Effective theory for low-energy nuclear energy density functionals

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F. Raimondi[a]
in collaboration with
K. Bennaceur[b], J. Dobaczewski[c,d]

[a] TRIUMF
[b] Université de Lyon, F-69003 Lyon, France; Institut de Physique Nucléaire de Lyon, CNRS/IN2P3, Université Lyon 1, F-69622 Villeurbanne Cedex, France
[c] Department of Physics, Post Office Box 35 (YFL), FI-40014 University of Jyväskylä, Finland.
[d] Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, ul. Hoża 69, PL-00-681 Warsaw, Poland

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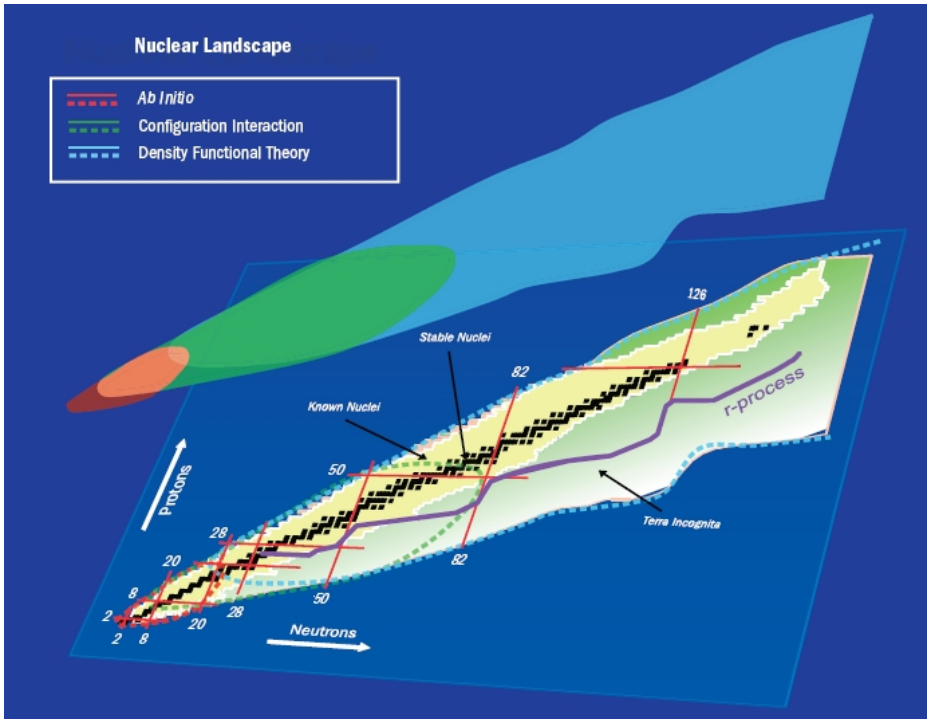
Nuclear Density Functional Theory



- Global theory for the entire nuclear chart (around 3000 nuclei identified, other 6000 expected)
- (quite) Accurate description of the ground-state properties (rms deviation for masses $\simeq$ 1 MeV)
- Reasonable computational cost (basic properties of all the nuclei in a single 24 wall-clock hour run on a 4 Tflop machine)

Outline

- Generalized Skyrme interaction to improve the form of the empirical nuclear functional
- Effective theory as theoretical framework to set the empirical nuclear functional

Energy Density Functional (EDF)

$$E\left[\rho(\mathbf{r})\right] = \frac{\hbar^2}{2m}\int d\mathbf{r}\,\tau(\mathbf{r}) + E^{int}\left[\rho(\mathbf{r})\right] - \lambda\int d\mathbf{r}\,\rho(\mathbf{r})$$

- No (physical) external potential term in the functional (nuclei are self bound)
- Kohn-Sham scheme achieved by mapping one-body density matrix to the local (or quasi-local) densities

Main features of the Energy Density Functional

- Existence of EDF predicted by Hohenberg-Kohn theorem
- Ground-state energy obtained through variational principle
$$E_{GS} = \mathrm{Min}_{\rho}\, E\left[\rho(\mathbf{r})\right]$$
- Different effects included through coupling constants
- I) Microscopically-constrained and II) phenomenological EDFs (both lacking of spectroscopic quality and predictive power)

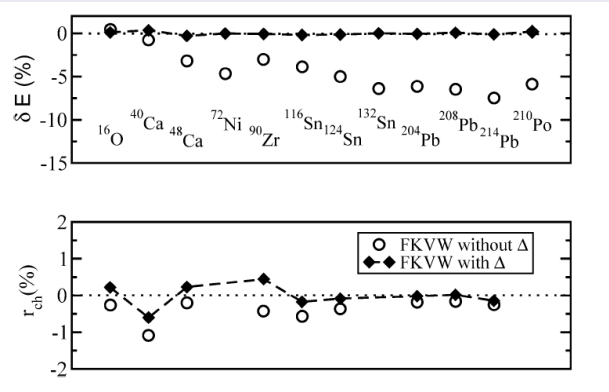
Two main classes of nuclear EDFs

I) Microscopically-constrained nuclear EDF

- Derived from the N-N potential in Ch EFT

$$V^{NN} = V_{1\pi}^{NN} + V_{2\pi}^{NN} + \cdots + V_{ct}^{NN}(\Lambda)$$

- Density-dependent coupling constants associated with the underlying meson-exchange interactions
- Mapping of the in-medium nucleonic effects at the two-pion-mass scale or heavier-meson scales in a local EDF

