Low-energy effective theory for phenomenological nuclear functionals

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

[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, Lund University, P.O. Box 118 Lund 22100,Sweden
[d] Department of Physics, Post Office Box 35 (YFL), FI-40014 University of Jyväskylä, Finland.
[e] Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, ul. Hoża 69, PL-00-681 Warsaw, Poland

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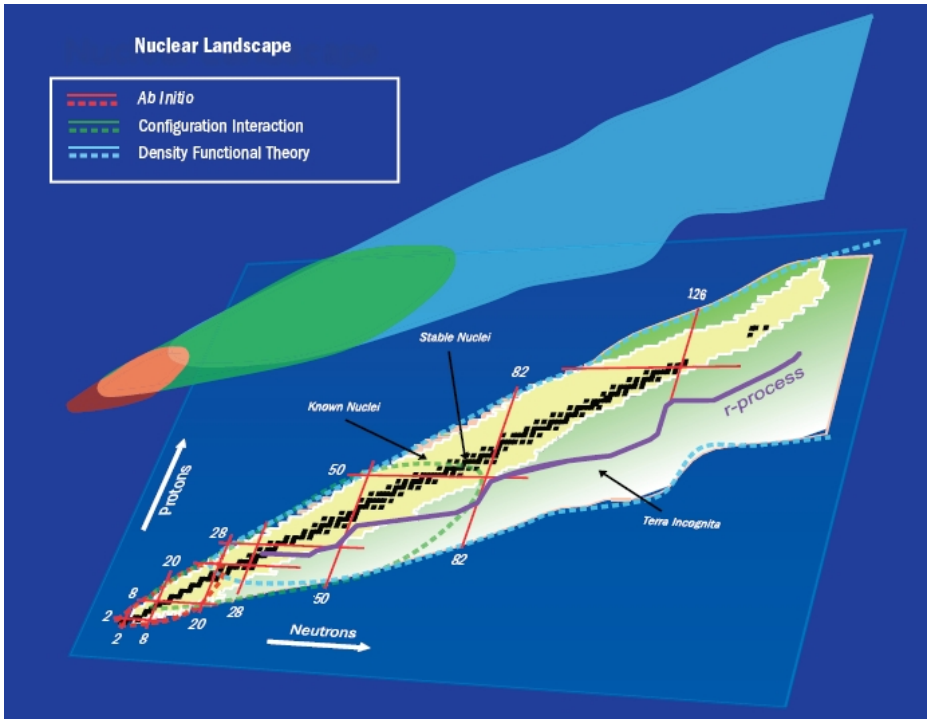
Outline

1. Introduction and Motivation
2. Effective pseudopotential with higher-order derivatives (Raimondi et al., Phys Rev C83, 054311 (2011))
3. Continuity equation for the N^3LO nuclear energy density functionals (Raimondi et al., Phys Rev C84, 064303 (2011))
4. Effective theory for nuclear EDFs (Dobaczewski et al., J. Phys. G39, 125103 (2012))
   - Introduce an expansion scale by regularizing zero-range pseudopotential
   - Fit the coupling constants of the regularized pseudopotential
   - Check independence and convergence properties of the expansion with respect to the expansion scale
   - Check naturalness of the coupling constants

Nuclear Density Functional Theory



- Nuclear DFT is still the only computationally-feasible method giving a global description of the entire nuclear chart (around 3100 nuclei identified, other 6000 expected)
- Description of the nuclear bulk properties (ground-state energies, nucleon-separation energies, charge radius, deformations,...)
- For phenomenological functionals, the best root-means-square deviation relative to thousands of measured masses is around 1 MeV

Ongoing research

- Existing functionals are still not predictive and lacking of true spectroscopic quality
  $\Rightarrow$ Improve the analytical form of the empirical nuclear functional
  $\Rightarrow$ Establish empirical EDF theory on solid theoretical ground

Energy Density Functional (EDF)

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

- Existence of EDF predicted by Hohenberg-Kohn theorem (issue on systematic presence of the symmetry dilemma for nuclear functionals)
- 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
- Ground-state energy obtained through variational principle, $E_{GS} = \mathrm{Min}_{\rho}\, E\left[\rho(\mathbf{r})\right]$

Standard phenomenological nuclear functional [Perlinska et alii, Phys Rev C **69, 014316 (2004)**]

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

- enriched with different kind of densities $\rho(\mathbf{r}),\tau(\mathbf{r}),j(\mathbf{r}),\cdots$ equipped with the corresponding coupling constants $C^{\rho},C^{\tau},C^{j},\cdots$

Motivation

Three questions to be addressed

1. How nuclear energy density functionals can be constrained by an effective interaction?

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1. How nuclear energy density functionals can be constrained by an effective interaction?
2. Is the continuity equation still valid for the higher-order energy density functional?
3. Is the "ab-initio" formulation the only way to put phenomenological nuclear functionals on a firm theoretical ground?

Problems...

1. Phenomenological functionals can be affected by the self-interaction problem [J. P. Perdew, Phys. Rev. B (1981)]
2. Fits of the extended functionals are made more complicated by the increased number of the parameters of the model (instabilities and interdependencies issues arise) [M. Kortelainen et al., J. Phys. G (2010)]
3. The presence of higher powers of momenta in the expansion of the energy density functional (EDF) can be incompatible with the continuity equation
4. Full derivation of phenomenological functionals from underlying vacuum NN and 3N nuclear forces is still incomplete [M. Stoitsov et al., Phys. Rev. C (2010)]

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...solutions

1. Derive an extended pseudopotential that gives the higher-order functional within the Hartree-Fock approximation
2. Reduce the number of the free coupling constants by relating the higher-order EDF to the zero-range extended pseudopotential
3. Derive the constraints among the coupling constants of the general EDF that guarantee the validity of the continuity equation
4. Provide a consistent formulation of the low-energy EDF approach in term of effective theory

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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

Extended Skyrme interaction: building blocks I

Building blocks in spherical tensor representation:

$$k_{1,\mu=\{-1,0,1\}} = -i\left\{\frac{1}{\sqrt{2}}\left(k_x - ik_y\right), k_z, \frac{-1}{\sqrt{2}}\left(k_x + ik_y\right)\right\}$$

where the relative momentum is defined,

$$\boldsymbol{k} = (\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)/2i$$

Pauli matrices acting on spin coordinates,

$$\begin{aligned} \sigma^{(i)}_{00} &= \hat{1}, \\ \sigma^{(i)}_{1,\mu=\{-1,0,1\}} &= -i\left\{\frac{1}{\sqrt{2}}\left(\sigma^{(i)}_x - i\sigma^{(i)}_y\right), \sigma^{(i)}_z, \frac{-1}{\sqrt{2}}\left(\sigma^{(i)}_x + i\sigma^{(i)}_y\right)\right\} \end{aligned}$$

Symmetrized two-body spin operators

$$\hat{S}_{v_{12}S} = \left(1 - \tfrac{1}{2}\delta_{v_1,v_2}\right)\left([\sigma^{(1)}_{v_1}\sigma^{(2)}_{v_2}]_S + [\sigma^{(1)}_{v_2}\sigma^{(2)}_{v_1}]_S\right)$$

Extended Skyrme interaction: building blocks II

Higher-order derivatives tensor

$K_{\tilde{n}\tilde{L}}$ are spherical tensor derivatives of order $\tilde{n}$ and rank $\tilde{L}$ (Carlsson et al., Phys. Rev. C (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

