Nowe idee w jądrowych zastosowaniach metody funkcjonału gęstości

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Seminarium „Struktura jądra atomowego”
Uniwersytet Warszawski
28 kwietnia 2010

JYVÄSKYLÄN YLIOPISTO

Present FiDiPro group members

Nicolas Michel, senior researcher

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Plan seminarium

1. Wstęp - poszukiwanie nowych funkcjonałów gęstości o jakości spektroskopowej.
2. Funkcjonał gęstości do szóstego rzędu w pochodnych (N^3LO).
3. Program HOSPHE – samozgodne rozwiązania N^3LO

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Focus issue on open problems in nuclear structure theory

multipolowych w jądrach sferycznych.
5. Przywracanie naruszonych symetrii metodą Lipkina.
6. Rozwinięcia macierzy gęstości (Negele-Vautherin i Damped Taylor), porównanie nielokalnych i quasilokalnych funkcjonałów gęstości.

Nuclear Energy Density Functional

We consider the EDF in the form,

$$\mathcal{E} = \int d^3r \mathcal{H}(r),$$

where the energy density $\mathcal{H}(r)$ can be represented as a sum of the kinetic energy and of the potential-energy isoscalar ($t = 0$) and isovector ($t = 1$) terms,

$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(r) + \mathcal{H}_1(r),$$

which for the time-reversal and spherical symmetries imposed read:

$$\mathcal{H}_t(r) = C_t^{\rho}\rho_t^2 + C_t^{\tau}\rho_t\tau_t + C_t^{\Delta\rho}\rho_t\Delta\rho_t + \tfrac{1}{2}C_t^{J}J_t^2 + C_t^{\nabla J}\rho_t\nabla\cdot J_t.$$

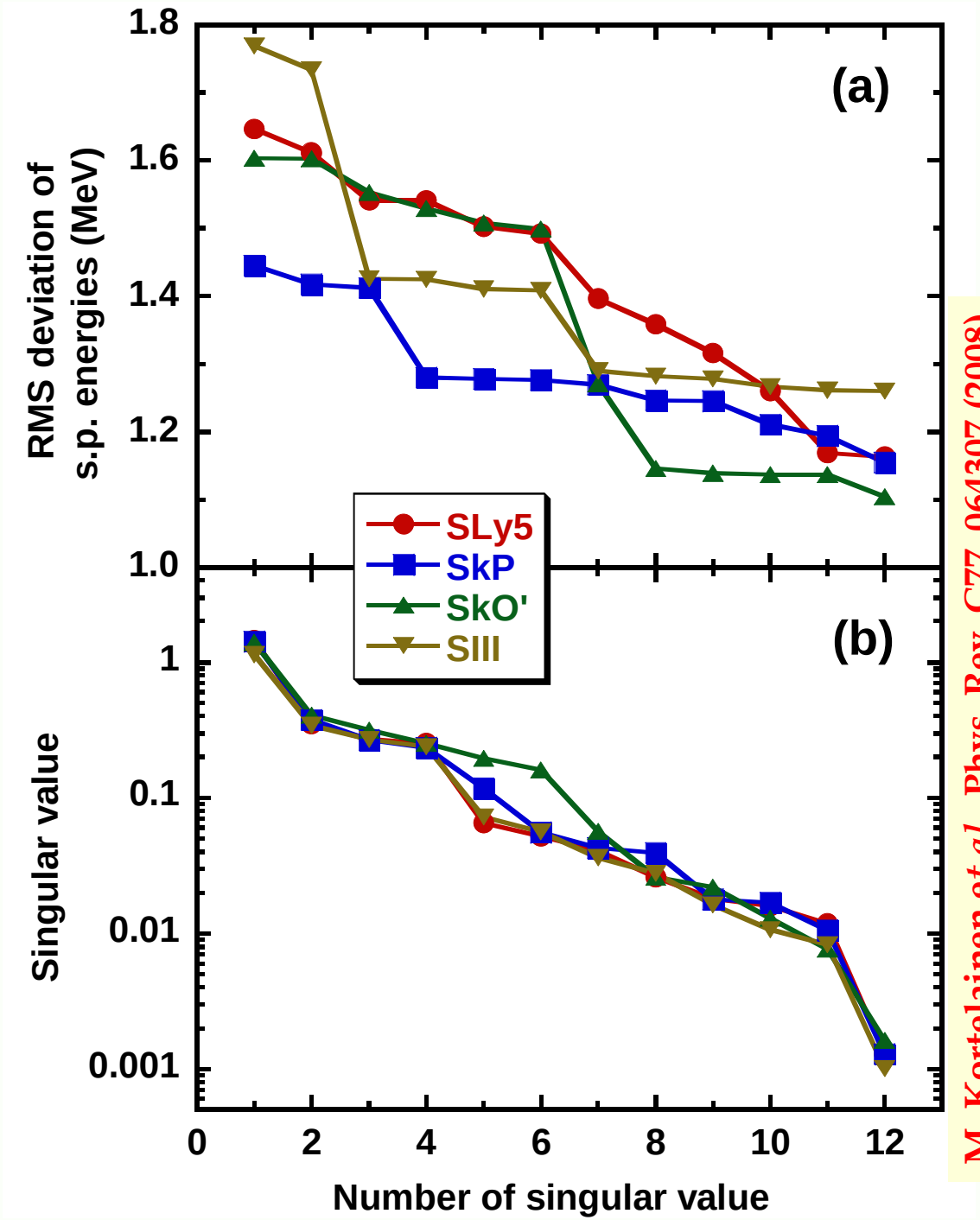
Following the parametrization used for the Skyrme forces, we assume the dependence of the coupling parameters C_t^{ρ} on the isoscalar density ρ_0 as:

$$C_t^{\rho} = C_{t0}^{\rho} + C_{t\mathrm{D}}^{\rho}\rho_0^{\alpha}.$$

The standard EDF depends linearly on 12 coupling constants,

$$C_{t0}^{\rho},\quad C_{t\mathrm{D}}^{\rho},\quad C_t^{\tau},\quad C_t^{\Delta\rho},\quad C_t^{\mathrm{J}},\quad \text{and}\quad C_t^{\nabla\mathrm{J}},$$

for $t = 0$ and 1.



Fits of s.p. energies

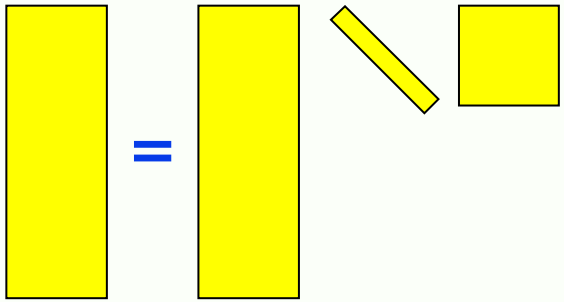
$$\epsilon_i - \epsilon_i^{\rm EXP} = -\sum_m \beta_{im} \Delta C_m,$$

EXP: M.N. Schwierz, I. Wiedenhover, and A. Volya, arXiv:0709.3525

M. Kortelainen *et al.*, Phys. Rev. C77, 064307 (2008)

Singular value decomposition

$$\beta_{im} = \sum_\mu V_{i\mu} d_\mu U^T_{\mu m},$$



$$\sum_i V_{i\mu} V_{i\nu} = \delta_{\mu\nu},$$

$$\sum_m U_{m\mu} U_{m\nu} = \delta_{\mu\nu},$$

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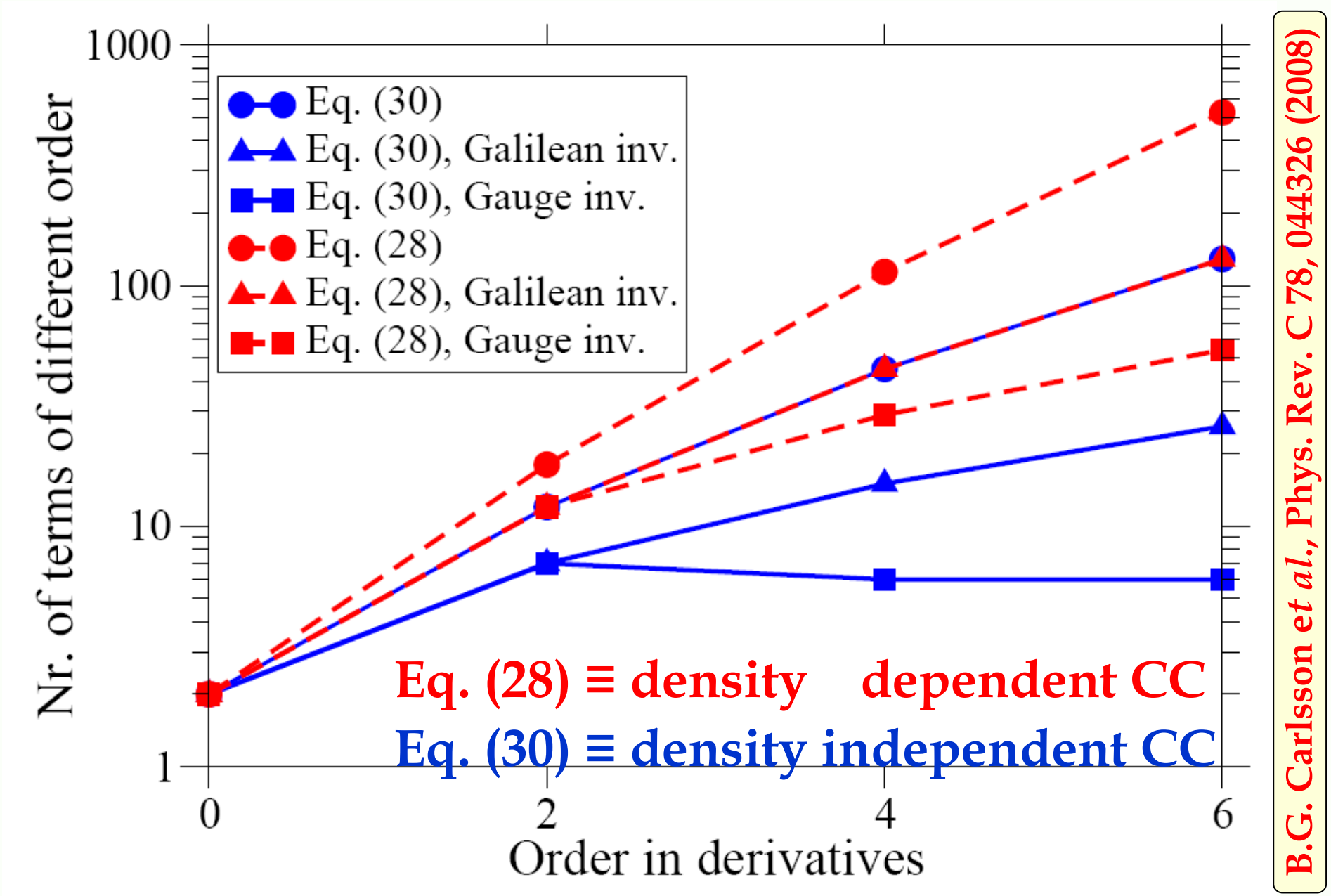
Numbers of terms in the density functional up to N^{3}LO



Energy density functional for spherical nuclei (I)

For conserved spherical, space-inversion, and time-reversal symmetries, all non-zero densities can be defined as:

$$
\begin{aligned}
R_0 &= \rho, \\
R_2 &= \vec{k}^2\rho = \tau - \tfrac{1}{4}\Delta\rho, \\
\overleftrightarrow{R}_{2ab} &= \vec{k}_a\vec{k}_b\rho, \\
R_4 &= \vec{k}^4\rho, \\
\overleftrightarrow{R}_{4ab} &= \vec{k}^2\vec{k}_a\vec{k}_b\rho, \\
R_6 &= \vec{k}^6\rho,
\end{aligned}
$$

and

$$
\begin{aligned}
\vec{J}_{1a} &= (\vec{k}\times\vec{s})_a, \\
\vec{J}_{3a} &= \vec{k}^2(\vec{k}\times\vec{s})_a, \\
\overleftrightarrow{J}_{3abc} &= \vec{k}_a\vec{k}_b(\vec{k}\times\vec{s})_c + \vec{k}_b\vec{k}_c(\vec{k}\times\vec{s})_a \\
&\quad + \vec{k}_c\vec{k}_a(\vec{k}\times\vec{s})_b, \\
\vec{J}_{5a} &= \vec{k}^4(\vec{k}\times\vec{s})_a,
\end{aligned}
$$

where $\vec{k}^2 = \sum_a \vec{k}_a\vec{k}_a$ and the Cartesian indices are defined as $a, b, c = x, y, z$. To lighten the notation, in these definitions we have omitted the arguments of local densities, $\vec{r}$, and limits of $\vec{r}\,' = \vec{r}$.