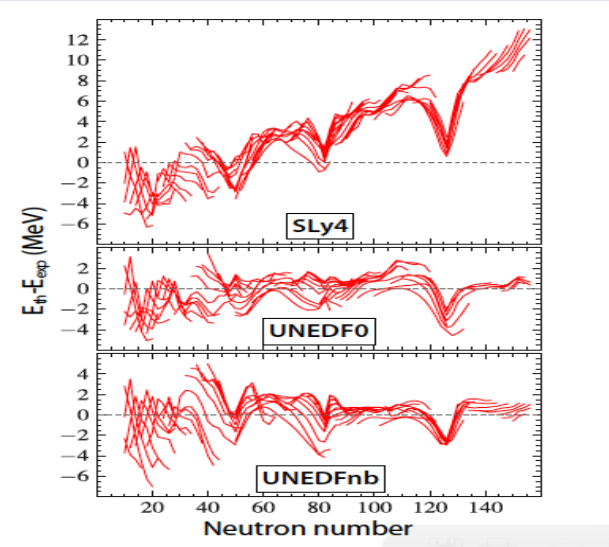


from [P. Finelli et alii, Nucl Phys A **770**, (2006)]

II) Phenomenological nuclear EDF

- Only nucleonic degrees of freedom are explicitely included
- The connection to the strong interaction is limited to the role of symmetries in building the relevant terms of the EDF
- Coupling constants are fitted to the experimental data

from M. Kortelainen et alii, Phys Rev C **82**, (2010)



The Skyrme EDF

Standard Skyrme EDF [Perlinska et alii, Phys Rev C **69, 014316 (2004)**]

$$E\left[\rho(\mathbf{r}),\tau(\mathbf{r}),j(\mathbf{r}),\cdots\right]=\int d\mathbf{r}\, C^{\rho}\rho(\mathbf{r})^2+C^{\tau}\rho(\mathbf{r})\tau(\mathbf{r})+C^{j}j(\mathbf{r})^2+\cdots$$

- Bilinear terms composed by local densities (equipped with coupling constants)

$$\begin{aligned}\tau(\mathbf{r}) &= \left[\nabla\cdot\nabla'\rho(\mathbf{r},\mathbf{r}')\right]_{\mathbf{r}=\mathbf{r}'}\\ j(\mathbf{r}) &= \frac{1}{2i}\left[\left(\nabla-\nabla'\right)\rho(\mathbf{r},\mathbf{r}')\right]_{\mathbf{r}=\mathbf{r}'}\end{aligned}$$

- Order of each term given by the number of derivatives (up to NLO)

The two-body term of the Skyrme interaction [Skyrme, Nuclear Physics **9 615 (1959)**]

$$\begin{aligned}t(\mathbf{k}',\mathbf{k}) &= t_0(1+x_0P^\sigma)+\tfrac{1}{2}t_1(1+x_1P^\sigma)(\mathbf{k}'^2+\mathbf{k}^2)\\ &+ t_2[1+x_2(P^\sigma-\tfrac{4}{5})]\mathbf{k}'\cdot\mathbf{k}\\ &+ \tfrac{1}{2}T[\sigma_1\cdot\mathbf{k}\sigma_2\cdot\mathbf{k}-\tfrac{1}{3}\sigma_1\cdot\sigma_2\mathbf{k}^2+\text{conj.}]\\ &+ \tfrac{1}{2}U[\sigma_1\cdot\mathbf{k}'\sigma_2\cdot\mathbf{k}-\tfrac{1}{3}\sigma_1\cdot\sigma_2\mathbf{k}'\cdot\mathbf{k}+\text{conj.}]\\ &+ V[i(\sigma_1+\sigma_2)\cdot\mathbf{k}'\times\mathbf{k}],\end{aligned}$$

4.png

- expansion in relative momenta of a finite-range interaction (low-momentum range)
- consistent with the symmetries of the nucleon-nucleon interaction
- contact force (easier calculation)
- fitted to experimental data

New-generation nuclear EDFs

Standard phenomenological functionals need to be improved:

- Experimental single-particle energies difficult to reproduce with Skyrme functionals
- Macroscopic models still better (Liquid Drop Models)

Different possible ways to extend the Skyrme EDF:

- by enriching the structure of the functional with density-dependent coupling constants or higher powers of density:

$$\begin{aligned} C &\implies C(\rho(\mathbf{r})); \\ \rho(\mathbf{r})\tau(\mathbf{r}) &\implies \rho^2(\mathbf{r})\tau^2(\mathbf{r}) \end{aligned}$$

- by extending the functional with higher-order derivatives:

$$E\left[\rho(\mathbf{r}), \tau(\mathbf{r}), j(\mathbf{r}), \cdots\right]$$

Simple Taylor expansion on one-body density matrix is performed

$$\rho\left(\mathbf{R}+\frac{\mathbf{r}}{2}\right) = \mathrm{e}^{\frac{1}{2}\mathbf{r}\cdot\nabla}\rho(\mathbf{R}) = \sum_n \frac{1}{n!}\left(\frac{1}{2}\mathbf{r}\cdot\nabla\right)^n \rho(\mathbf{R})$$

Extended Skyrme interaction

Building blocks are higher-order derivatives tensors

$K_{\tilde{n}\tilde{L}}$ are spherical tensor derivatives of order $\tilde{n}$ and rank $\tilde{L}$ [Carlsson et al., Phys. Rev. C **78**, 044326 (2008)]