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

where $C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}$ is the strength parameter corresponding to the term,

$$\begin{aligned}\hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S} = \quad & \frac{1}{2} i^{v_{12}} \left(\left[\left[K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}} \right]_S \hat{S}_{v_{12}S} \right]_0 + (-1)^{v_{12}+S} \left[\left[K'_{\tilde{n}\tilde{L}} K_{\tilde{n}'\tilde{L}'} \right]_S \hat{S}_{v_{12}S} \right]_0 \right) \\ & \times \left(1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau \right) \hat{\delta}_{12}(\boldsymbol{r}'_1 \boldsymbol{r}'_2; \boldsymbol{r}_1 \boldsymbol{r}_2)\end{aligned}$$

1. Central-like form of the tensor, i.e. derivatives operators are coupled together and then coupled to the spin operators to give a rotational scalar
2. Locality and zero-range character ensured by the Dirac delta function
3. Exchange term explicitely embedded in the pseudopotential with $\hat{P}^M \hat{P}^\sigma \hat{P}^\tau$
4. $\{\tilde{n}', \tilde{L}', \tilde{n}, \tilde{L}, v_{12}, S\}$ are the allowed indices of the tensors according to the symmetries
5. Terms up to next-to-next-to-next-to-leading order (N^3LO) in derivatives are considered (Skyrme interaction corresponds to a NLO expansion)

Symmetries of the pseudopotential

1. Rotational invariance (spherical tensors coupled to rank 0)
2. Time reversal and parity invariance ($\tilde{n}' + \tilde{n}$ must be even)
3. Hermiticity (parameters $C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}$ must be real)
4. Invariance under permutation of particles indices 1 and 2
5. Galilean invariance

Gauge symmetry

The additional gauge symmetry can be considered. The gauge-invariant pseudopotential must verify the condition

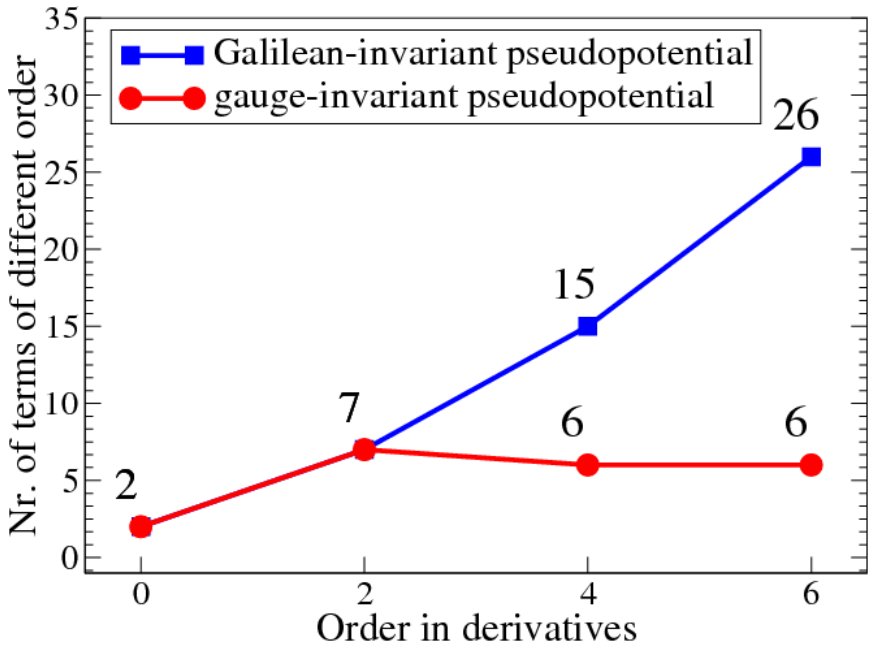
$$\hat{V} = e^{-i\phi(r_2')} e^{-i\phi(r_1')} \hat{V} e^{i\phi(r_1)} e^{i\phi(r_2)}$$

This condition imposes constraints among the parameters, which can be classified as

- vanishing parameters, $C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S} = 0$
- stand-alone gauge invariant parameters (unrestricted parameters)
- independent parameters
- dependent parameters (expressed as linear combinations of the independent ones)

Number of terms of the N^{3}LO pseudopotential

Number of terms of the N^{3}LO pseudopotential plotted as a function of the order in derivatives



- Total number of free terms in the Galilean-invariant pseudopotential is 50, whereas the total number of free terms in the gauge-invariant pseudopotential is 21
- The numbers of terms of the Galilean-(gauge-)invariant pseudopotential are exactly equal to those corresponding to the Galilean-(gauge-)invariant functional in each isospin channel
- At second order, all the terms of the pseudopotential are stand-alone gauge-invariant terms
- Higher-order spin-orbit terms, with $\tilde{n} + \tilde{n}' > 2$, do violate the gauge symmetry

Relations between the pseudopotential and energy density functional

The N^{3}LO EDF is obtained by averaging the N^{3}LO pseudopotential $\hat{V}$ over the uncorrelated wavefunction (a Slater determinant)

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

with the sum $\sum$ running over the allowed values of the indices for the terms of the functional $T^{n'L'v'J',t}_{mI,nLvJ}$ and the corresponding coupling constants $C^{n'L'v'J',t}_{mI,nLvJ}$

Building blocks in energy density functional (Carlsson et al., Phys. Rev. C (2008))

$$T^{n'L'v'J',t}_{mI,nLvJ} = \left[\left[\rho^t_{n'L'v'J'}(\boldsymbol{r})\left[D_{mI}\rho^t_{nLvJ}(\boldsymbol{r})\right]_{J'}\right]_0\right]^0$$

Local densities formed by acting on non-local densities with the relative momentum tensors $K_{\tilde{n}\tilde{L}}$ and taking the limit $\boldsymbol{r}' = \boldsymbol{r}$

$$\rho^t_{nLvJ}(\boldsymbol{r}) = \left\{[K_{nL}\rho^t_v(\boldsymbol{r},\boldsymbol{r}')]_J\right\}_{\boldsymbol{r}'=\boldsymbol{r}}$$

Results

The EDF obtained from the pseudopotential has the following features:

- The obtained EDF coupling constants obey the Galilean-invariant constraints (in general, the EDF is equipped by the same symmetries as the pseudopotential)

- The obtained EDF is free from self-interaction problems

- Owing to the zero range of the pseudopotential, we expect that the number of independent coupling constants of the functional is reduced by a factor of 2

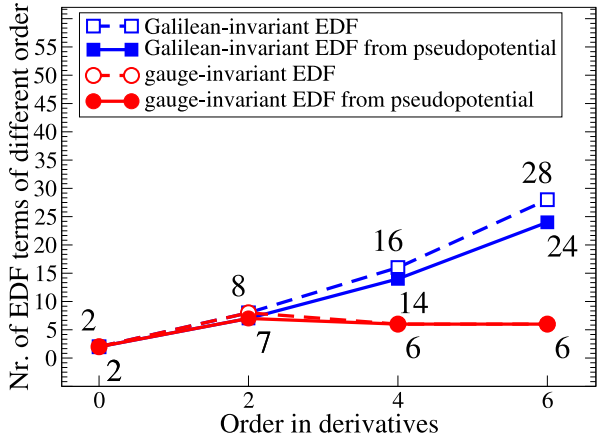
Zero-order EDF case

We can express the isovector coupling constants through the isoscalar ones

$$C^{0000,1}_{00,0000} = -\frac{2}{\sqrt{3}} C^{0000,0}_{00,0000} - C^{0011,0}_{00,0011}$$

$$C^{0011,1}_{00,0011} = -C^{0000,0}_{00,0000}$$

Spherical EDF case



- Spherical, space-inversion, and time-reversal symmetries of the EDF are assumed (selection of symmetries suitable for even-even nuclei)
- Gauge symmetry is considered as further symmetry of the EDF (red lines)
- The reduction in the spherical magic nuclei related to imposing the pseudopotential origins on the EDF is less important than the general case of deformed, odd, nuclei.
- For the Galilean-invariant case (blue lines) the reduction of free coupling constants is due the dependence between spin-orbit isovector and isoscalar coupling constants