Numbers of terms of different orders in the EDF up to N^{3}LO, evaluated for the conserved spherical, space-inversion, and time-reversal symmetries. The last two columns give numbers of terms when the Galilean or gauge invariance is assumed, respectively.

order	Total	Galilean	Gauge
0	1	1	1
2	4	4	4
4	12	9	3
6	28	16	3
N^{3}LO	45	30	11

B.G. Carlsson *et al.*, Phys. Rev. C 78, 044326 (2008)
Phys. Rev. C 81, 029904(E) (2010)

Energy density functional for spherical nuclei (II)

We can write the N^{3}LO spherical energy density as a sum of contributions from zero, second, fourth, and sixth orders:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_2 + \mathcal{H}_4 + \mathcal{H}_6,$$

where

$$\mathcal{H}_0 = C_{00}^0 R_0 R_0,$$

$$\begin{aligned}\mathcal{H}_2 &= C_{20}^0 R_0 \Delta R_0 + C_{02}^0 R_0 R_2 \\ &+ C_{11}^0 R_0 \vec{\nabla}\cdot\vec{J}_1, + C_{01}^1 \vec{J}_1^2,\end{aligned}$$

Energy densities $\mathcal{H}_0$ and $\mathcal{H}_2$ correspond, of course, to the standard Skyrme functional with $C_{00}^0 = C^\rho$, $C_{20}^0 = C^{\Delta\rho} + \frac{1}{4}C^\tau$, $C_{02}^0 = C^\tau$, $C_{11}^0 = C^{\nabla J}$, and $C_{01}^1 = C^{J1}$. At fourth order, the energy density reads

$$\begin{aligned}\mathcal{H}_4 &= C_{40}^0 R_0 \Delta^2 R_0 + C_{22}^0 R_0 \Delta R_2 \\ &+ C_{04}^0 R_0 R_4 + C_{02}^2 R_2 R_2 \\ &+ D_{22}^0 R_0 \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + D_{02}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \overleftrightarrow{R}_{2ab} \\ &+ C_{21}^1 \vec{J}_1 \cdot \Delta \vec{J}_1 + C_{03}^1 \vec{J}_1 \cdot \vec{J}_3 \\ &+ \otimes \vec{J}_1 \cdot \vec{\nabla}\left(\vec{\nabla}\cdot\vec{J}_1\right) \\ &+ C_{31}^0 R_0 \Delta\left(\vec{\nabla}\cdot\vec{J}_1\right) + C_{13}^0 R_0 \left(\vec{\nabla}\cdot\vec{J}_3\right) \\ &+ C_{11}^2 R_2 \left(\vec{\nabla}\cdot\vec{J}_1\right) + D_{11}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{J}_{1b},\end{aligned}$$

At sixth order, the energy density reads

$$\begin{aligned}\mathcal{H}_6 &= C_{60}^0 R_0 \Delta^3 R_0 + C_{42}^0 R_0 \Delta^2 R_2 \\ &+ C_{24}^0 R_0 \Delta R_4 + C_{06}^0 R_0 R_6 \\ &+ C_{22}^2 R_2 \Delta R_2 + C_{04}^2 R_2 R_4 \\ &+ D_{42}^0 R_0 \Delta \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + D_{24}^0 R_0 \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{4ab} \\ &+ D_{22}^2 R_2 \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + E_{22}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \Delta \overleftrightarrow{R}_{2ab} \\ &+ \otimes \sum_{abc} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{\nabla}_c \overleftrightarrow{R}_{2cb} + E_{04}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \overleftrightarrow{R}_{4ab} \\ &+ C_{41}^1 \vec{J}_1 \cdot \Delta^2 \vec{J}_1 + C_{23}^1 \vec{J}_1 \cdot \Delta \vec{J}_3 \\ &+ C_{05}^1 \vec{J}_1 \cdot \vec{J}_5 + C_{03}^3 \vec{J}_3 \cdot \vec{J}_3 \\ &+ \otimes \vec{J}_1 \cdot \Delta \vec{\nabla}\left(\vec{\nabla}\cdot\vec{J}_1\right) + \otimes \vec{J}_1 \cdot \vec{\nabla}\left(\vec{\nabla}\cdot\vec{J}_3\right) \\ &+ E_{23}^1 \sum_{abc} \vec{J}_{1a} \vec{\nabla}_b \vec{\nabla}_c \overleftrightarrow{J}_{3abc} + D_{03}^3 \sum_{abc} \overleftrightarrow{J}_{3abc} \overleftrightarrow{J}_{3abc} \\ &+ C_{51}^0 R_0 \Delta^2 \left(\vec{\nabla}\cdot\vec{J}_1\right) + C_{33}^0 R_0 \Delta \left(\vec{\nabla}\cdot\vec{J}_3\right) \\ &+ C_{15}^0 R_0 \left(\vec{\nabla}\cdot\vec{J}_5\right) + C_{31}^2 R_2 \Delta \left(\vec{\nabla}\cdot\vec{J}_1\right) \\ &+ C_{13}^2 R_2 \left(\vec{\nabla}\cdot\vec{J}_3\right) + C_{11}^4 R_4 \left(\vec{\nabla}\cdot\vec{J}_1\right) \\ &+ D_{33}^0 R_0 \sum_{abc} \vec{\nabla}_a \vec{\nabla}_b \vec{\nabla}_c \overleftrightarrow{J}_{3abc} + D_{13}^2 \sum_{abc} \overleftrightarrow{R}_{2ab} \vec{\nabla}_c \overleftrightarrow{J}_{3abc} \\ &+ D_{31}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \Delta \vec{\nabla}_a \vec{J}_{1b} + E_{13}^2 \sum_{ab} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{J}_{3b} \\ &+ D_{11}^4 \sum_{ab} \overleftrightarrow{R}_{4ab} \vec{\nabla}_a \vec{J}_{1b} \\ &+ \otimes \sum_{ab} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{\nabla}_b \left(\vec{\nabla}\cdot\vec{J}_1\right).\end{aligned}$$

The energy densities above are given in terms of 45 coupling constants $C_{mn}^{n'}$, $D_{mn}^{n'}$, $E_{mn}^{n'}$, and $F_{mn}^{n'}$.

B.G. Carlsson *et al.*, Phys. Rev. C 78, 044326 (2008)
Phys. Rev. C 81, 029904(E) (2010)

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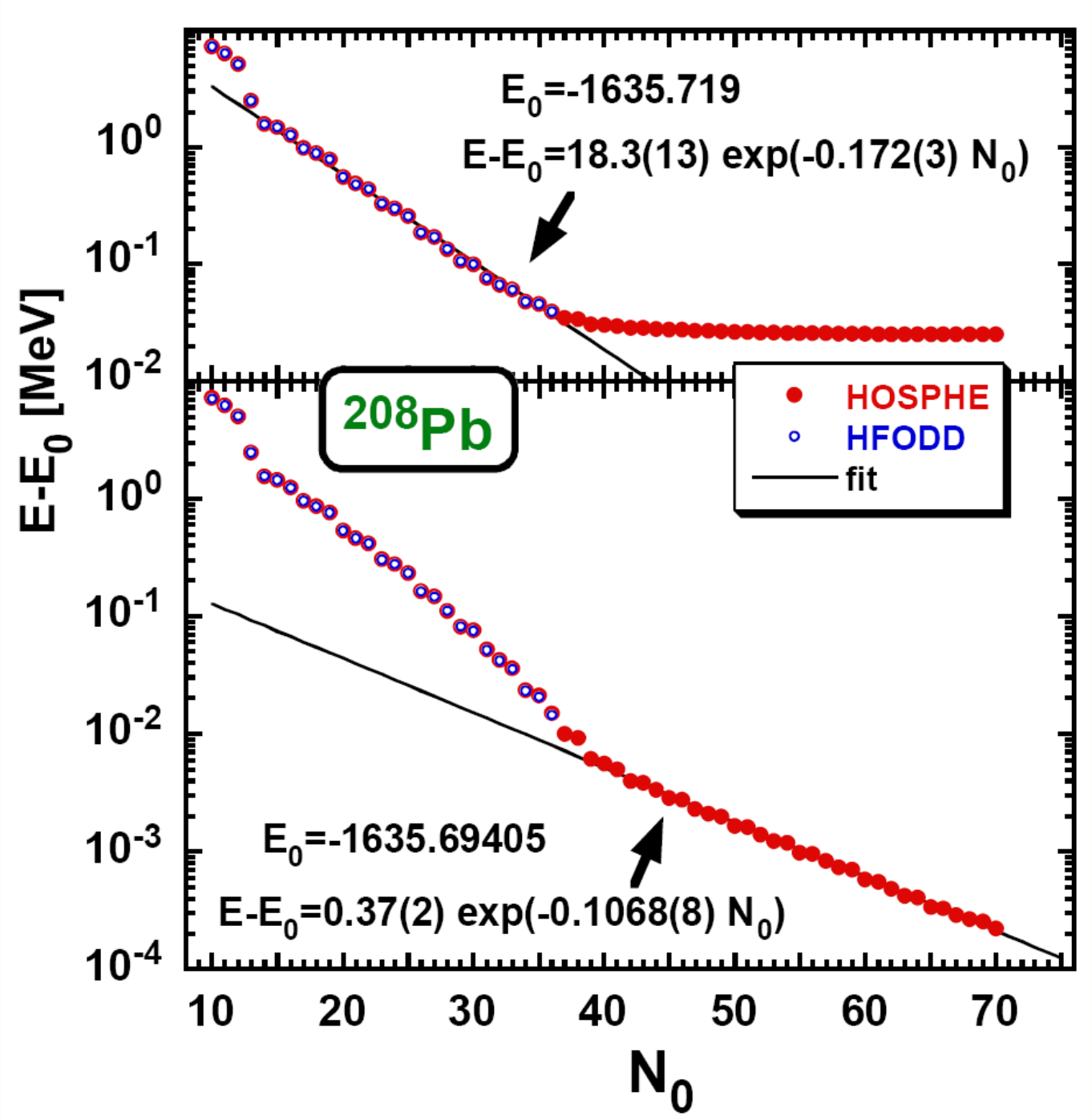

Program HOSPHE

Solution of self-consistent equations for the N³LO nuclear energy density functional in spherical symmetry