No.	tensor K_{nL}	order n	rank L
1	1	0	0
2	k	1	1
3	$[kk]_0$	2	0
4	$[kk]_2$	2	2
5	$[kk]_0 k$	3	1
6	$[k[kk]_2]_3$	3	3
7	$[kk]_0^2$	4	0
8	$[kk]_0[kk]_2$	4	2
9	$[k[k[kk]_2]_3]_4$	4	4
10	$[kk]_0^2 k$	5	1
11	$[kk]_0[k[kk]_2]_3$	5	3
12	$[k[k[k[kk]_2]_3]_4]_5$	5	5
13	$[kk]_0^3$	6	0
14	$[kk]_0^2[kk]_2$	6	2
15	$[kk]_0[k[k[kk]_2]_3]_4$	6	4
16	$[k[k[k[k[kk]_2]_3]_4]_5]_6$	6	6

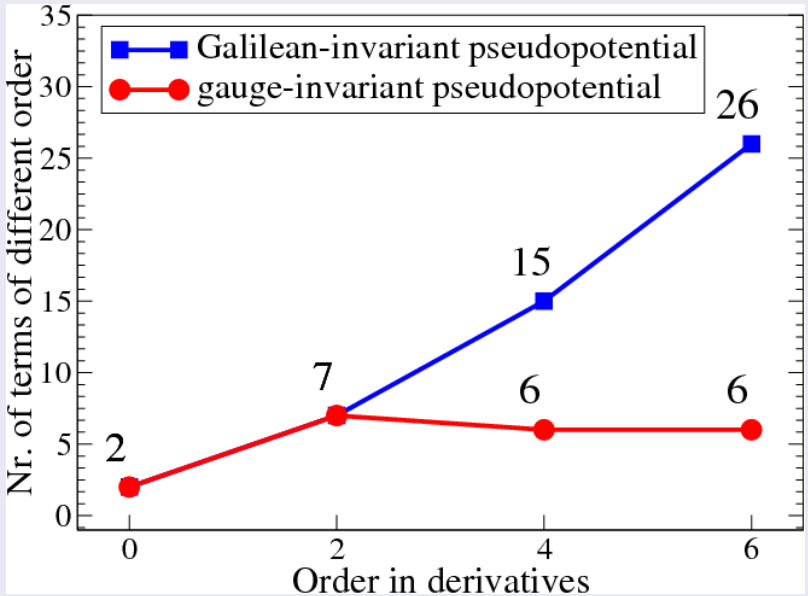
Extended Skyrme interaction: higher-order pseudopotential

Two-body pseudopotential [Raimondi et alii, Phys Rev C **83**, 054311 (2011)][Raimondi et alii, Phys Rev C **84**, 064303 (2011)]

$$\hat{V} = \sum_{\substack{\tilde{n}'\tilde{L}',\\ \tilde{n}\tilde{L},v_{12}S}} C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S} \hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}$$

$C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}$ coupling constant corresponding to tensor $\hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}$ coupled with spin operators.

1. $\{\tilde{n}', \tilde{L}', \tilde{n}, \tilde{L}, v_{12}, S\}$ allowed indices according to the symmetries
2. Pseudopotential is a scalar, local and zero-range operator
3. Expansion up to N^{3}LO



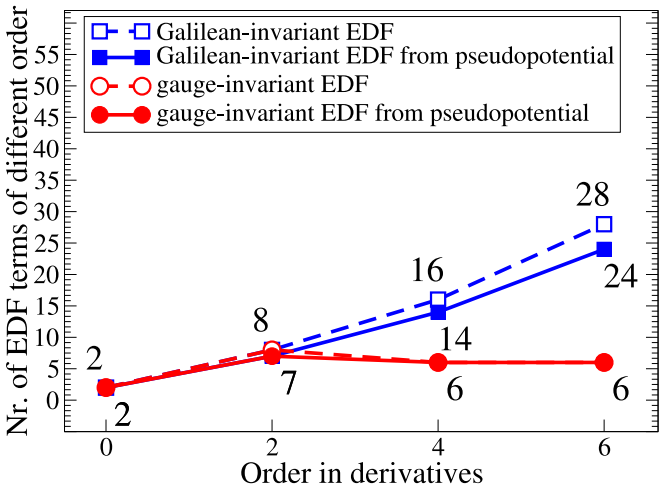
N^{3}LO EDF obtained from the pseudopotential

The average of the pseudopotential with respect to the nuclear many-body wavefunction

$$\langle C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}\hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}\rangle = \sum C^{n'L'v'J',t}_{mI,nLvJ}T^{n'L'v'J',t}_{mI,nLvJ}$$

gives the EDF coupling constants $C^{n'L'v'J',t}_{mI,nLvJ}$ as linear combinations of the pseudopotential coupling constants $C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}$

Results for N^{3}LO EDF



- The EDF has the same symmetries of the pseudopotential
- EDF free from self-interaction problems
- Reduced number of independent coupling constants of the functional

Nuclear phenomenological EDFs based on Effective Theory

Nuclear functionals need to be put on a firm theoretical ground:

- necessity of a regularization procedure to cure the UV divergence of zero-range interactions
- consistent expansion scheme for the functional based on a (length) scale

Methodology of effective theory for nuclear functionals:

1. Introduce an expansion scale by regularizing zero-range pseudopotential
2. Fit the coupling constants
3. Check independence and convergence properties of the expansion
4. Check naturalness of the coupling constants

Scales of energy

We can extract three different scales for nuclear phenomena:

1. Scale of the spontaneous chiral symmetry breaking $\sim$ 1 GeV (Hard)
2. Scale of the boson-exchange interaction (Soft/Hard):
   - Pion mass scale $m_\pi \simeq$135 MeV$/c^2$
   - Fermi momentum scale $k_F \simeq$ 260 MeV$/\hbar c$
3. Low-energy nuclear phenomena scale (Soft):
   - Nucleon separation energy $\delta E \simeq$ 8 MeV corresponding to $\delta k \simeq$ 32 MeV$/\hbar c$
   - Shell effects $E \leqslant$ 1 MeV corresponding to $\delta k \leqslant$ 4 MeV$/\hbar c$