Outline

Generalized continuity equation CE

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_v^t(\boldsymbol{r}) = -\frac{\hbar}{m}\boldsymbol{\nabla}\cdot\boldsymbol{J}_v^t(\boldsymbol{r})$$

where the generalized current is defined,

$$\boldsymbol{J}_v^t(\boldsymbol{r}) = \frac{1}{2i}\left(\boldsymbol{\nabla}-\boldsymbol{\nabla}'\right)\rho_v^t(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}'=\boldsymbol{r}}$$

and the spin-isospin densities are the traces of one-body density matrix,

$$\rho_v^t(\boldsymbol{r},\boldsymbol{r}') = \sum_{\sigma\tau,\sigma'\tau'}\sigma_v^{\sigma'\sigma}\tau_{\tau'\tau}^t\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma'\tau')$$

- Scalar-isoscalar $(v=0,t=0)$, $\frac{\mathrm{d}}{\mathrm{d}t}\rho_0^0(\boldsymbol{r},t) = -\frac{\hbar}{m}\boldsymbol{\nabla}\cdot\boldsymbol{J}_0^0(\boldsymbol{r},t)$
- Scalar-isovector $(v=0,t=1)$, $\frac{\mathrm{d}}{\mathrm{d}t}\rho_0^1(\boldsymbol{r},t) = -\frac{\hbar}{m}\boldsymbol{\nabla}\cdot\boldsymbol{J}_0^1(\boldsymbol{r},t)$
- Vector-isoscalar $(v=1,t=0)$, $\frac{\mathrm{d}}{\mathrm{d}t}\rho_1^0(\boldsymbol{r},t) = -\frac{\hbar}{m}\boldsymbol{\nabla}\cdot\boldsymbol{J}_1^0(\boldsymbol{r},t)$
- Vector-isovector $(v=1,t=1)$, $\frac{\mathrm{d}}{\mathrm{d}t}\rho_1^1(\boldsymbol{r},t) = -\frac{\hbar}{m}\boldsymbol{\nabla}\cdot\boldsymbol{J}_1^1(\boldsymbol{r},t)$

A theorem in time-dependent density functional theory

Statement

The gauge invariance of the potential energy density is a necessary and sufficient condition for the validity of the continuity equation

Ingredients of the theorem

- The self-consistent symmetry of the potential energy $E_p\{\rho\}$ with respect to a unitary transformation U

$$E_p\{\rho\} = E_p\{U\rho U^+\}$$

- The self-consistent field (one-body pseudopotential), $\Gamma_{\alpha\beta} = \frac{\partial E_p\{\rho\}}{\partial \rho_{\beta\alpha}}$
- The equation of the time evolution of an operator G

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle G\rangle = i\hbar \mathrm{Tr} G\frac{\mathrm{d}}{\mathrm{d}t}\rho = \mathrm{Tr} G[h,\rho]$$

The theorem follows trivially by specializing U to a gauge transformation and assuming the gauge invariance of the one-body pseudopotential

Application of the theorem to the N^{3}LO EDF

The four local spin-isospin groups of local gauge transformation

$$U_v^t(\boldsymbol{r}) = \exp\left(i\left[\left[\gamma_v^t(\boldsymbol{r})\sigma_v\right]_0\tau^t\right]^0\right)$$

where $\gamma_v^t(\boldsymbol{r})$ is the gauge angle, an arbitrary function of $\boldsymbol{r}$, and σ_v (τ^t) are the generators of the transformation in the spin (isospin) space.

- $U_0^0(\boldsymbol{r})$ gives the standard abelian gauge group U(1)
- $U_1^0(\boldsymbol{r})$ forms the non-abelian gauge groups SU(2) in the spin space
- $U_0^1(\boldsymbol{r})$ forms the non-abelian gauge groups SU(2) in the isospin space
- $U_1^1(\boldsymbol{r})$ corresponds to the non-abelian gauge group SU(2)$\times$SU(2) in the spin-isospin product space

The theorem for N^{3}LO functional

The invariance of the N^{3}LO EDF with respect to each of the four local gauge transformations is equivalent to the validity of the generalized continuity equation in the four spin-isospin channels

Derivation of the continuity equation for N^{3}LO one-body pseudopotential

Starting from the Schrödinger equation that gives the time evolution of single-particle Kohn-Sham wave functions

$$i\hbar\frac{\partial}{\partial t}\phi_i(\boldsymbol{r}\sigma\tau,t) = -\frac{\hbar^2}{2m}\Delta\phi_i(\boldsymbol{r}\sigma\tau,t) + \sum_{\sigma'\tau'}\hat{\Gamma}^{\sigma\sigma'}_{\tau\tau'}(\boldsymbol{r})\phi_i(\boldsymbol{r}\sigma'\tau',t)$$

we obtain the time-evolution equation for the density matrix,

$$i\hbar\frac{\partial}{\partial t}\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma'\tau',t) = -\frac{\hbar^2}{2m}\left(\Delta-\Delta'\right)\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma'\tau',t)$$
$$+\sum_{\sigma''\tau''}\left(\hat{\Gamma}^{\sigma\sigma''}_{\tau\tau''}(\boldsymbol{r})\rho(\boldsymbol{r}\sigma''\tau'',\boldsymbol{r}'\sigma'\tau',t) - \hat{\Gamma}^{\sigma'\sigma''*}_{\tau'\tau''}(\boldsymbol{r}')\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma''\tau'',t)\right)$$

Condition for the validity of CE

$$\sum_{\sigma''\tau''}\left(\Gamma^{\sigma\sigma''}_{\tau\tau''}(\mathbf{r})\rho(\mathbf{r}\sigma''\tau'',\mathbf{r}'\sigma'\tau') - \Gamma^{\sigma'\sigma''*}_{\tau'\tau''}(\mathbf{r}')\rho(\mathbf{r}\sigma\tau,\mathbf{r}'\sigma''\tau'')\right)_{\boldsymbol{r}'=\boldsymbol{r}} = 0$$

This condition can be separated in the four spin-isospin channels, relative to the four channels of the generalized continuity equation

N^{3}LO one-body pseudopotential

The functional derivative of the N^{3}LO potential energy with respect to the local densities

$$\hat{\Gamma}^{\sigma\sigma'}_{\tau\tau'}(\boldsymbol{r}) = \sum_{a\alpha\beta,\gamma t} C^{\beta,t}_{a,\alpha} \frac{\partial T^{\beta,t}_{a,\alpha}(\boldsymbol{r})}{\partial \rho_\gamma}$$

where the grouped indices notation is adopted (for instance, $C^{\beta,t}_{a,\alpha} \equiv C^{n_\beta L_\beta v_\beta J_\beta, t}_{m_a I_a, n_\alpha L_\alpha v_\alpha J_\alpha}$)

N^{3}LO one-body pseudopotential [Carlsson et al., Comput. Phys. Commun. (2010)]

$$\hat{\Gamma}^{\sigma\sigma'}_{\tau\tau'}(\boldsymbol{r}) = \sum_{\gamma,t} \left[\left[U^t_\gamma(\boldsymbol{r}) \left[D_{n_\gamma L_\gamma} \sigma^{\sigma\sigma'}_{v_\gamma} \right]_{J_\gamma} \right]_0 \tau^t_{\tau\tau'} \right]^0$$

composed by the potentials derived as secondary densities,

$$U^t_\gamma(\boldsymbol{r}) = \sum_{a\alpha\beta;d\delta} C^{\beta,t}_{a,\alpha} \chi^{\beta;d\delta}_{a,\alpha;\gamma} \left[D_d \rho^t_\delta(\boldsymbol{r}) \right]_{J_\gamma} ,$$

where $\chi^{\beta;d\delta}_{a,\alpha;\gamma}$ are numerical coefficients (1494 up to N^{3}LO)

