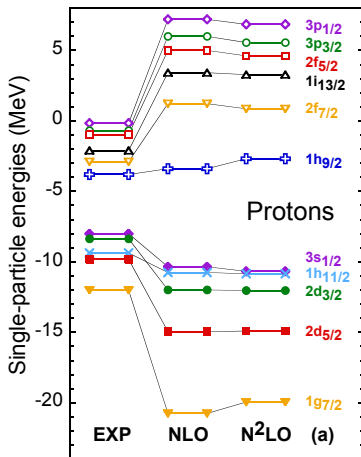
- Infinite nuclear matter properties

	ρ_{sat} (fm ⁻³)	B (MeV)	K_{∞} (MeV)	m^*/m	J (MeV)	L (MeV)
NLO	0.1599	-16.17	229.8	0.4076	31.96	64.04
N ² LO	0.1601	-16.09	230.0	0.4061	31.95	64.68

- Binding energies of semi-magic nuclei



Single particle energies with a low effective mass...



How to increase the effective mass ?

A three-body interaction seems to be the only way...

- ▶ Finite-range three-body: **not doable** in 3D codes
- ▶ Semi-contact three-body: **not doable either** in 3D codes 😞
D. Lacroix, K.B., Phys. Rev. C 91, 011302(R) (2015)
- ▶ Zero-range contact interaction: **too repulsive** in the pairing channel
- ▶ Non-local zero-range contact 3-body interaction
(*i.e.* Finite-range 2-body and 3-body with gradients):

Original idea:

N. Onishi and J. Negele, Nuclear Physics A 301 (1978) 336

Three-body terms with gradients

Same as in J. Sadoudi *et al.*, Phys. Rev. C 88 (2013) 064326

- ▶ Symmetrized expression built from

$$v_3(x_1, x_2, x_3; x_4, x_5, x_6) = [v_{30} + v_{31} + v_{32}] \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}_3) \\ \times \delta(\mathbf{r}_1 - \mathbf{r}_4) \delta(\mathbf{r}_2 - \mathbf{r}_5) \delta(\mathbf{r}_3 - \mathbf{r}_6) \delta_{q_1 q_4} \delta_{q_2 q_5} \delta_{q_3 q_6}$$

with

$$v_{30} = u_0 \delta_{s_1 s_4} \delta_{s_2 s_5} \delta_{s_3 s_6}$$

$$v_{31} = \frac{u_1}{2} (\delta_{s_1 s_4} \delta_{s_2 s_5} + y_1 \delta_{s_1 s_5} \delta_{s_2 s_4}) \delta_{s_3 s_6} (\hat{\mathbf{k}}_{12}^{*2} + \hat{\mathbf{k}}_{45}^2)$$

$$v_{32} = u_2 [\delta_{s_1 s_4} \delta_{s_2 s_5} \delta_{s_3 s_6} + y_{21} \delta_{s_1 s_5} \delta_{s_2 s_4} \delta_{s_3 s_6} \\ + y_{22} (\delta_{s_1 s_6} \delta_{s_2 s_5} \delta_{s_3 s_4} + \delta_{s_1 s_4} \delta_{s_2 s_6} \delta_{s_3 s_5})] \hat{\mathbf{k}}_{12}^* \cdot \hat{\mathbf{k}}_{45}$$

- ▶ 6 additional parameters...

Fit of the parameters and infinite nuclear matter properties

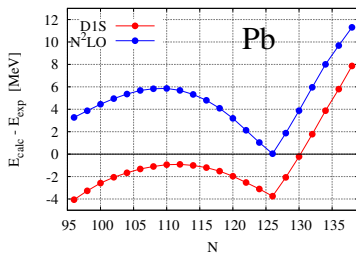
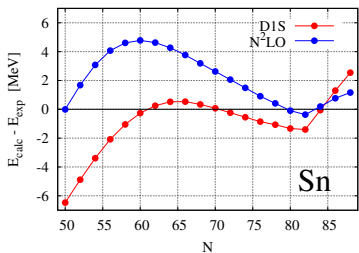
- ▶ Finite-range local terms + spin-orbit + 3-body → 19 parameters...
- ▶ Setting ρ_{sat} , m^*/m and J to the empirical values leaves 16 free parameters
- ▶ Infinite nuclear matter