Two observations:

- The small-energy scale in QCD chiral dynamics becomes a short-range high-energy of nucleon-nucleon force acting on nucleons in nuclei.
- In finite nuclei surface effects decrease the infinite-matter binding energies

First step: regularized pseudopotential

A possible way to regularized the potential is to consider Gaussian function

$$\delta(\boldsymbol{r}) = \lim_{a \to 0} g_a(\boldsymbol{r}) = \lim_{a \to 0} \frac{e^{-\frac{\boldsymbol{r}^2}{a^2}}}{(a\sqrt{\pi})^3}$$

Central two-body regularized pseudopotential

$$V(\boldsymbol{r}_1', \boldsymbol{r}_2'; \boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_{i=1}^{4} \hat{P}_i \hat{O}_i(\boldsymbol{k}, \boldsymbol{k}') \delta(\boldsymbol{r}_1' - \boldsymbol{r}_1) \delta(\boldsymbol{r}_2' - \boldsymbol{r}_2) g_a(\boldsymbol{r}_1 - \boldsymbol{r}_2),$$

- $\hat{P}_i$ are the spin and isospin exchange operators, giving the different channels of the interaction
- $\delta(\boldsymbol{r}_1' - \boldsymbol{r}_1)\delta(\boldsymbol{r}_2' - \boldsymbol{r}_2)$ are the locality delta functions
- $\hat{O}_i(\boldsymbol{k}, \boldsymbol{k}')$ are relative momentum operators:
  - 0^{th} order: $\mathbf{1}$ (LO)
  - 2^{nd} order: $\boldsymbol{k}^2$, $\boldsymbol{k}'^2$, ... (NLO)
  - 4^{th} order: $\boldsymbol{k}^4$, $\boldsymbol{k}'^2\boldsymbol{k}^2$, ... ($\mathrm{N^2LO}$)
  - ...

Simplified version of the regularized pseudopotential

Assumption: The pseudopotential depends only on the sum of relative momenta

$$\hat{O}_i(\boldsymbol{k}, \boldsymbol{k}') \equiv \hat{O}_i(\boldsymbol{k} + \boldsymbol{k}')$$

For instance, at NLO, we have (two coupling constants $T_1^{(i)}$ and $T_2^{(i)}$ become dependent),

$$T_0^{(i)} + \frac{1}{2} T_1^{(i)} \left(\boldsymbol{k}^2 + \boldsymbol{k}'^{*2}\right) + T_2^{(i)} \boldsymbol{k} \cdot \boldsymbol{k}'^{*} \equiv T_0^{(i)} + \frac{1}{2} T_1^{(i)} \left(\boldsymbol{k} + \boldsymbol{k}'^{*}\right)^2$$

Local central two-body regularized pseudopotential

$$V(\boldsymbol{r}) = \sum_{i=1}^{4} \hat{P}_i \hat{O}_i(\boldsymbol{k}) g_a(\boldsymbol{r}) = \sum_{i=1}^{4} \hat{P}_i \sum_{n=0}^{n_{\max}} V_{2n}^{(i)} \Delta^n g_a(\boldsymbol{r})$$

- $V(\boldsymbol{r})$ is function of the relative distance $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$
- scalar potential as expansion in powers of Laplacians Δ in $\boldsymbol{r}$
- $V_{2n}^{(i)}$ are coupling constants to be adjusted to data, at a given fixed scale a

Second step: fitting the coupling constants

Standard optimization procedure

1. define a large set of experimental observables
2. optimize values of the coupling constants so as to reproduce experiments
3. test the predictability of the parametrization obtained

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Derivation of the coupling constants

Gogny interaction is a phenomenological finite-range interaction,

$$G(\boldsymbol{r}) = \sum_{i=1}^{4} \hat{P}_i G_i(\boldsymbol{r}) = \sum_{i=1}^{4} \hat{P}_i \sum_{k=1,2} G_k^{(i)} g_{a_k}(\boldsymbol{r})$$

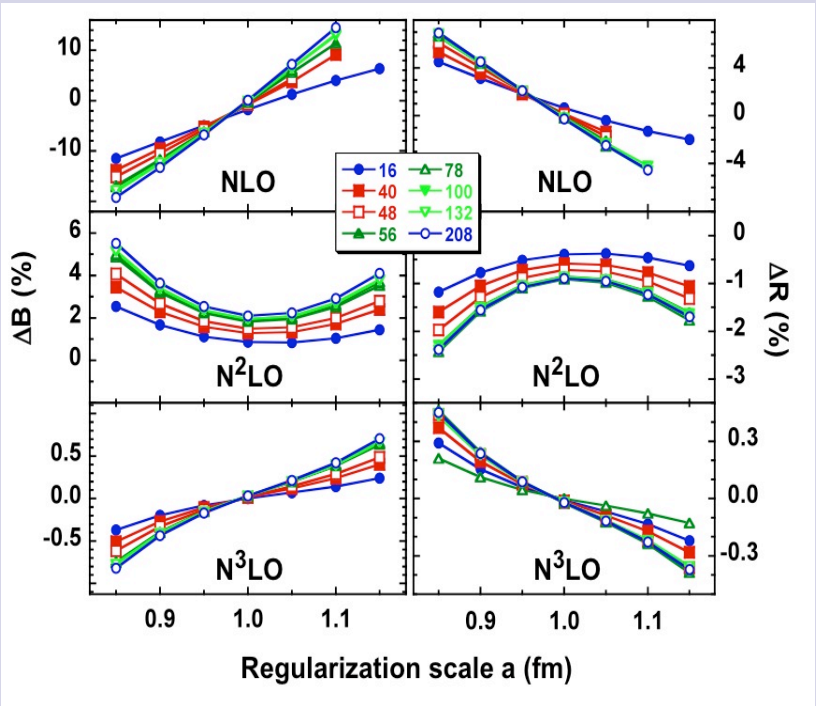
Strategy: for a given value of the range a, derive the pseudopotential coupling constants $V_{2n}^{(i)}$ from the Gogny coupling constants $G_k^{(i)}$ and a_k. This is achieved by requiring that the lowest moments of both potentials are equal