Results (scalar-isoscalar channel $\Leftrightarrow$ Abelian gauge group)

- For the standard CE in the scalar-isoscalar channel, the constraints among the coupling constants which guarantee the validity of the CE are the same as those defining the gauge-invariant functional up to $\mathrm{N^3LO}$ (perfect agreement with the gauge-invariance constraints of the functional found in [Carlsson et al., Phys. Rev. C (2008)])

- Scalar-isoscalar constraints do not mix coupling constants in spin and isospin (index t) spaces

At second order $(t = 0, 1)$

$$
\begin{aligned}
C^{0000,t}_{00,2000} &= -C^{1101,t}_{00,1101} \\
C^{1110,t}_{00,1110} &= -\tfrac{1}{3} C^{0011,t}_{00,2011} - \tfrac{1}{3}\sqrt{5} C^{0011,t}_{00,2211} \\
C^{1111,t}_{00,1111} &= \tfrac{1}{2}\sqrt{\tfrac{5}{3}} C^{0011,t}_{00,2211} - \tfrac{1}{\sqrt{3}} C^{0011,t}_{00,2011} \\
C^{1112,t}_{00,1112} &= -\tfrac{1}{3}\sqrt{5} C^{0011,t}_{00,2011} - \tfrac{1}{6} C^{0011,t}_{00,2211} \\
C^{0000,t}_{11,1111} &= C^{1101,t}_{11,0011}
\end{aligned}
$$

the unconstrained coupling constants $C^{0000,t}_{20,0000}$, $C^{0011,t}_{20,0011}$ and $C^{0011,t}_{22,0011}$

Results for non-Abelian gauge groups

Non-Abelian gauge-invariant functionals are more restricted than the Abelian one (spin-orbit coupling constants are forced to be zero by the non-Abelian transformation)

scalar-isovector channel

- The condition for the continuity equation in the scalar-isovector channel gives constraints that mix coupling constants in the isospin space
- When the proton-neutron symmetry is assumed ($\tau_1^1 = \tau_2^1 = 0$), the continuity equations for protons and neutrons decouple and become independently valid

vector-isoscalar channel

- The condition for the continuity equation in the vector-isoscalar channel gives constraints that mix coupling constants in the spin space

vector-isovector channel

- The condition for the continuity equation in the vector-isovector channel gives constraints that relate coupling constants in both spin and isospin spaces

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Nuclear phenomenological EDFs based on Effective Theory

Consistent formulation of phenomenological EDFs within an effective theory

An example: Effective theory for deformed nuclei (Papenbrock and Zhang, Nucl Phys A (2011), Phys Rev C (2013))

1. Exploit separation of energy scales between vibrational ($\Omega \sim 1$ MeV) and rotational ($\xi \sim$ tens of KeV) degrees of freedom in rare earth nuclei
2. Low-energy (rotational) degrees of freedom treated as (approximated) Nambu-Goldstone modes of spontaneous breaking of the rotational symmetry (SO(3) down to SO(2))
3. Restored full rotational symmetry is the guiding principle in building the Hamiltonian from the rotational and vibrational degrees of freedom
4. Higher-order terms in Nambu-Goldstone modes, with empirical coupling constants, are introduced to include omitted physics at the breakdown scale
5. Expansion is controlled by a power counting based on the ratio $\frac{\xi}{\Omega}$
6. More flexibility of the effective Hamiltonian compared to the old phenomenological models (i.e. Bohr Hamiltonian)

Outline

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

Outline

1. Introduction and Motivation
2. Effective pseudopotential with higher-order derivatives (Raimondi et al., Phys Rev C83, 054311 (2011))
3. Continuity equation for the N^3LO nuclear energy density functionals (Raimondi et al., Phys Rev C84, 064303 (2011))
4. Effective theory for nuclear EDFs (Dobaczewski et al., J. Phys. G39, 125103 (2012))
   - Introduce an expansion scale by regularizing zero-range pseudopotential
   - Fit the coupling constants of the regularized pseudopotential
   - Check independence and convergence properties of the expansion with respect to the expansion scale
   - Check naturalness of the coupling constants

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

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

Methodology of effective theory for higher-order in derivatives functionals

1. Introduction and Motivation
2. Effective pseudopotential with higher-order derivatives (Raimondi et al., Phys Rev C83, 054311 (2011))
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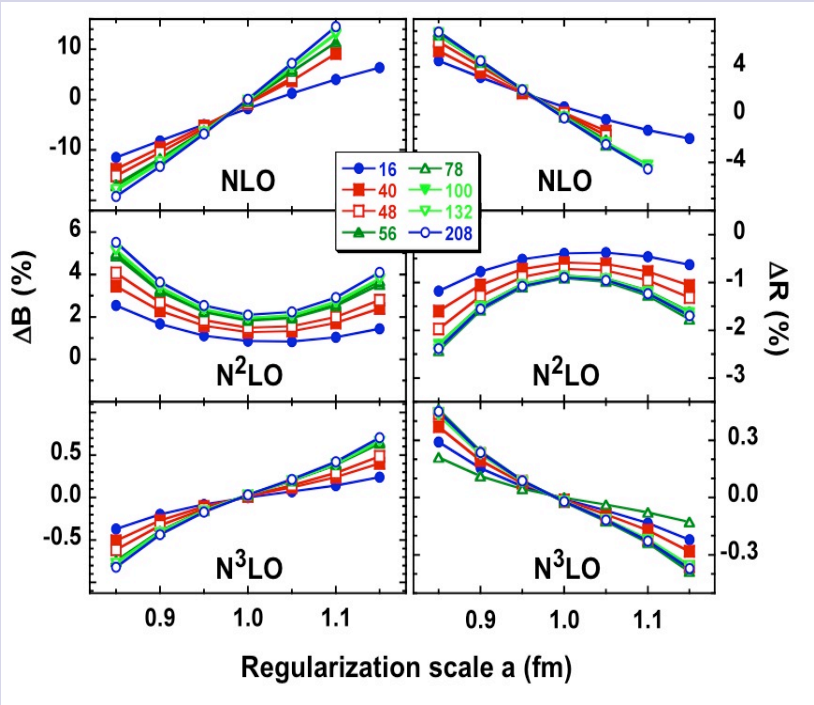
Compute observables