B.G. Carlsson *et al.*, arXiv:0912.3230

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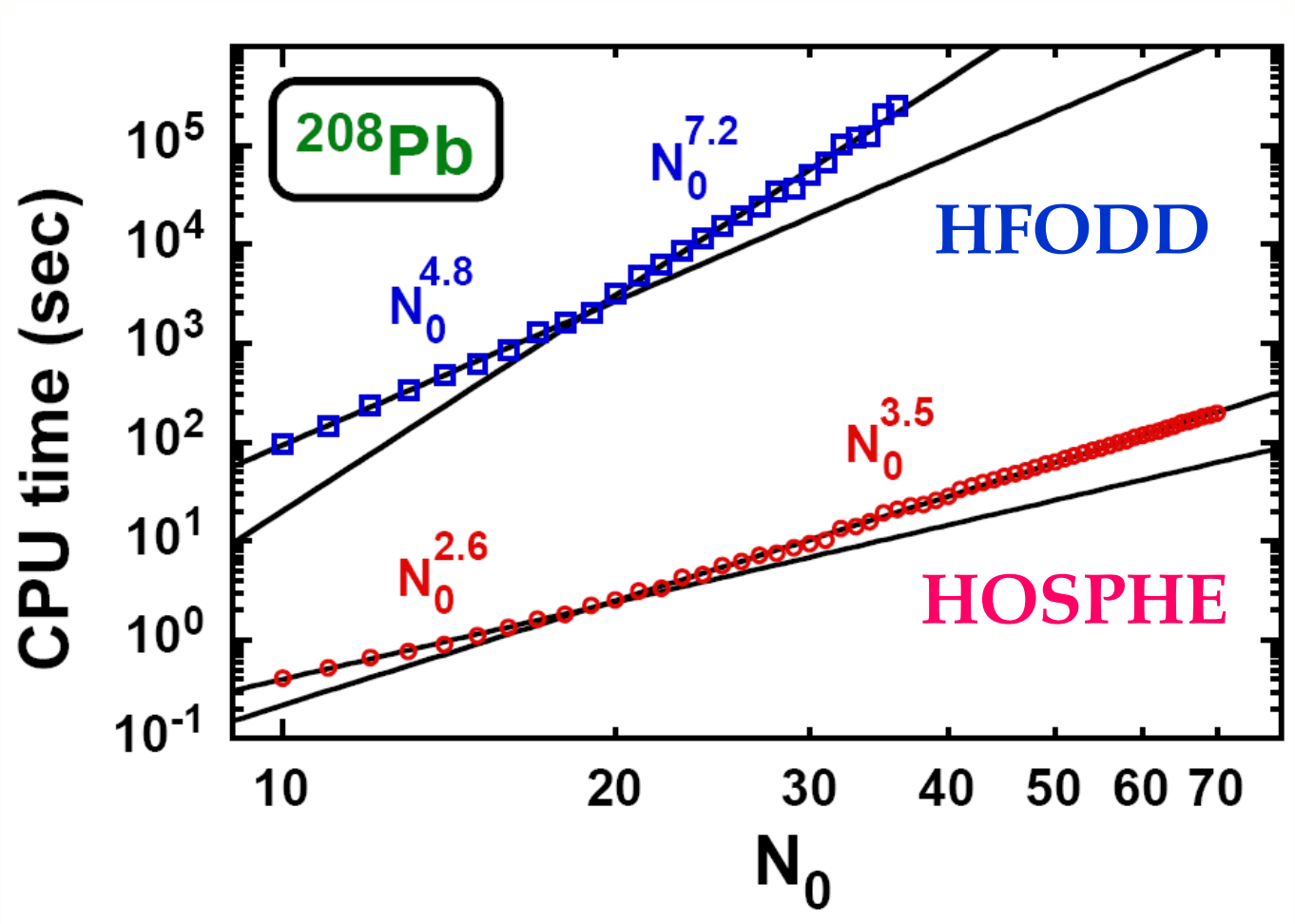

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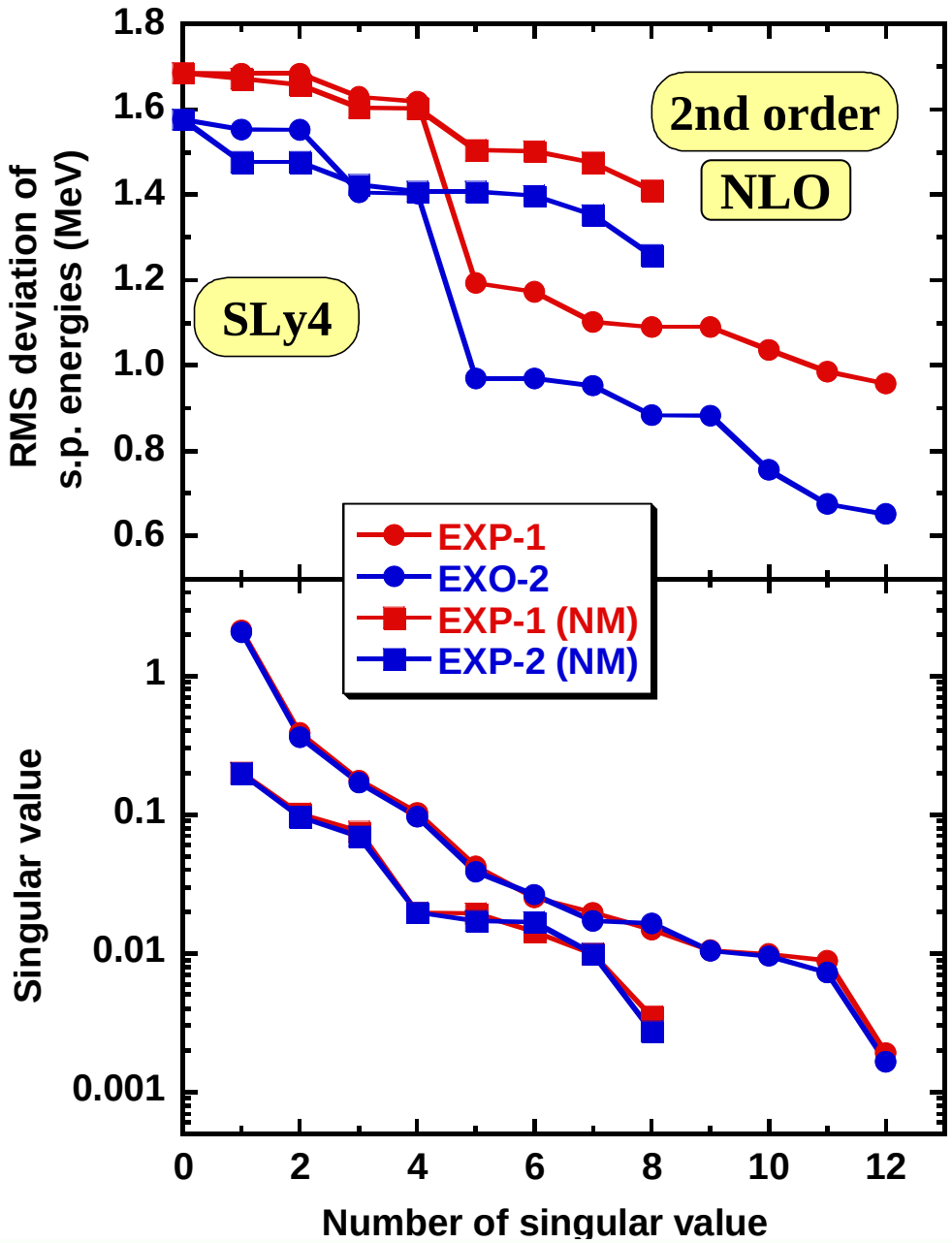
Fits of s.p. energies – regression analysis



B.G. Carlsson *et al.*, to be published

EXP-1:
M.N. Schwierz,
I. Wiedenhover, and
A. Volya, arXiv:0709.3525

EXP-2:
M.G. Porquet *et al.*,
to be published

NM:
Nuclear-matter constraints on:

- saturation density
- energy per particle
- incompressibility
- effective mass

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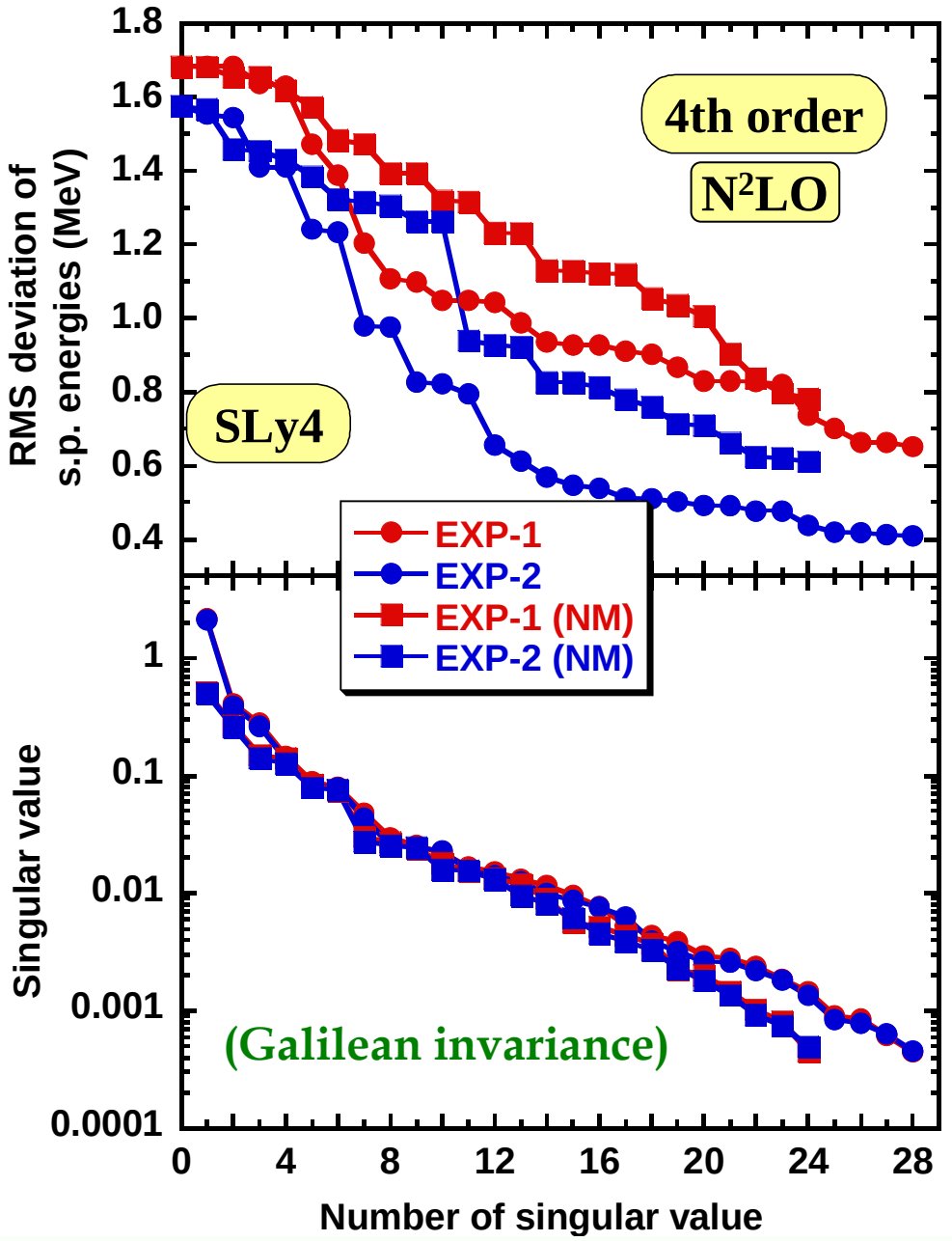