$$M_{2m}^{(i)} \equiv \int \boldsymbol{r}^{2m} G_i(\boldsymbol{r}) \mathrm{d}^3\boldsymbol{r} = \int \boldsymbol{r}^{2m} V_i(\boldsymbol{r}) \mathrm{d}^3\boldsymbol{r}$$

Third step: compute observables

Eight doubly magic nuclei are considered for calculation: ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{78}Ni, ^{100}Sn, ^{132}Sn and ^{208}Pb

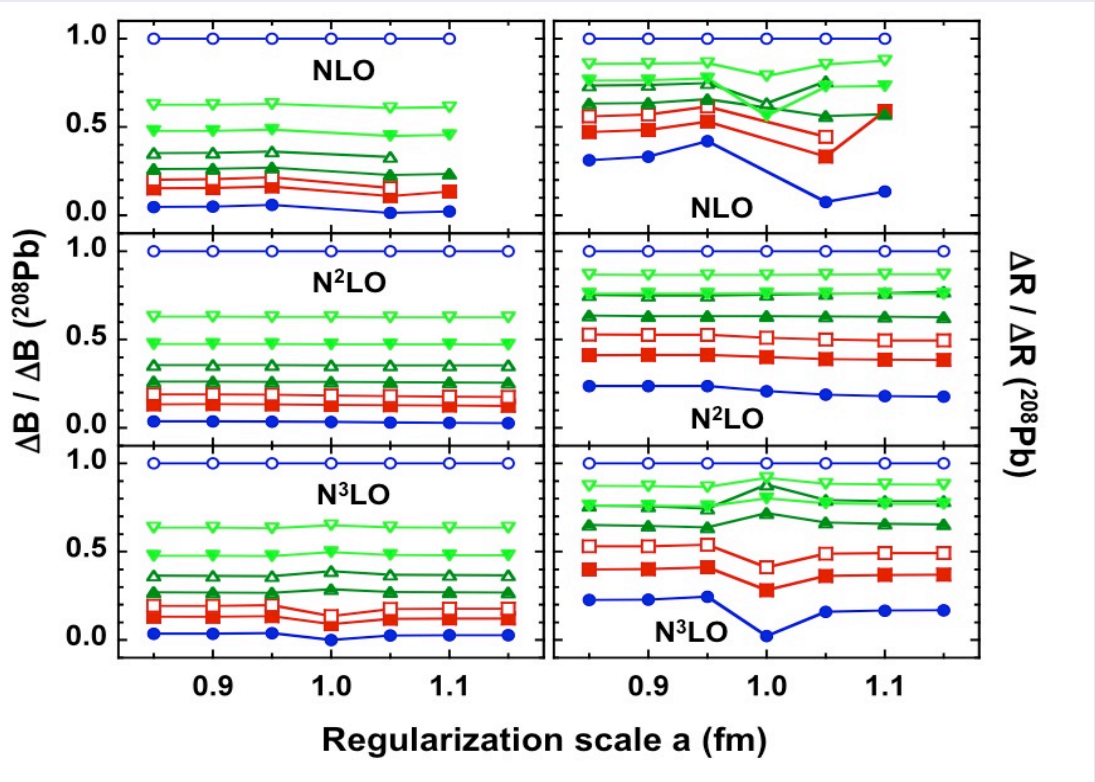
Deviations of binding energies and radii relative to Gogny interaction results



- Convergence very rapid: decreasing by about a factor of four at each order
- Deviations below 1% at N^{3}LO
- Smooth trends of the lines may be ascribed to many-body effects physics

Independence of the regularization scale

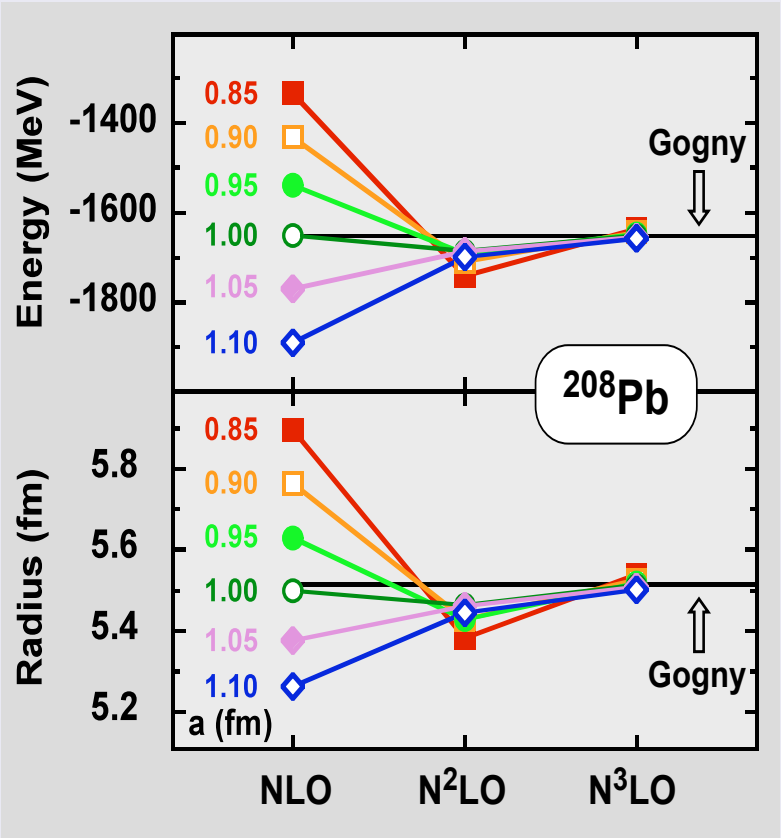
Deviations of binding energies and radii relative to those obtained for ^{208}Pb