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

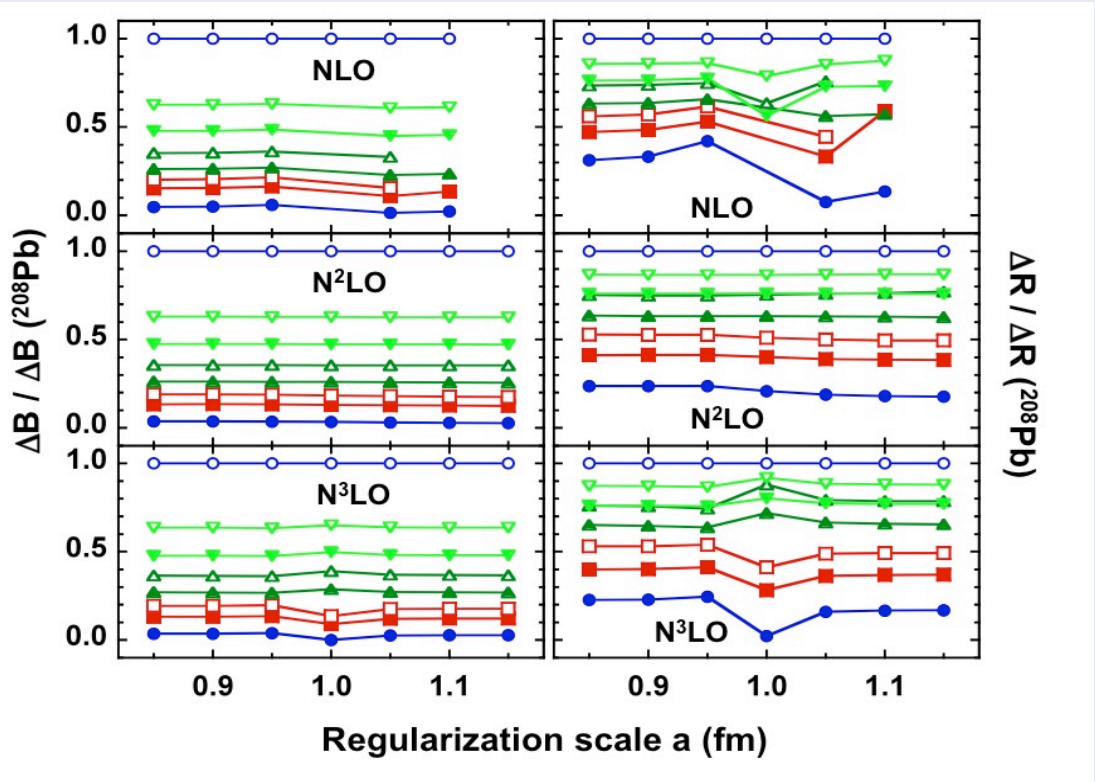
Deviations of binding energies and radii relative to Gogny interaction results



- 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 very sensitive to the values of coupling constants

Independence of the regularization scale

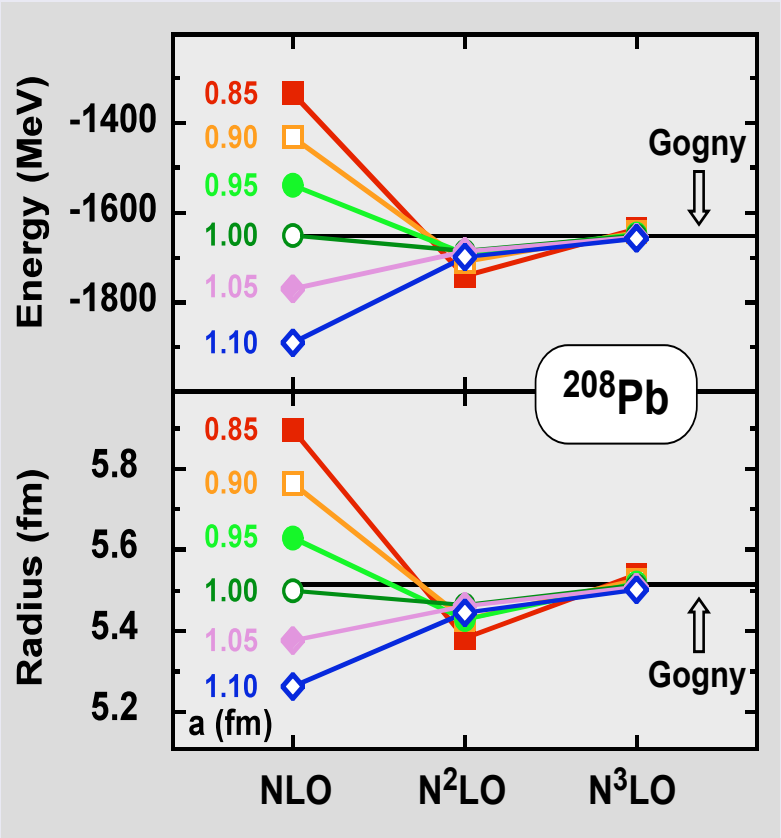
Deviations of binding energies and radii relative to those obtained for ^{208}Pb



- 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

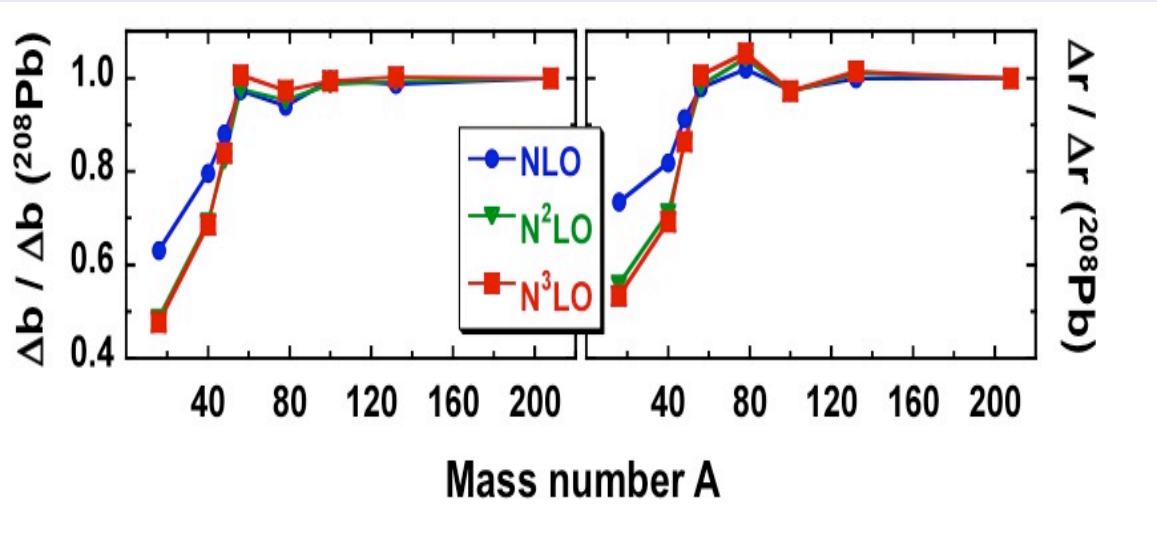


- At N^{2}LO the independence with respect to the scale is reached
- At N^{3}LO the convergence of the energy and radius are reached

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

Outline

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

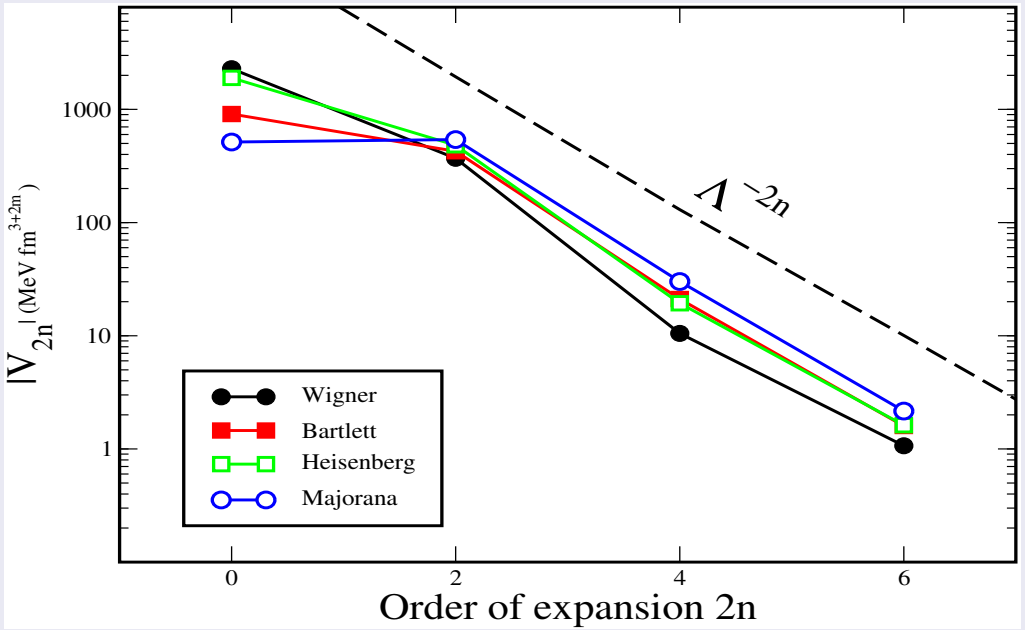
$$S = f^{2(l-1)}\Lambda^{n+l-2}$$

- 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})