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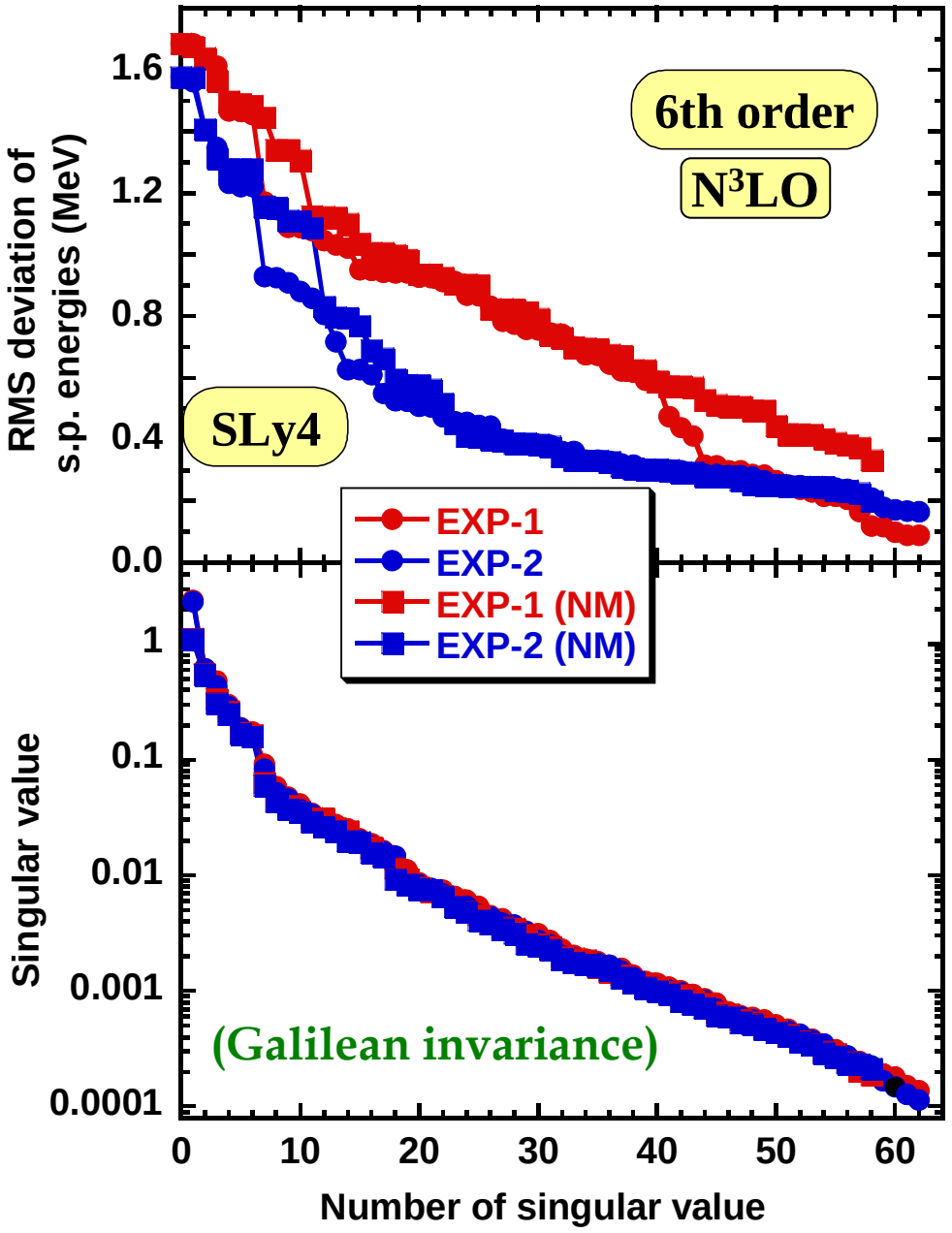

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Pseudopotentials vs. energy density functional

The most general pseudopotentials up to next-to-next-to-next-to-leading order (N^3LO) have been determined together with their gauge-invariance and continuity-equation properties (Ph.D. thesis of Francesco Raimondi).

$$\left[\left[K'_{n'L'}\delta K_{nL}\right]_\nu \left[\sigma_{\nu_1}\sigma_{\nu_2}\right]_\nu\right]_0$$

Table 3: Fourth order terms

	n	L	n'	L'	$n+n'$	ν	$\nu_1+\nu_2$
1	0	0	4	0	4	0	0
2	0	0	4	0	4	0	2
3	0	0	4	2	4	2	2
4	1	1	3	1	4	0	0
5	1	1	3	1	4	0	2
6	1	1	3	1	4	1	1
7	1	1	3	1	4	2	2
8	1	1	3	3	4	2	2
9	2	0	2	0	4	0	0
10	2	0	2	0	4	0	2
11	2	0	2	2	4	2	2
12	2	2	2	2	4	0	0
13	2	2	2	2	4	0	2
14	2	2	2	2	4	1	1
15	2	2	2	2	4	2	2

This approach is fully analogous to the N^3LO expansion in the chiral perturbation effective field theory: W.C. Haxton, Phys. Rev. C77, 034005 (2008)

Fast RPA and QRPA + Arnoldi method

Within RPA, let ρ denote the one-body projective density matrix, $\rho^2 = \rho$, and $h(\rho) = \partial E/\partial\rho$ denote the mean-field Hamiltonian calculated for ρ. The TDHF equation for $\rho(t)$ then reads:

$$i\hbar\frac{d}{dt}\rho = [h(\rho), \rho].$$

The RPA method approximates the TDHF solution by a single-mode vibrational state $\rho(t)$ in the vibrating mean field $h(t) = h(\rho(t))$:

$$\rho(t) = \rho_0 + \tilde{\rho}e^{-i\omega t} + \tilde{\rho}^+e^{i\omega t}, \qquad h(t) = h_0 + \tilde{h}e^{-i\omega t} + \tilde{h}^+e^{i\omega t}$$

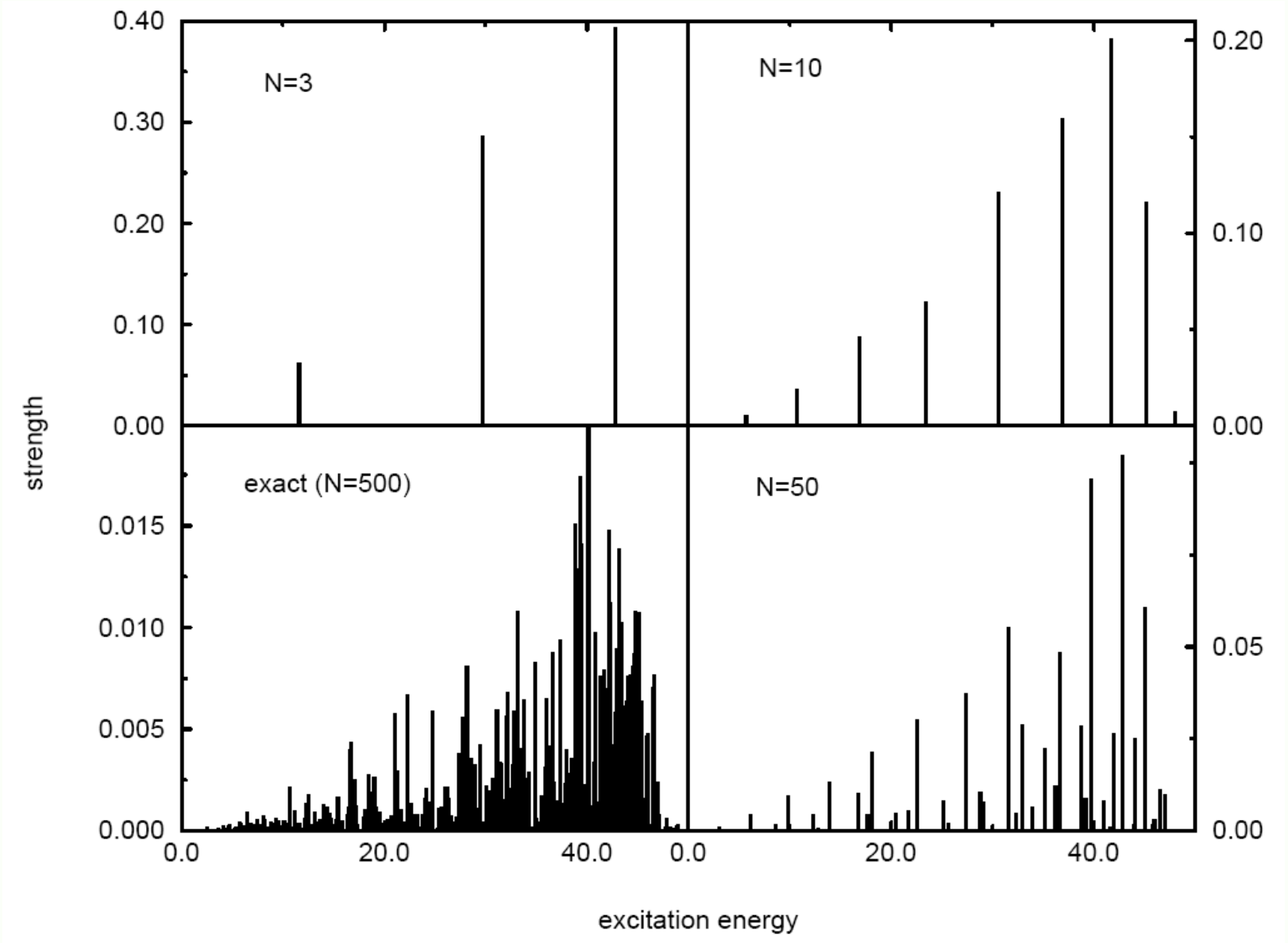
where ρ_0 is the self-consistent solution, $[h_0, \rho_0] = 0$ for $h_0 = h(\rho_0)$, $\tilde{\rho}$ is the RPA amplitude, and $\tilde{h} = h(\tilde{\rho})$. This allows for transforming the TDHF into the RPA equation in the form

$$\hbar\omega\tilde{\rho} = \mathrm{H}_0\tilde{\rho} = [h_0, \tilde{\rho}] + [\tilde{h}, \rho_0],$$

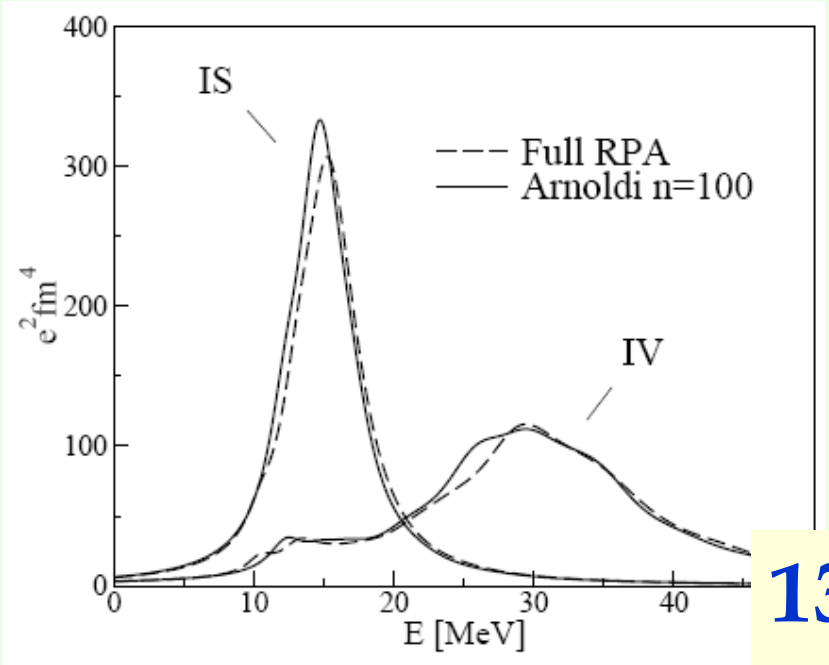
by which the right-hand side becomes a linear operator H_0 depending on ρ_0 and acting on $\tilde{\rho}$.