- The flatness of lines shows a good degree of independence of the regularization scale
- The choice of ^{208}Pb as nucleus of reference is irrelevant

Independence of the regularization scale for ^{208}Pb

Convergence properties for ^{208}Pb at different scales



- At N^{2}LO the independence with respect to the scale is reached
- At N^{3}LO the convergence of the energy and radius are reached

Comparison between pseudopotential and Gogny form factors of the interaction

- Nuclear observables are weakly dependent on the regularization scale a
- a as parameter to be optimized with respect to the Gogny interaction
- The optimized value of a can be interpreted as range of the effective interaction

Optimization of the pseudopotential coupling constants (included a) has been performed by matching the form factors of the pseudopotential at NLO to the ones of the Gogny interaction

General expressions for the form factors

Gogny form factor

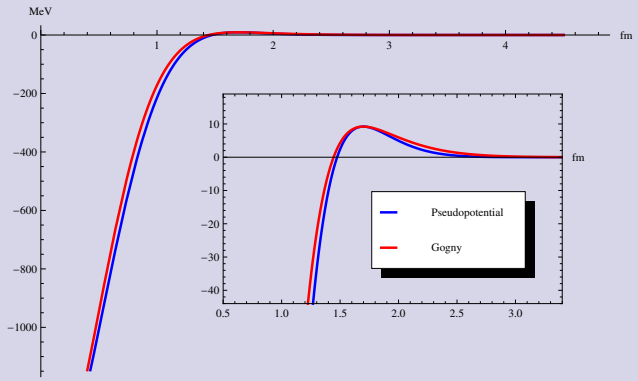
$$\sum_{k=1}^{2} C_k^{(G)} \mathrm{e}^{-\frac{\boldsymbol{r}^2}{a_k^2}}$$

Regularized pseudopotential form factor

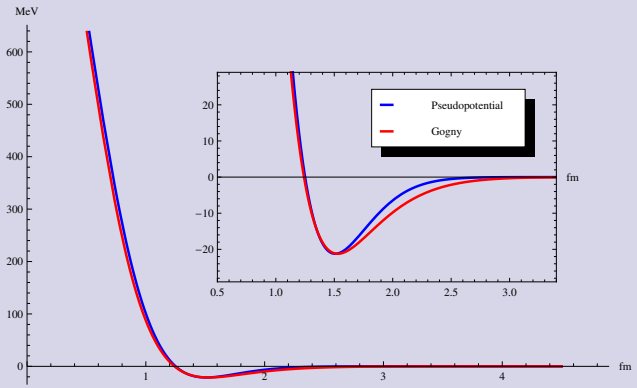
$$\mathrm{e}^{-\frac{\boldsymbol{r}^2}{a^2}} \left(C_0 + C_2 \frac{\boldsymbol{r}^2}{a^2} \right)$$

Plots of the pseudopotential and Gogny form factors of the interaction (a= 0.85 fm)

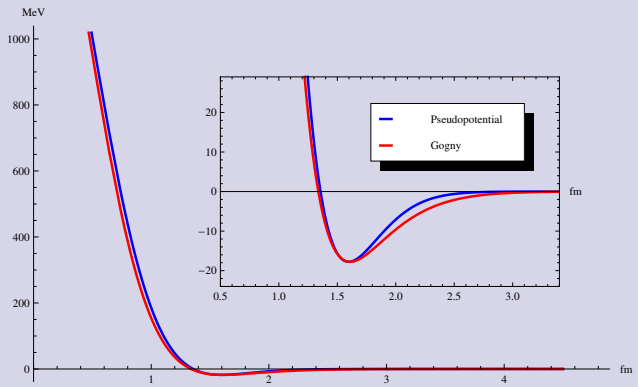
Channel without spin and isospin exchange operators