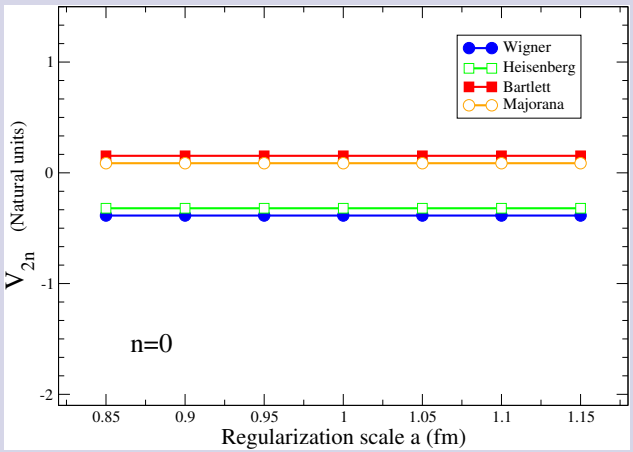
Coupling constants in natural units (I)

- Natural coupling constants

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

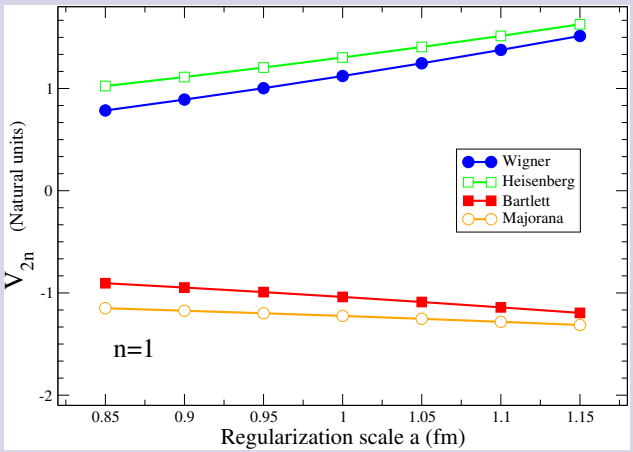
- $v_{2n}^{(i)}$ natural if $f \simeq 35$ MeV$/(\hbar c)^{3/2}$

Zero-order coupling constants



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

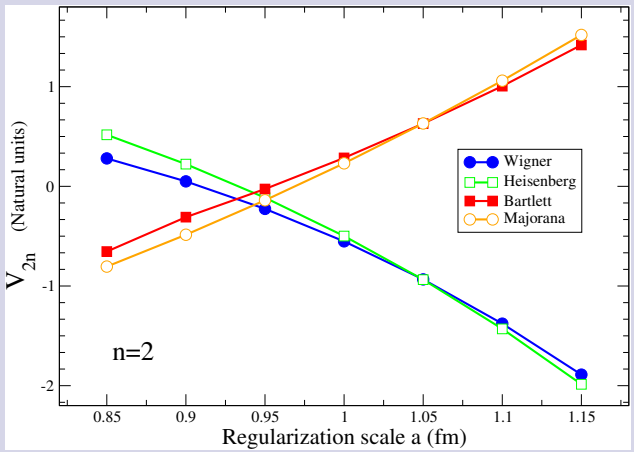
Second-order coupling constants



- NLO coupling constants are natural at all the scales

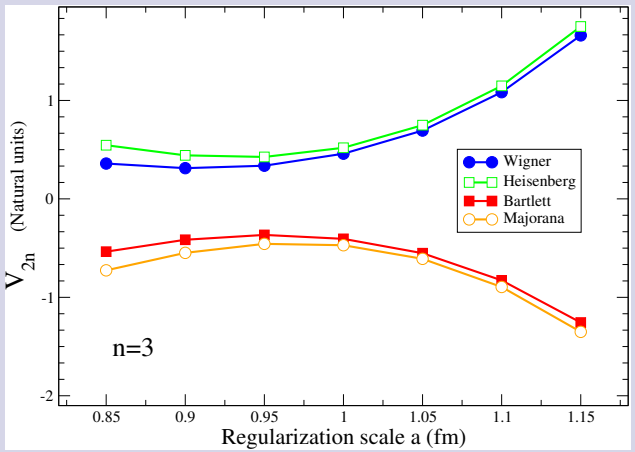
Coupling constants in natural units (II)

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

1. Some aspects of the N^{3}LO EDF have been investigated
   - Relation of the functional to the N^{3}LO pseudopotential and reduction of the free coupling constants of the functional
   - Link between the validity of continuity equation and the gauge invariance of the functional
2. Effective-theory principles have been applied to low-energy nuclear theory
   - Construction of the expansion scheme allowing for a systematic improvement of nonlocal EDFs and/or finite-range effective interactions 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 both the higher-order and regularized pseudopotential to experimental data

BACK UP

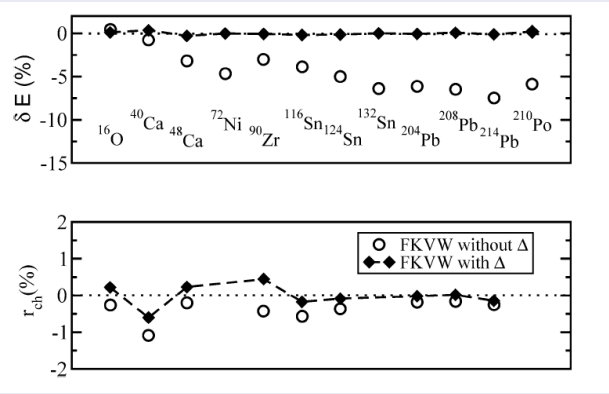
Two main classes of nuclear EDFs

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

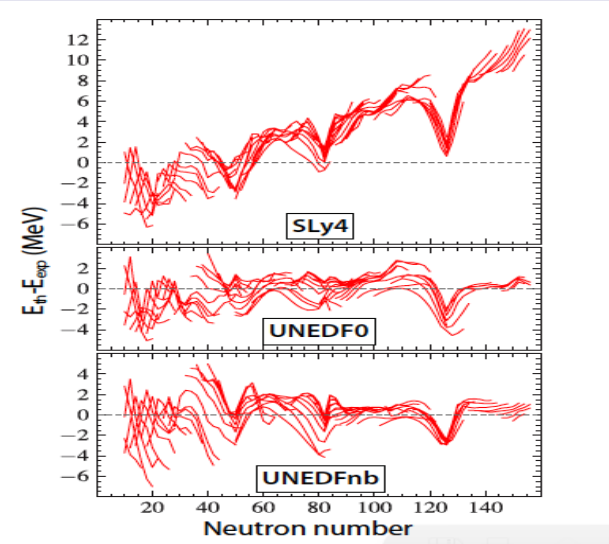


from [P. Finelli et alii, Nucl Phys A **770**, (2006)]

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)