J. Toivanen et *al.*, Phys. Rev. C 81, 034312 (2010)

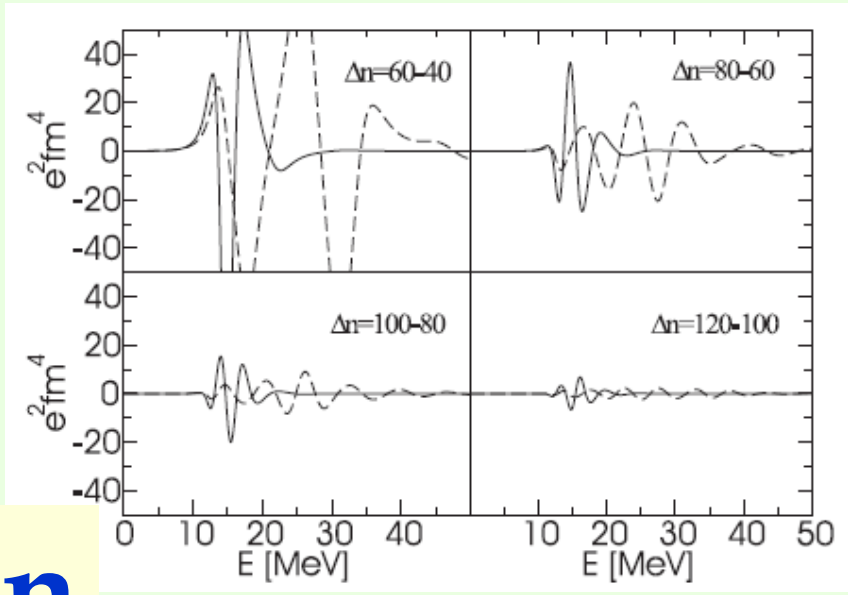
Figure taken from C. W. Johnson, G. F. Bertsch and W. D. Hazelton, Computer Physics Communications **120**, 155-161 (1999).



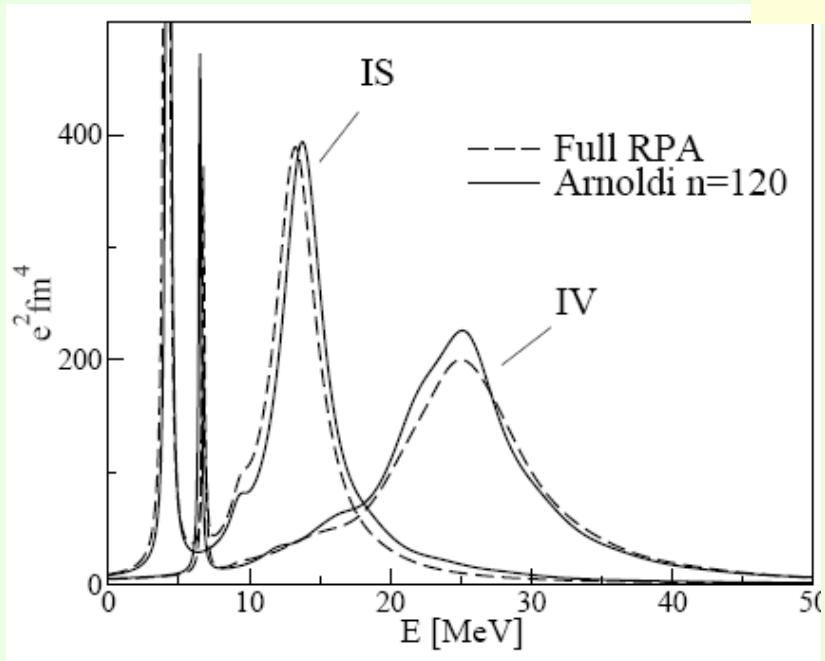
Fast RPA and QRPA + Arnoldi method



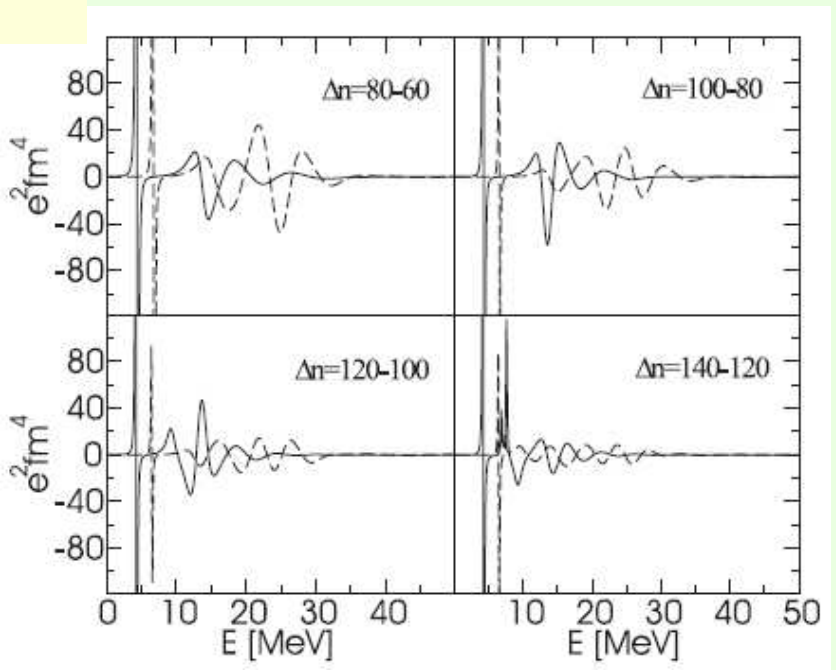
0^+



^{132}Sn

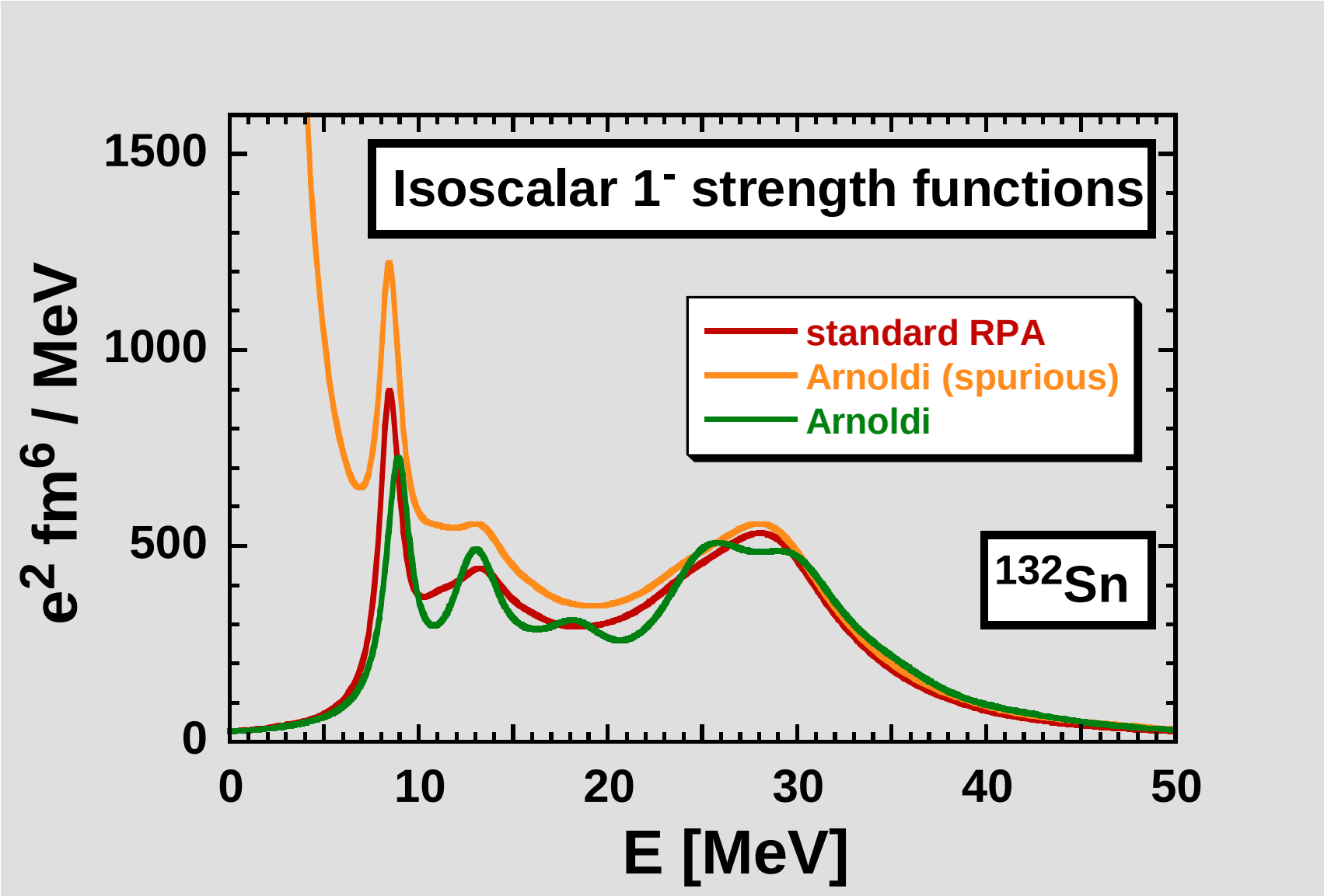


2^+



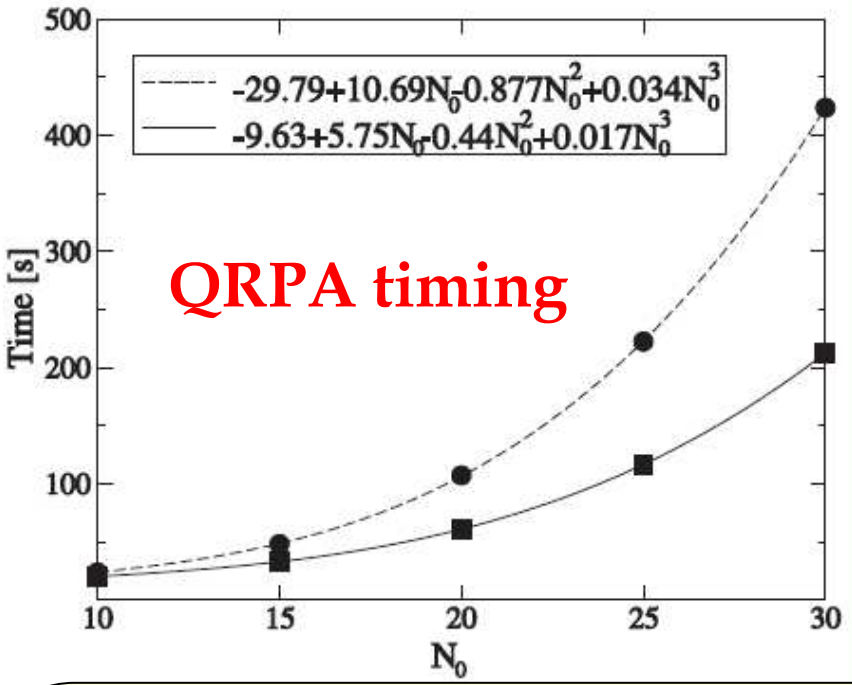
J. Toivanen *et al.*, Phys. Rev. C 81, 034312 (2010)

Removal of spurious modes



J. Toivanen *et al.*, Phys. Rev. C 81, 034312 (2010)

Scaling properties



- Spherical QRPA+Arnoldi scales linearly with the size of the single-particle space Ω.
- Deformed QRPA+Arnoldi expected to scale quadratically, that is, as Ω^2
- Standard QRPA scales quartically, that is, as Ω^4 !