	ρ_{sat} (fm^{-3})	B (MeV)	K_{∞} (MeV)	m^*/m	J (MeV)	L (MeV)
NLO	0.1599	-16.17	229.8	0.4076	31.96	64.04
N ² LO	0.1601	-16.09	230.0	0.4061	31.95	64.68
N ² LO + 3B	0.1600	-16.02	258.6	0.7000	32.00	35.94

- ▶ The three-body terms with gradients allows to increase the effective mass and *seems* to give attractive pairing

Results

- ▶ Equations of states are OK...
- ▶ Pairing strong enough...
- ▶ Binding energies of spherical nuclei



Very encouraging results, but...

Yet another illustration of Murphy's law

- ▶ Calculations of spherical nuclei with a spherical code give **nice** results
- ▶ Calculations for the **same** spherical nuclei with a code allowing deformation give **calamitous** results
 - ▶ Collapse of the local part of the pairing density $\tilde{\rho}(\mathbf{r}, \mathbf{r}) = 0$
 - ▶ Huge pairing energies
 - ▶ Unphysical binding energies
 - ▶ Although nuclei are perfectly spherical...
- ▶ No bug found so far...
- ▶ So what ?

The culprit

The contact (local) 3-body term (mainly added to increase the effective mass) is **always** too repulsive in the pairing channel.

So, if it hurts, don't do it...

$$v_3(x_1, x_2, x_3; x_4, x_5, x_6) = [v_{30} + v_{31} + v_{32}] \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}_3) \\ \times \delta(\mathbf{r}_1 - \mathbf{r}_4) \delta(\mathbf{r}_2 - \mathbf{r}_5) \delta(\mathbf{r}_3 - \mathbf{r}_6) \delta_{q_1 q_4} \delta_{q_2 q_5} \delta_{q_3 q_6}$$

with

$$v_{30} = 0$$

$$v_{31} = \frac{u_1}{2} (\delta_{s_1 s_4} \delta_{s_2 s_5} + y_1 \delta_{s_1 s_5} \delta_{s_2 s_4}) \delta_{s_3 s_6} (\hat{\mathbf{k}}_{12}^{*2} + \hat{\mathbf{k}}_{45}^2)$$

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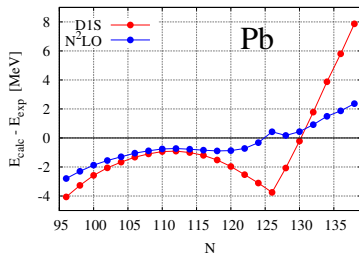
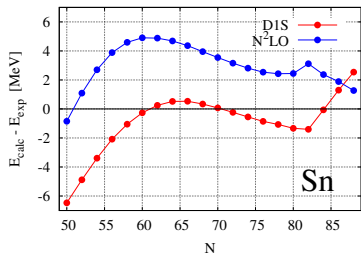
☺ One less parameter to fit !

Fit of the parameters and infinite nuclear matter properties

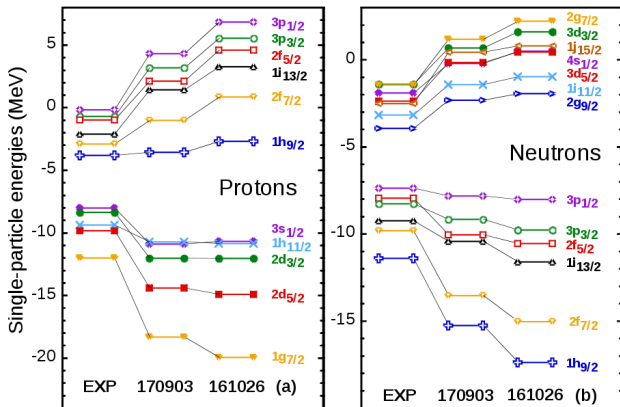
- ▶ Preliminary fit with 4 spherical nuclei
- ▶ Saturation density ρ_{sat} , symmetry energy coefficient J and effective mass m^*/m fixed
- ▶ Pairing adjusted by tuning the contribution of the finite-range interaction in the pairing channel
- ▶ Empirical constraints to avoid finite-size instabilities