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

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

The N^{3}LO energy density functional I

One-body density matrix

Separation into spin $(v = 0, 1)$ and isospin $(t = 0, 1)$ channels

$$\rho(\boldsymbol{r}\sigma\tau, \boldsymbol{r}'\sigma'\tau') = \frac{1}{4} \sum_{\substack{v=0,1 \\ t=0,1}} \left(\sqrt{3}\right)^{v+t} \left[\sigma_v^{\sigma\sigma'} \left[\tau_{\tau\tau'}^t \rho_v^t(\boldsymbol{r}, \boldsymbol{r}')\right]^0\right]_0$$

non-local densities

$$\begin{aligned}
\rho_0^0(\boldsymbol{r}, \boldsymbol{r}') &= \rho(\boldsymbol{r}, \boldsymbol{r}') \\
\rho_1^0(\boldsymbol{r}, \boldsymbol{r}')_{1,\mu=\{-1,0,1\}} &= -i \left\{ \tfrac{1}{\sqrt{2}} \left(\boldsymbol{s}_x(\boldsymbol{r}, \boldsymbol{r}') - i\boldsymbol{s}_y(\boldsymbol{r}, \boldsymbol{r}')\right), \boldsymbol{s}_z(\boldsymbol{r}, \boldsymbol{r}'), \right. \\
&\quad \left. \tfrac{-1}{\sqrt{2}} \left(\boldsymbol{s}_x(\boldsymbol{r}, \boldsymbol{r}') + i\boldsymbol{s}_y(\boldsymbol{r}, \boldsymbol{r}')\right) \right\} \\
\rho_0^1(\boldsymbol{r}, \boldsymbol{r}')_{1,\mu=\{-1,0,1\}} &= -i \left\{ \tfrac{1}{\sqrt{2}} \left(\vec{\rho}_x(\boldsymbol{r}, \boldsymbol{r}') - i\vec{\rho}_y(\boldsymbol{r}, \boldsymbol{r}')\right), \vec{\rho}_z(\boldsymbol{r}, \boldsymbol{r}'), \right. \\
&\quad \left. \tfrac{-1}{\sqrt{2}} \left(\vec{\rho}_x(\boldsymbol{r}, \boldsymbol{r}') + i\vec{\rho}_y(\boldsymbol{r}, \boldsymbol{r}')\right) \right\} \\
\rho_1^1(\boldsymbol{r}, \boldsymbol{r}')_{1,\mu=\{-1,0,1\}} &= -i \left\{ \tfrac{1}{\sqrt{2}} \left(\vec{\boldsymbol{s}}_x(\boldsymbol{r}, \boldsymbol{r}') - i\vec{\boldsymbol{s}}_y(\boldsymbol{r}, \boldsymbol{r}')\right), \vec{\boldsymbol{s}}_z(\boldsymbol{r}, \boldsymbol{r}'), \right. \\
&\quad \left. \tfrac{-1}{\sqrt{2}} \left(\vec{\boldsymbol{s}}_x(\boldsymbol{r}, \boldsymbol{r}') + i\vec{\boldsymbol{s}}_y(\boldsymbol{r}, \boldsymbol{r}')\right) \right\}
\end{aligned}$$

The N^{3}LO energy density functional II

Local densities

Formed by acting on non-local densities with the relative momentum tensors $K_{\tilde{n}\tilde{L}}$ and taking the limit $\boldsymbol{r}' = \boldsymbol{r}$

$$\rho^t_{nLvJ}(\boldsymbol{r}) = \left\{ [K_{nL} \rho^t_v(\boldsymbol{r}, \boldsymbol{r}')]_J \right\}_{\boldsymbol{r}'=\boldsymbol{r}}$$

Terms in the energy density functional

$$T^{n'L'v'J',t}_{mI,nLvJ} = \left[\left[\rho^t_{n'L'v'J'}(\boldsymbol{r}) \left[D_{mI} \rho^t_{nLvJ}(\boldsymbol{r}) \right]_{J'} \right]_0 \right]^0$$

The terms are required to be:

- quadratic in densities
- time-reversal invariant
- space-inversion invariant
- rotational invariant

The corresponding density-independent coupling constants is denoted $C^{n'L'v'J',t}_{mI,nLvJ}$

Comparison with standard Skyrme interaction

The pseudopotential up to second order is equivalent to the Skyrme interaction, expressed traditionally in Cartesian coordinates

	Terms	Cartesian representation (Skyrme force)
1	$\hat{V}^{20}_{00,00}$	$\frac{1}{\sqrt{3}}(\boldsymbol{k'}^2\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)+\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\boldsymbol{k}^2)$
2	$\hat{V}^{20}_{00,20}$	$\frac{1}{3}(\boldsymbol{k'}^2\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)+\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\boldsymbol{k}^2)(\boldsymbol{\sigma^{(1)}}\cdot\boldsymbol{\sigma^{(2)}})$
3	$\hat{V}^{22}_{00,22}$	$\frac{1}{\sqrt{5}}((\boldsymbol{k'}\cdot\boldsymbol{\sigma^{(1)}})(\boldsymbol{k'}\cdot\boldsymbol{\sigma^{(2)}})\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)+\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)(\boldsymbol{k}\cdot\boldsymbol{\sigma^{(1)}})(\boldsymbol{k}\cdot\boldsymbol{\sigma^{(2)}}))$ $-\frac{1}{3\sqrt{5}}((\boldsymbol{k'}^2\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)+\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\boldsymbol{k}^2)(\boldsymbol{\sigma^{(1)}}\cdot\boldsymbol{\sigma^{(2)}}))$
4	$\hat{V}^{11}_{11,00}$	$\frac{1}{\sqrt{3}}(\boldsymbol{k'}\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\cdot\boldsymbol{k})$
5	$\hat{V}^{11}_{11,20}$	$\frac{1}{3}(\boldsymbol{k'}\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\cdot\boldsymbol{k})(\boldsymbol{\sigma^{(1)}}\cdot\boldsymbol{\sigma^{(2)}})$
6	$\hat{V}^{11}_{11,11}$	$\frac{1}{\sqrt{6}}i(\boldsymbol{k'}\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\times\boldsymbol{k})(\boldsymbol{\sigma^{(1)}}+\boldsymbol{\sigma^{(2)}})$
7	$\hat{V}^{11}_{11,22}$	$\frac{1}{\sqrt{5}}(\boldsymbol{k'}\cdot\boldsymbol{\sigma^{(1)}})\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)(\boldsymbol{k}\cdot\boldsymbol{\sigma^{(2)}})-\frac{1}{3\sqrt{5}}(\boldsymbol{k'}\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\cdot\boldsymbol{k})(\boldsymbol{\sigma^{(1)}}\cdot\boldsymbol{\sigma^{(2)}})$

Density dependent terms are missing (however important to guarantee proper saturation)

Results

Number of independent parameters and coupling constants up to N^3LO

	Pseudopotential		EDF							
			Not related to pseudopotential				Related to pseudopotential			
			General		Spherical		General		Spherical	
Order	Galilean	Gauge	Galilean	Gauge	Galilean	Gauge	Galilean	Gauge	Galilean	Gauge
0	2	2	4	4	2	2	2	2	2	2
2	7	7	14	14	8	8	7	7	7	7
4	15	6	30	12	16	6	15	6	14	6
6	26	6	52	12	28	6	26	6	24	6
N^3LO	50	21	100	42	54	22	50	21	47	21

- In the general case (no spherical symmetry) the number of independent coupling constants of the EDF obtained from the pseudopotential is twice smaller than that of the EDF not related to the pseudopotential
- One-half of the coupling constants (for instance the isovector ones) can be expressed through the other half (for instance the isocalar ones)