Future plans:

- Full implementation and testing of the spherical QRPA + Arnoldi method in the code HOSPHE with new-generation separable pairing interactions. Systematic calculations of multipole giant-resonance modes to be used in the EDF adjustments.
- Deformed QRPA + Arnoldi method implemented in the code HFODD. Systematic calculations of β-decay strengths functions and β-delayed neutron emission probabilities to be used in the EDF adjustments.

Including dynamical effects of symmetry restoration

The research program to restore simultaneously the main broken symmetries (translational, rotational, particle-number, and isospin) has been formulated within the Lipkin method.

J. Phys. G: Nucl. Part. Phys. **36** (2009) 105105 (13pp)

Lipkin translational-symmetry restoration in the mean-field and energy–density-functional methods

Jacek Dobaczewski

Future plans:

- **Implementation of the Lipkin method within the code HFODD [Ph.D. thesis of Pekka Toivanen]**

Goal:

Improved description of experimental nuclear masses at shell closures.

Phenomenological effective interactions

- Gogny force.*

$$\tilde{G}_{xyx'y'} = \delta(\vec{x}-\vec{x}')\delta(\vec{y}-\vec{y}')G(x,y),$$

where the tilde denotes a non-antisymmetrized matrix element ($G_{xyx'y'} = \tilde{G}_{xyx'y'} - \tilde{G}_{xyy'x'}$), and $G(x,y)$ is a sum of two Gaussians, plus a zero-range, density dependent part,

$$G(x,y) = \sum\nolimits_{i=1,2} e^{-(\vec{x}-\vec{y})^2/\mu_i^2} \times (W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau)$$

$$+t_3(1+P_\sigma)\delta(\vec{x}-\vec{y})\rho^{1/3}\left[\tfrac{1}{2}(\vec{x}+\vec{y})\right].$$

In this Equation, $P_\sigma = \frac{1}{2}(1+\vec{\sigma}_1\cdot\vec{\sigma}_2)$ and $P_\tau = \frac{1}{2}(1+\vec{\tau}_1\cdot\vec{\tau}_2)$ are, respectively, the spin and isospin exchange operators of particles 1 and 2, $\rho(\vec{r})$ is the total density of the system at point $\vec{r}$, and $\mu_i = 0.7$ and $1.2\,\mathrm{fm}$, W_i, B_i, H_i, M_i, and t_3 are parameters.

- Skyrme force.*

$$\tilde{G}_{xyx'y'} = \Big\{t_0(1+x_0P^\sigma) + \tfrac{1}{6}t_3(1+x_3P^\sigma)\rho^\alpha\left(\tfrac{1}{2}(\vec{x}+\vec{y})\right)$$

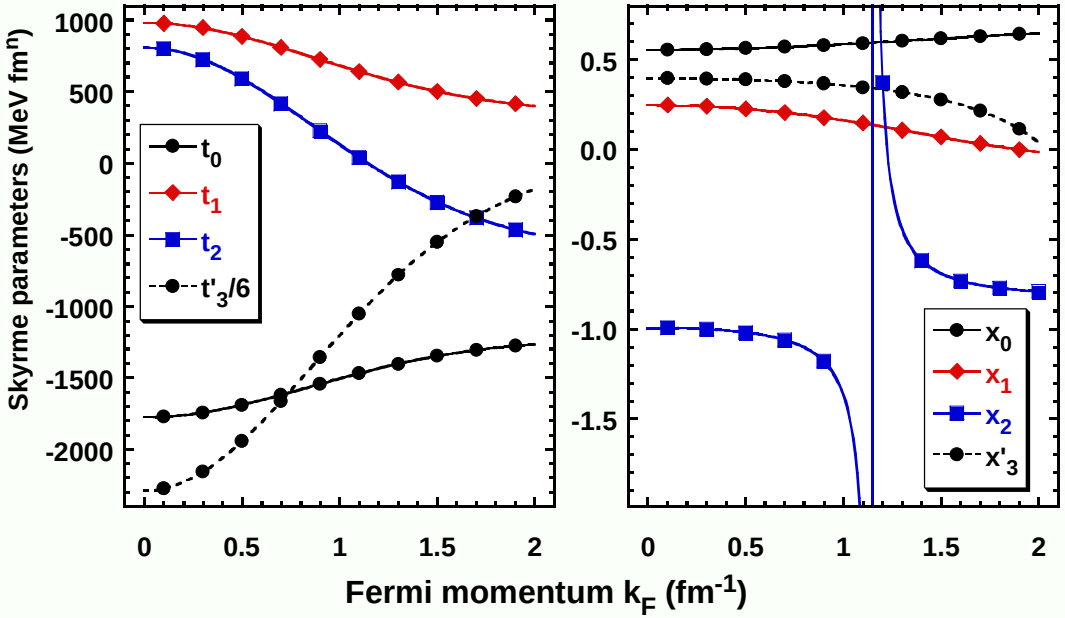
$$+\tfrac{1}{2}t_1(1+x_1P^\sigma)[\vec{k}^2+\vec{k}'^2] + t_2(1+x_2P^\sigma)\vec{k}^*\cdot\vec{k}'\Big\}\delta(\vec{x}-\vec{x}')\delta(\vec{y}-\vec{y}')\delta(\vec{x}-\vec{y}),$$

where the relative momentum operators read

$$\hat{\vec{k}} = \frac{1}{2i}\left(\vec{\nabla}_x - \vec{\nabla}_y\right), \qquad \hat{\vec{k}}' = \frac{1}{2i}\left(\vec{\nabla}'_x - \vec{\nabla}'_y\right).$$

*We omit the spin-orbit and tensor terms for simplicity.

Local density approximation from density-matrix expansions



Based on the Negele-Vautherin density-matrix expansion, we have derived the NLO Skyrme-functional parameters corresponding to the finite-range Gogny interaction. The method has been extended to derive the coupling constants of local N^{3}LO functionals

J. Dobaczewski, B.G. Calsson, M. Kortelainen, arXiv:1002.3646

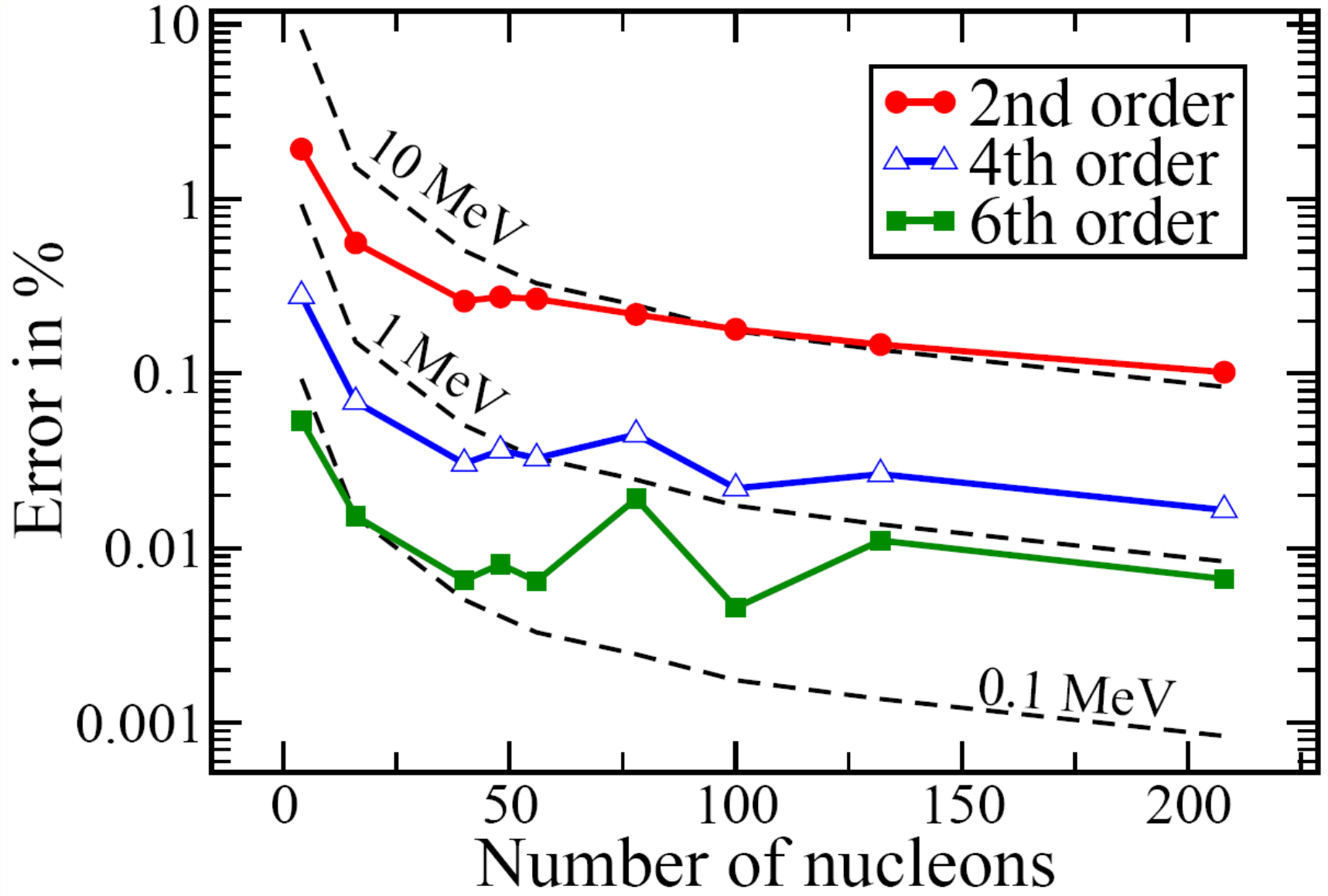
Local density approximation from density-matrix expansions

Table 4. Binding energies E of seven doubly magic nuclei calculated by using the Skyrme-force parameters S1Sa, S1Sb, and S1Sc (see text) compared with the Gogny-force energies E_G. All energies are in MeV.