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N ² LO + 3B	0.1600	-16.02	258.6	0.7000	32.00	35.94
N ² LO + 3B ($U_0 = 0$)	0.1600	-16.42	276.3	0.5500	35.00	44.99

Sherical nuclei

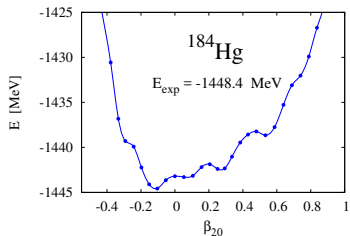
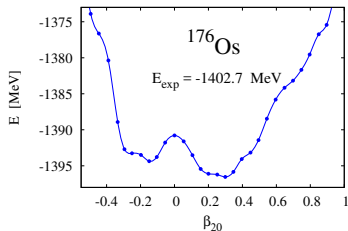
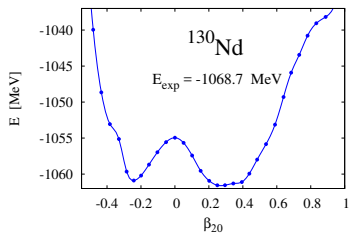
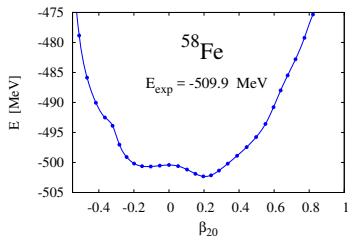


Results are not too bad but it's easy to find examples with less encouraging agreement...

Single particle energies in ^{208}Pb 

Density of state scales as expected

Deformed nuclei



Conclusion

- ▶ The two-body finite-range pseudopotential complemented with a non-local three-body contact term gives acceptable results but not competitive yet with other existing effective interactions
- ▶ It does not contain density dependent terms and is used consistently in all channels: usable with no technical difficulties in beyond mean-field calculations
- ▶ The local version of the two-body terms give encouraging results, the non local version will not hurt
- ▶ Local version implemented in FINRES₄ (spherical solver), under construction in 3D codes HFBTEMP (M. Kortelainen) and HFODD (J. Dobaczewski *et al.*)

Open questions: Different “flavors” of spherical results

- ▶ Calculations of spherical nuclei with a spherical code give **nice** results
- ▶ Calculations for the **same** spherical nuclei with a code allowing deformation give **calamitous** results
 - ▶ Collapse of the local part of the pairing density $\tilde{\rho}(\mathbf{r}, \mathbf{r}) = 0$
 - ▶ Huge pairing energies
 - ▶ Unphysical binding energies
 - ▶ Although nuclei are perfectly spherical...
- ▶ No bug found so far...
- ▶ So what ?
- ▶ On a deformed basis, non local densities might not fulfill

$$\rho_q(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\ell j m_\ell} \rho_q(r_1, r_2) Y_{m_\ell}^{(\ell)*}(\hat{r}_1) Y_{m_\ell}^{(\ell)}(\hat{r}_2)$$

even for a spherical nucleus ?

Open questions: Effective mass, how large should it be ?

	ρ_{sat} (fm^{-3})	B (MeV)	K_{∞} (MeV)	m^*/m	J (MeV)	L (MeV)
NLO	0.1599	-16.17	229.8	0.4076	31.96	64.04
N ² LO	0.1601	-16.09	230.0	0.4061	31.95	64.68
N ² LO + 3B	0.1600	-16.02	258.6	0.7000	32.00	35.94
N ² LO + 3B ($U_0 = 0$)	0.1600	-16.42	276.3	0.5500	35.00	44.99

- ▶ For mean-field calculations ?
- ▶ For beyond mean-field calculations ?

Open questions: What drives the parameters to regions with finite-size instabilities ?

- ▶ Several Skyrme interactions are plagued with finite-size instabilities
- ▶ Isovector instabilities are more likely to occur when the interaction is tuned to give attractive pairing
- ▶ Can it be avoided ?
- ▶ Does a finite-range help ?