Results

The averaging expression

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

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

Zero-order EDF case

For instance, at zero-order, we get,

$$\begin{aligned}
C^{0000,0}_{00,0000} &= \frac{3}{8}C^{00}_{00,00} + \frac{\sqrt{3}}{8}C^{00}_{00,20} \\
C^{0011,0}_{00,0011} &= -\frac{\sqrt{3}}{8}C^{00}_{00,00} - \frac{5}{8}C^{00}_{00,20} \\
C^{0000,1}_{00,0000} &= -\frac{\sqrt{3}}{8}C^{00}_{00,00} + \frac{3}{8}C^{00}_{00,20} \\
C^{0011,1}_{00,0011} &= -\frac{3}{8}C^{00}_{00,00} - \frac{\sqrt{3}}{8}C^{00}_{00,20}
\end{aligned}$$

Results for non-Abelian gauge groups (scalar-isovector channel)

- The condition for the continuity equation in the scalar-isovector channel gives constraints that mix coupling constants in the isospin space

At second order, the constraints for the scalar-isovector continuity equation

$$
\begin{aligned}
C^{0000,t}_{00,2000} &= -\frac{3^t}{\sqrt{3}} C^{1101,1-t}_{00,1101} \\
C^{1110,t}_{00,1110} &= -\frac{3^t}{3\sqrt{3}} C^{0011,1-t}_{00,2011} - \frac{3^t}{3}\sqrt{\frac{5}{3}} C^{0011,1-t}_{00,2211} \\
C^{1111,t}_{00,1111} &= -\frac{3^t}{3} C^{0011,1-t}_{00,2011} + \frac{3^t}{6}\sqrt{5} C^{0011,1-t}_{00,2211} \\
C^{1112,t}_{00,1112} &= -\frac{3^t}{3}\sqrt{\frac{5}{3}} C^{0011,1-t}_{00,2011} - \frac{3^t}{6\sqrt{3}} C^{0011,1-t}_{00,2211} \\
C^{0000,t}_{11,1111} &= C^{1101,t}_{11,0011} = C^{0000,1}_{20,0000} = C^{0011,1}_{20,0011} = C^{0011,1}_{22,0011} = 0
\end{aligned}
$$

the unconstrained coupling constants $C^{0000,1}_{20,0000}$, $C^{0011,1}_{20,0011}$ and $C^{0011,1}_{22,0011}$

- When the proton-neutron symmetry is assumed ($\tau_1 = \tau_2 = 0$), the continuity equations for protons and neutrons decouple and become independently valid

Results for non-Abelian gauge groups (vector-isoscalar channel)

- The condition for the continuity equation in the vector-isoscalar channel gives constraints that mix coupling constants in the spin space

At second order, the constraints for the vector-isoscalar continuity equation

$$
\begin{aligned}
C^{1101,t}_{00,1101} &= -\frac{1}{\sqrt{3}} C^{0011,t}_{00,2011}, \\
C^{1110,t}_{00,1110} &= -\frac{1}{\sqrt{3}} C^{0000,t}_{00,2000}, \\
C^{1111,t}_{00,1111} &= -C^{0000,t}_{00,2000}, \\
C^{1112,t}_{00,1112} &= -\sqrt{\frac{5}{3}} C^{0000,t}_{00,2000}, \\
C^{0011,t}_{20,0011} &= C^{0000,t}_{11,1111} = C^{1101,t}_{11,0011} = C^{0011,t}_{00,2211} = C^{0011,t}_{22,0011} = 0,
\end{aligned}
$$

the unconstrained coupling constants $C^{0000,t}_{20,0000}$

Results for non-Abelian gauge groups (vector-isovector channel)

- The condition for the continuity equation in the vector-isovector channel gives constraints that relate coupling constants in both spin and isospin spaces

For instance, at second order, the constraints for the vector-isovector continuity equation

$$
\begin{aligned}
C^{0000,t}_{00,2000} &= -\sqrt{3}(\sqrt{3})^t C^{1110,0}_{00,1110}, \\
C^{1101,t}_{00,1101} &= \sqrt{3}(\sqrt{3})^t C^{1110,0}_{00,1110}, \\
C^{1110,1}_{00,1110} &= \sqrt{3} C^{1110,0}_{00,1110}, \\
C^{1111,t}_{00,1111} &= \sqrt{3}(\sqrt{3})^t C^{1110,0}_{00,1110}, \\
C^{1112,t}_{00,1112} &= \sqrt{5}(\sqrt{3})^t C^{1110,0}_{00,1110}, \\
C^{0011,t}_{00,2011} &= -3(\sqrt{3})^t C^{1110,0}_{00,1110}, \\
C^{0011,t}_{20,0011} &= C^{0011,t}_{22,0011} = C^{0000,1}_{20,0000} = C^{0011,t}_{00,2211} = C^{0000,t}_{11,1111} = C^{1101,t}_{11,0011} = 0,
\end{aligned}
$$

- In general, Non-Abelian gauge-invariant functionals are more restricted than the Abelian one (spin-orbit coupling constants are always forced to be zero by the non-Abelian gauge transformation)

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

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

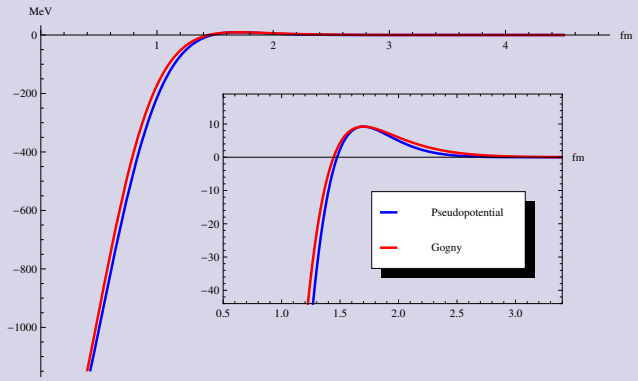
$$\sum_{k=1}^{2} C_k^{(G)} \mathrm{e}^{-\frac{\boldsymbol{r}^2}{a_k^2}}$$

Regularized pseudopotential form factor

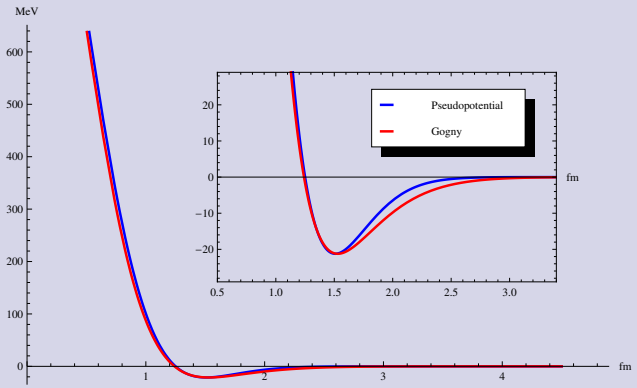
$$\mathrm{e}^{-\frac{\boldsymbol{r}^2}{a^2}} \left(C_0 + C_2 \frac{\boldsymbol{r}^2}{a^2} \right)$$

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

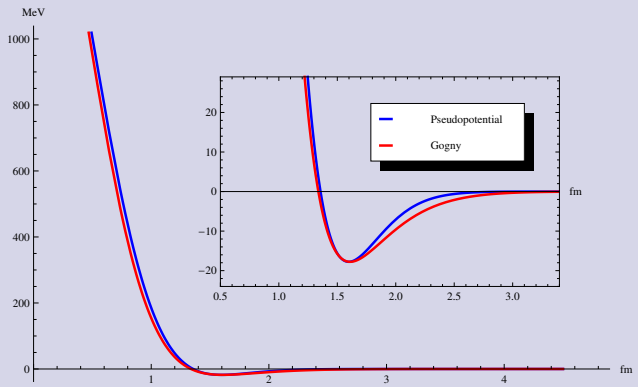
Channel without spin and isospin exchange operators



Channel with spin exchange operator



Channel with isospin exchange operator



Channel with both spin and isospin exchange operators