	D1S [33]	S1Sa		S1Sb		S1Sc	
	E_G	E	ΔE	E	ΔE	E	ΔE
^{40}Ca	−342.689	−335.312	2.15%	−340.642	0.60%	−339.369	0.97%
^{48}Ca	−414.330	−409.118	1.26%	−410.698	0.88%	−414.213	0.03%
^{56}Ni	−481.111	−473.497	1.58%	−471.970	1.90%	−479.843	0.26%
^{78}Ni	−637.845	−630.447	1.16%	−629.066	1.38%	−638.837	−0.16%
^{100}Sn	−828.024	−814.568	1.63%	−814.896	1.59%	−826.453	0.19%
^{132}Sn	−1101.670	−1086.272	1.40%	−1086.867	1.34%	−1101.445	0.02%
^{208}Pb	−1637.291	−1612.634	1.51%	−1617.419	1.21%	−1637.291	0.00%
RMS	n.a.	n.a.	1.56%	n.a.	1.33%	n.a.	0.39%

J. Dobaczewski, B.G. Calsson, M. Kortelainen, arXiv:1002.3646

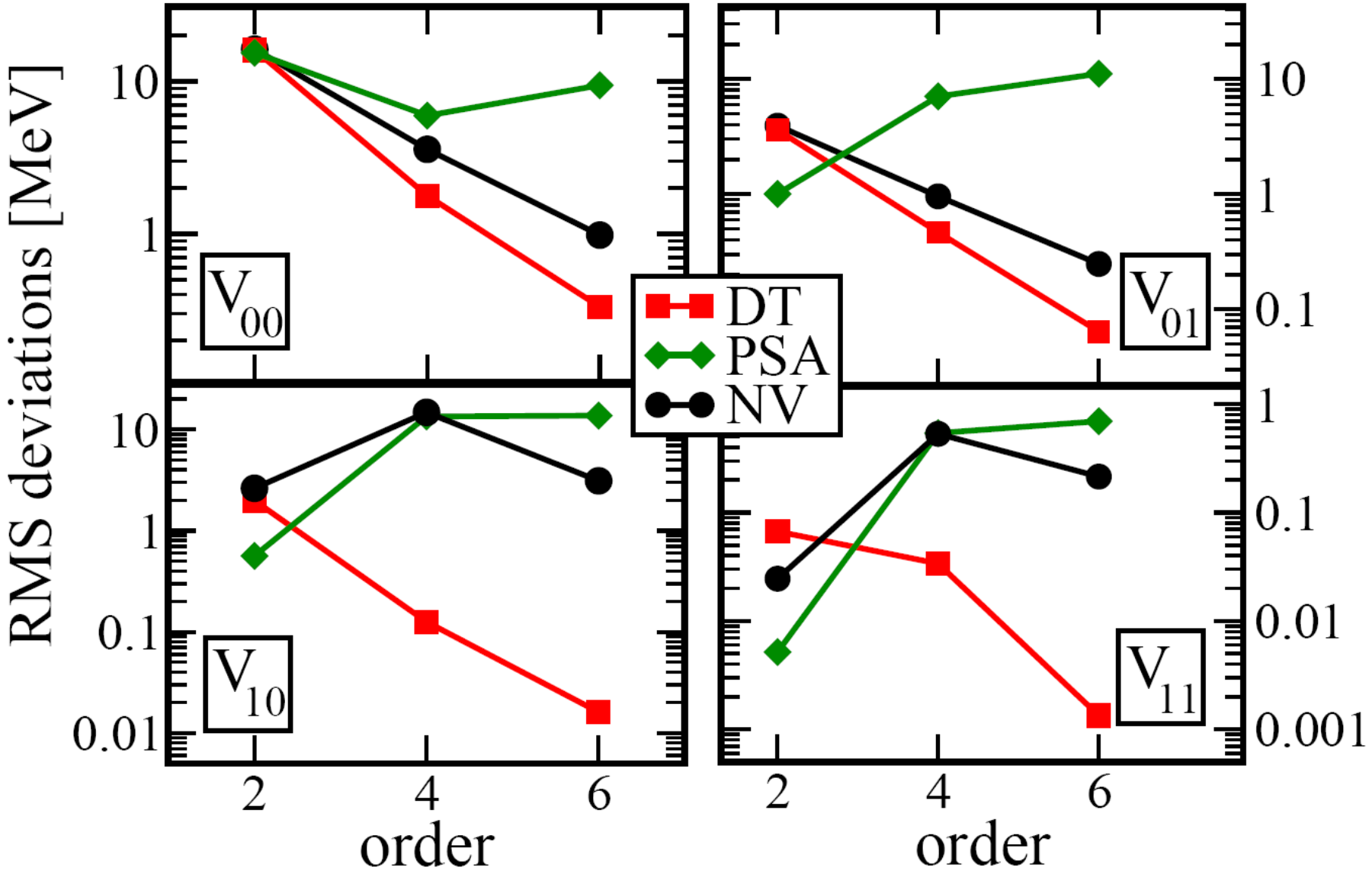
Convergence of density-matrix expansions for nuclear interactions (diect term)



B.G. Calsson, J. Dobaczewski, arXiv:1003.2543

JYVÄSKYLÄN YLIOPISTO

Convergence of density-matrix expansions for nuclear interactions (exchange term)



B.G. Calsson, J. Dobaczewski, arXiv:1003.2543

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SciDAC 2 UNEDF Project (USA)

http://www.unedf.org/

Building a Universal Nuclear Energy Density Functional

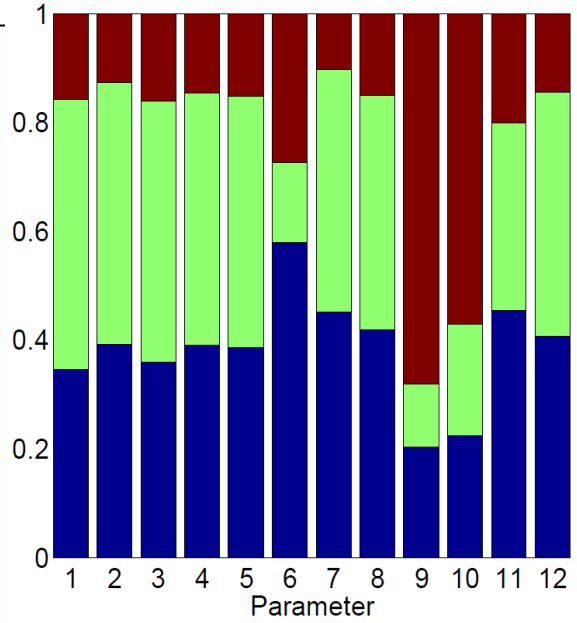
- Understand nuclear properties “for element formation, for properties of stars, and for present and future energy and defense applications”
- Scope is all nuclei, with particular interest in reliable calculations of unstable nuclei and in reactions
- Order of magnitude improvement over present capabilities
  - ➢ Precision calculations
- Connected to the best microscopic physics
- Maximum predictive power with well-quantified uncertainties

FIDIPRO Project (Finland)

http://www.jyu.fi/accelerator/fidipro/

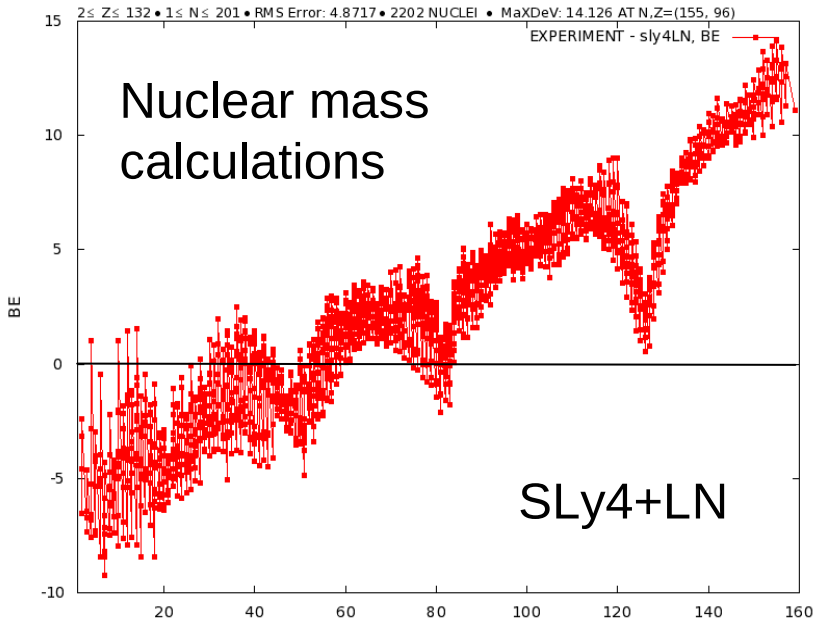
UNEDF-1 Skyrme Functional

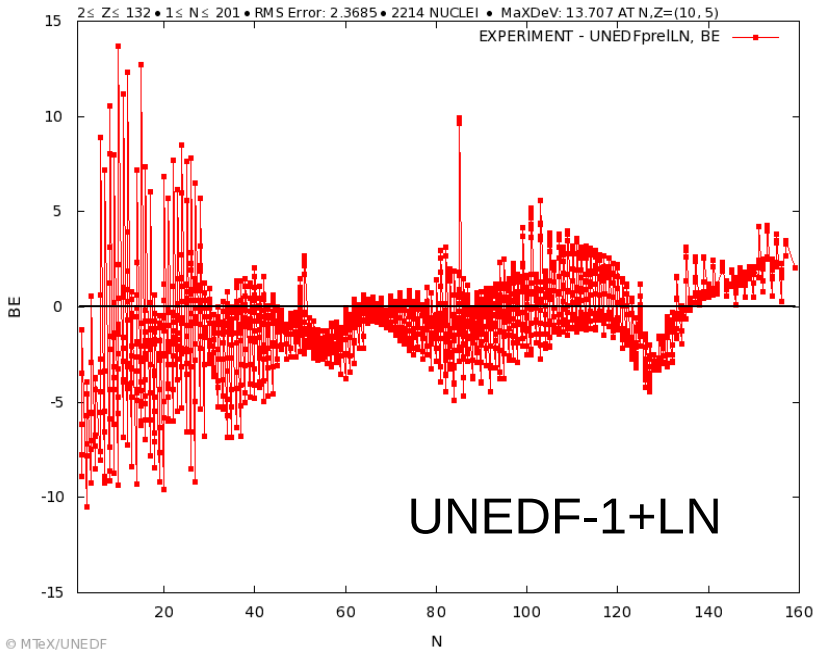
1. ρ
2. $\frac{E}{A}$
3. K
4. a_{sym}
5. L
6. $\frac{1}{M_s^*}$
7. $C_0^{\rho\Delta\rho}$
8. $C_1^{\rho\Delta\rho}$
9. $V_0^{(\nu)}$
10. $V_0^{(\pi)}$
11. $C_0^{\nabla J}$
12. $C_1^{\nabla J}$



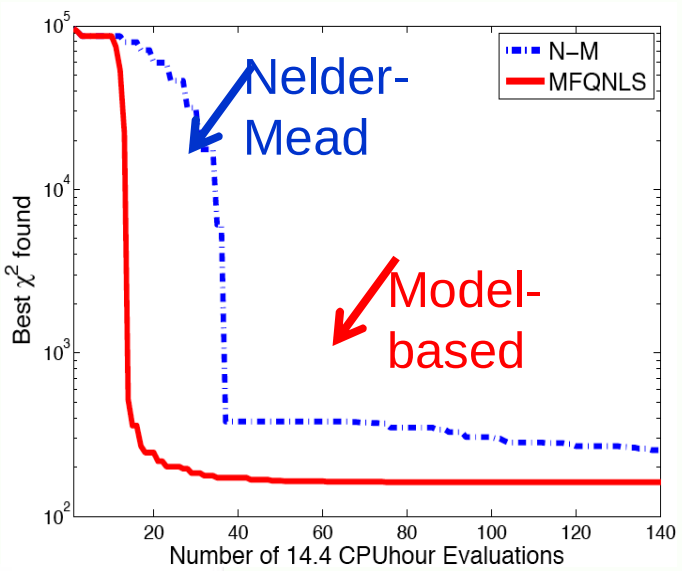
72 masses
28 rms radii
8 OEM differences