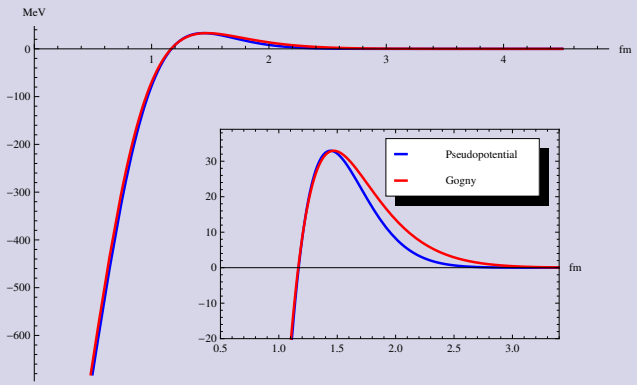
Channel with spin exchange operator



Channel with isospin exchange operator



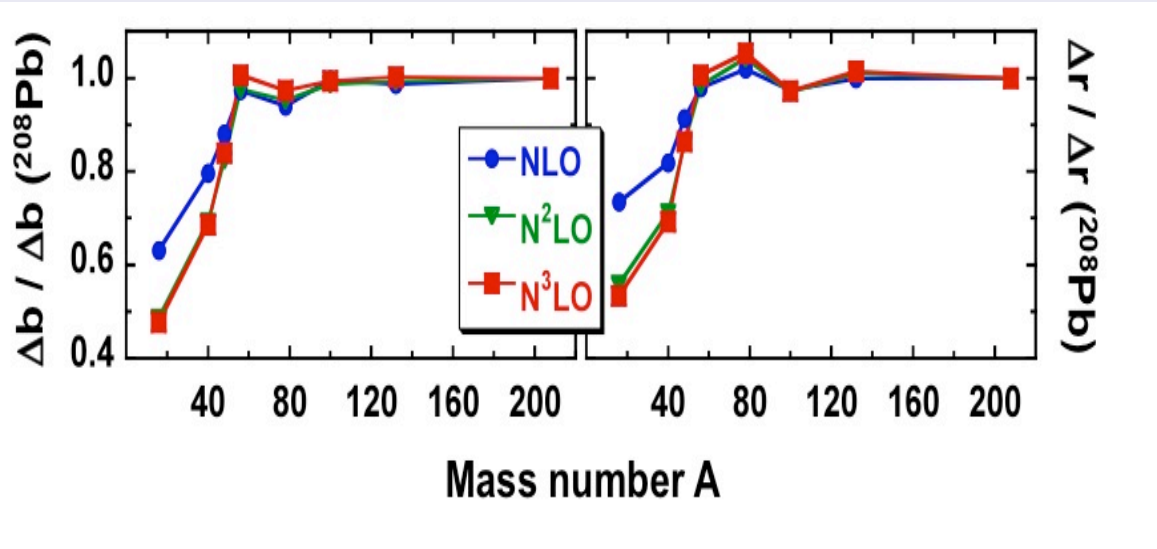
Channel with both spin and isospin exchange operators



Comparing different nuclei in the same scale

- Lepage plots show the dependence of the error in the description of a given observable on energy or a distance
- In nuclear structure (energy and length scales per particle roughly constants) we can study how the error depends on number of nucleons

Deviations of binding energies and radii scaled by number of particles



- Density-matrix expansion technique tells us that local functionals work better in nuclei where the bulk properties overcome surface effects
- Nucley beyond A$\simeq$48 scale in the same way as ^{208}Pb: different size does not change convergence properties
- Lighter nuclei have better convergence properties

Fourth step: naturalness of coupling constants

Naive dimensional analysis applied to effective nuclear Lagrangian

Naturalness: after extracting the dimensional scales from a term of the functional, the remaining dimensionless coefficient should be of order of unity

- The relevant scales of the effective point-coupling Lagrangian

$$c \left[\frac{\psi\dagger\psi}{f^2\Lambda}\right]^l \left[\frac{\nabla}{\Lambda}\right]^n f^2\Lambda^2$$

c dimensionless constant of order of unity,
l power of density expansion,
n power of gradient expansion,
Λ scale of the gradient,
f is the pion decay constant (for functionals derived from ChEFT)

- Scaling factor for the conversion from unnatural to natural coupling constants

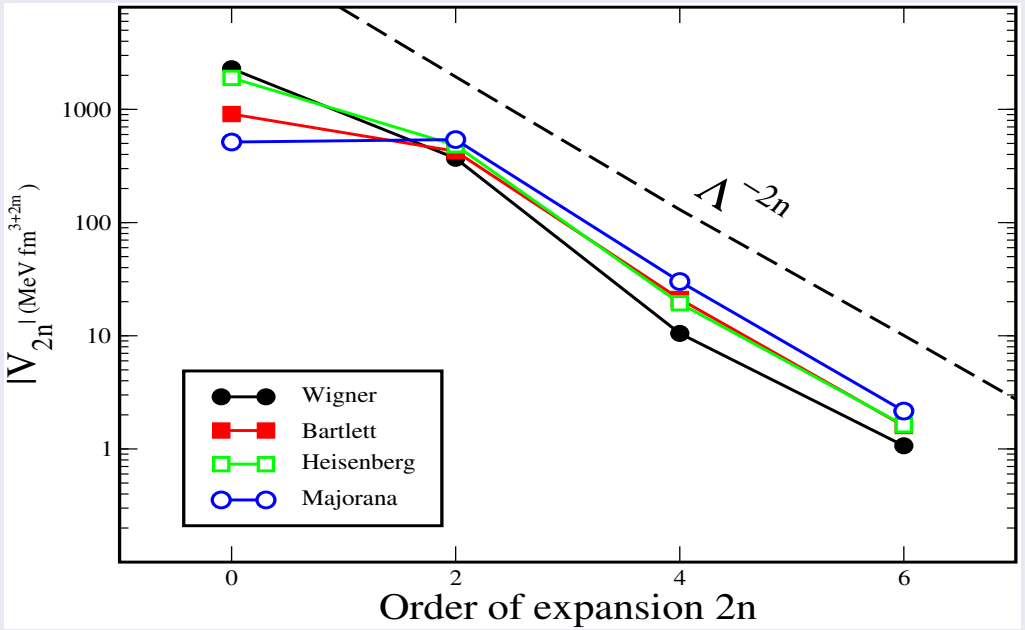
$$S = f^{2(l-1)}\Lambda^{n+l-2}$$

- Dimensionless coupling constants for the local effective pseudopotential ($l = 2$)

$$v_{2n}^{(i)} = f^2\Lambda^{2n}V_{2n}^{(i)}$$

Coupling constants before NDA

Coupling constants values for different channels of the interaction (a=0.85 fm)



- Coupling constants are derived from the coupling constants of the Gogny interaction (no direct adjustment to data)
- In logarithmic scale, coupling constants decrease almost linearly with n
- The slope of this decrease is Λ^{-2n} ($\Lambda \simeq$700 MeV/$\hbar c \simeq$ 3.5 fm^{-1})

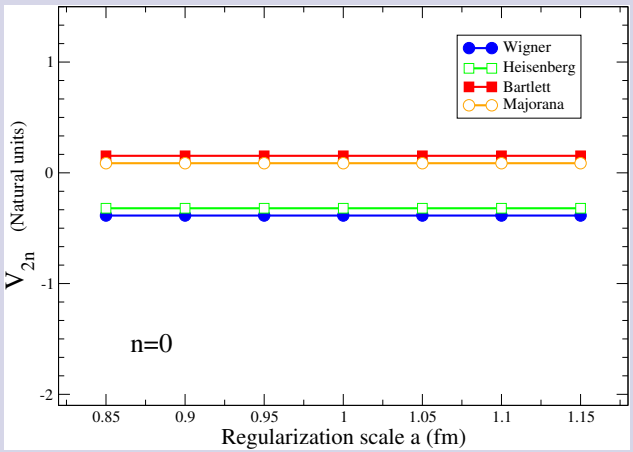
Coupling constants in natural units (I)

- Natural coupling constants

$$v_{2n}^{(i)} = f^2 \Lambda^{2n} V_{2n}^{(i)}$$

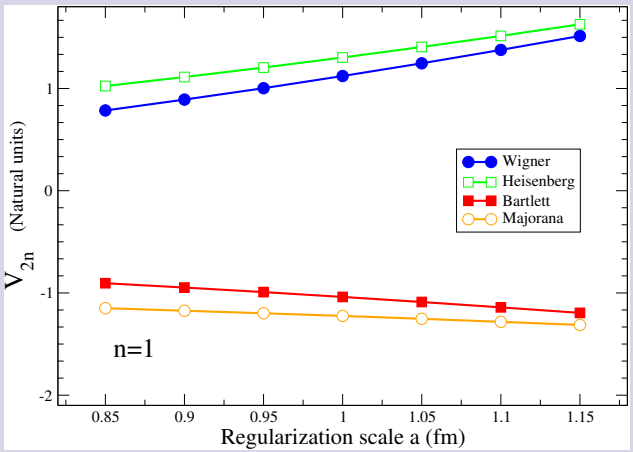
- $v_{2n}^{(i)}$ natural if $f \simeq 35$ MeV$/(\hbar c)^{3/2}$

Zero-order coupling constants



- LO coupling constants are less natural than higher-order ones

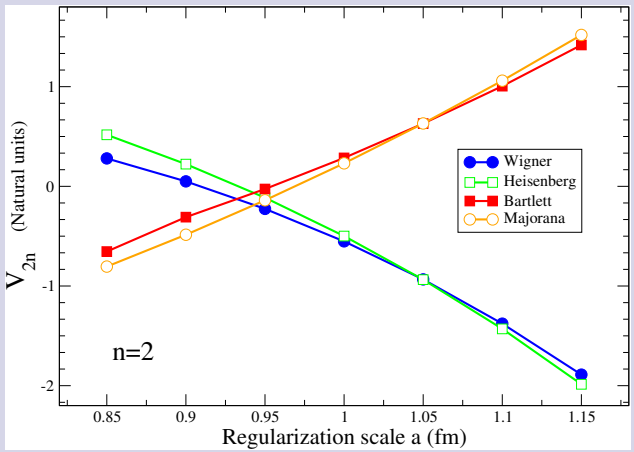
Second-order coupling constants



- NLO coupling constants are natural at all the scales

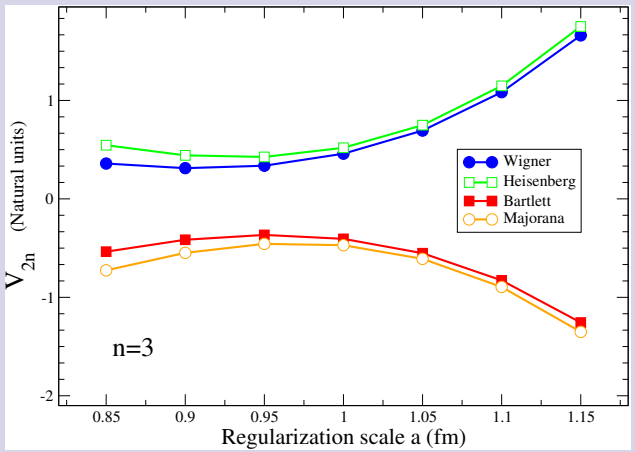
Coupling constants in natural units (II)

Fourth-order coupling constants



- N^2LO coupling constants are natural only at some scales

Sixth-order coupling constants



- N^3LO coupling constants are natural at all the scales

- Naturalness of the coupling constants provides a signature of a QCD hard scale in the low-energy effective functionals
- Future adjustments of the coupling constants to data $\Longrightarrow$ weaker scale dependence

Summary and perspective

Main results addressed

- Application of the effective-theory principles to low-energy nuclear theory
- Construction of the expansion scheme allowing for a systematic improvement of nonlocal EDFs and/or finite-range effective interactions
- Practical implementation of the proposed scheme in terms of Gaussian regulators
- Demonstration that such an expansion scheme rapidly converges
- Check of the naturalness of the pseudopotential coupling constants

Perspective

- Extension of the study to nonlocal regularized pseudopotential
- Optimization of the regularized pseudopotential to experimental data

THANK YOU