Relative change in value of the parameter when experimental data is changed





Comparison of performance between standard optimization algorithm (Nelder-Mead) and model-based approaches



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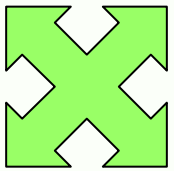

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Mean-field equations

Mean-field potentials:

$$\Gamma_t^{\rm even} = -\vec{\nabla}\cdot M_t(\vec{r})\vec{\nabla} + U_t(\vec{r}) + \tfrac{1}{2i}(\overleftrightarrow{\nabla\sigma}\cdot\overleftrightarrow{B}_t(\vec{r}) + \overleftrightarrow{B}_t(\vec{r})\cdot\overleftrightarrow{\nabla\sigma})$$
$$\Gamma_t^{\rm odd} = -\vec{\nabla}\cdot(\vec{\sigma}\cdot\vec{C}_t(\vec{r}))\vec{\nabla} + \vec{\sigma}\cdot\vec{\Sigma}_t(\vec{r}) + \tfrac{1}{2i}(\vec{\nabla}\cdot\vec{I}_t(\vec{r}) + \vec{I}_t(\vec{r})\cdot\vec{\nabla}) - \vec{\nabla}\cdot\vec{D}_t(\vec{r})\vec{\sigma}\cdot\vec{\nabla}$$

where

$$\begin{aligned}
U_t &= 2C_t^{\rho}\rho_t + 2C_t^{\Delta\rho}\Delta\rho_t + C_t^{\tau}\tau_t + C_t^{\nabla J}\vec{\nabla}\cdot\vec{J}_t,\\
\vec{\Sigma}_t &= 2C_t^{s}\vec{s}_t + 2C_t^{\Delta s}\Delta\vec{s}_t + C_t^{T}\vec{T}_t + C_t^{\nabla j}\vec{\nabla}\times\vec{j}_t, -2C_t^{\nabla s}\Delta\vec{s}_t + C_t^{F}\vec{F}_t - 2C_t^{\nabla s}\vec{\nabla}\times(\vec{\nabla}\times\vec{s}_t)\\
M_t &= C_t^{\tau}\rho_t,\\
\vec{C}_t &= C_t^{T}\vec{s}_t,\\
\overleftrightarrow{B}_t &= 2C_t^{J}\overleftrightarrow{J}_t - C_t^{\nabla J}\overleftrightarrow{\nabla}\rho_t,\\
\vec{I}_t &= 2C_t^{j}\vec{j}_t + C_t^{\nabla j}\vec{\nabla}\times\vec{s}_t,\\
\vec{D}_t &= C_t^{F}\vec{s}_t,
\end{aligned}$$

Neutron and proton mean-field Hamiltonians:

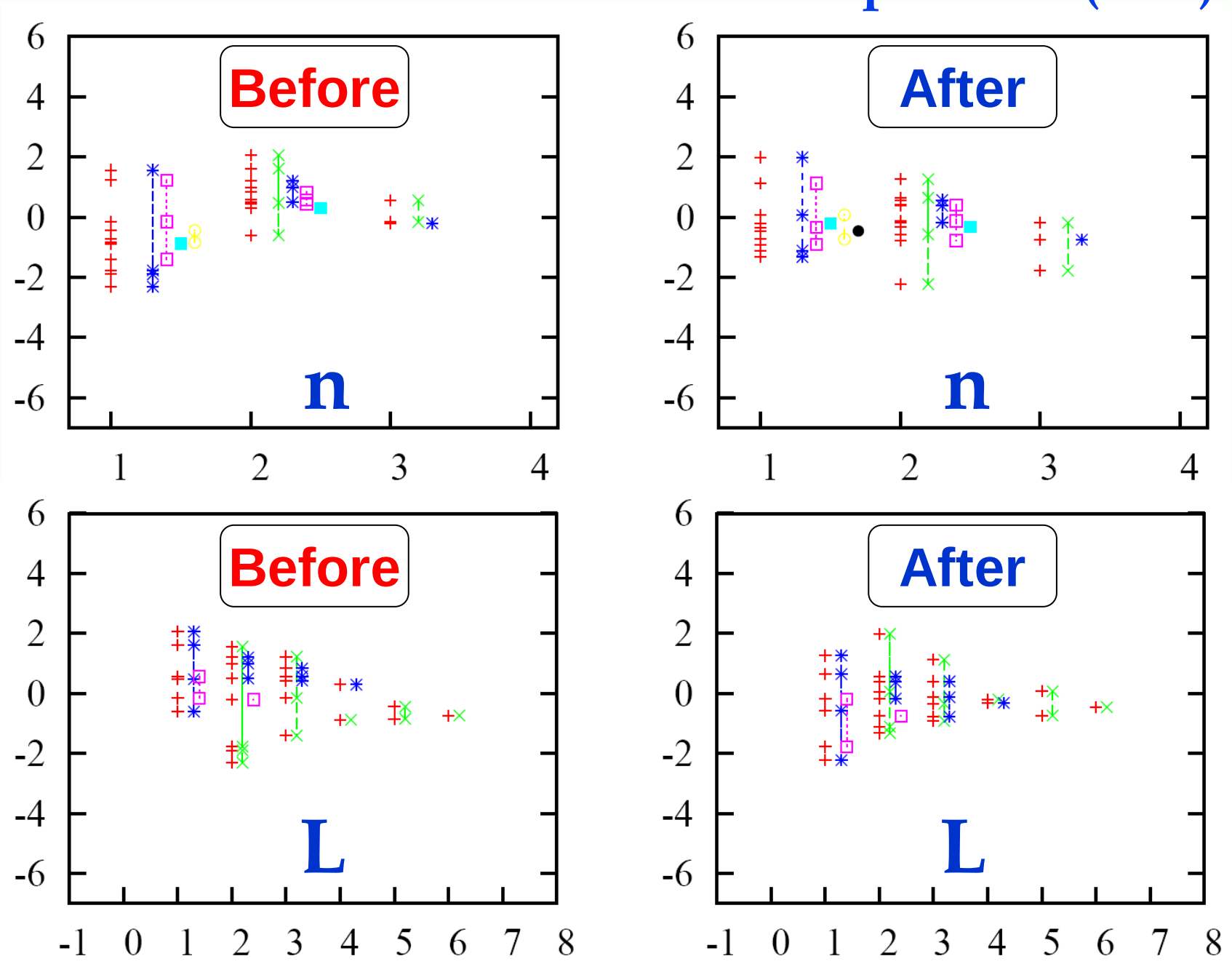
$$\begin{aligned}
h_n &= -\tfrac{\hbar^2}{2m}\Delta + \Gamma_0^{\rm even} + \Gamma_0^{\rm odd} + \Gamma_1^{\rm even} + \Gamma_1^{\rm odd},\\
h_p &= -\tfrac{\hbar^2}{2m}\Delta + \Gamma_0^{\rm even} + \Gamma_0^{\rm odd} - \Gamma_1^{\rm even} - \Gamma_1^{\rm odd}.
\end{aligned}$$

HF equation for single-particle wave functions:

$$h_\alpha\psi_{i,\alpha}(\vec{r}\sigma) = \epsilon_{i,\alpha}\psi_{i,\alpha}(\vec{r}\sigma),$$

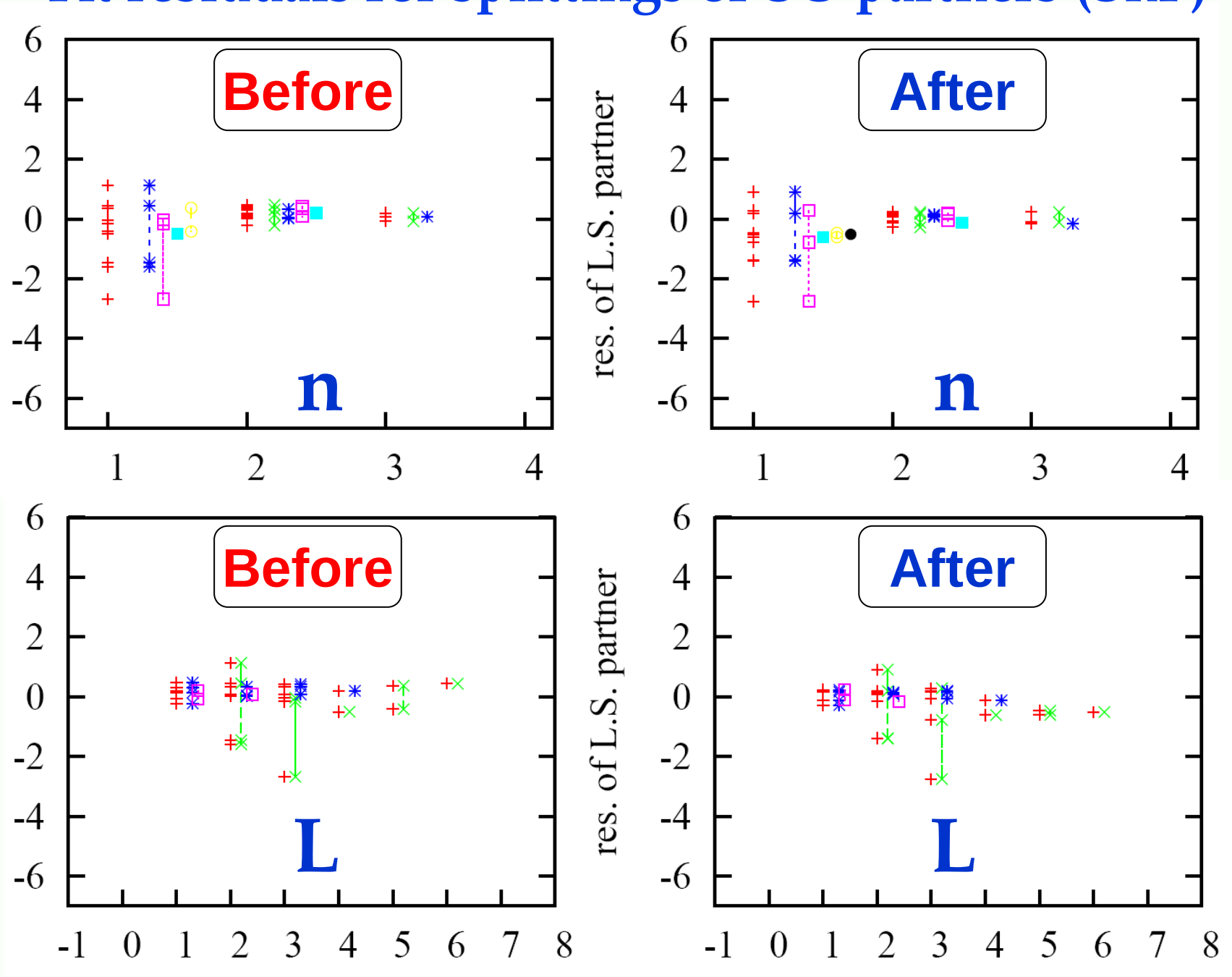
where i numbers the neutron ($\alpha{=}n$) and proton ($\alpha{=}p$) eigenstates.

Fit residuals for centroids of SO partners (SkP)



M. Kortelainen *et al.*, to be published

Fit residuals for splittings of SO partners (SkP)



M. Kortelainen *et al.*, to be published

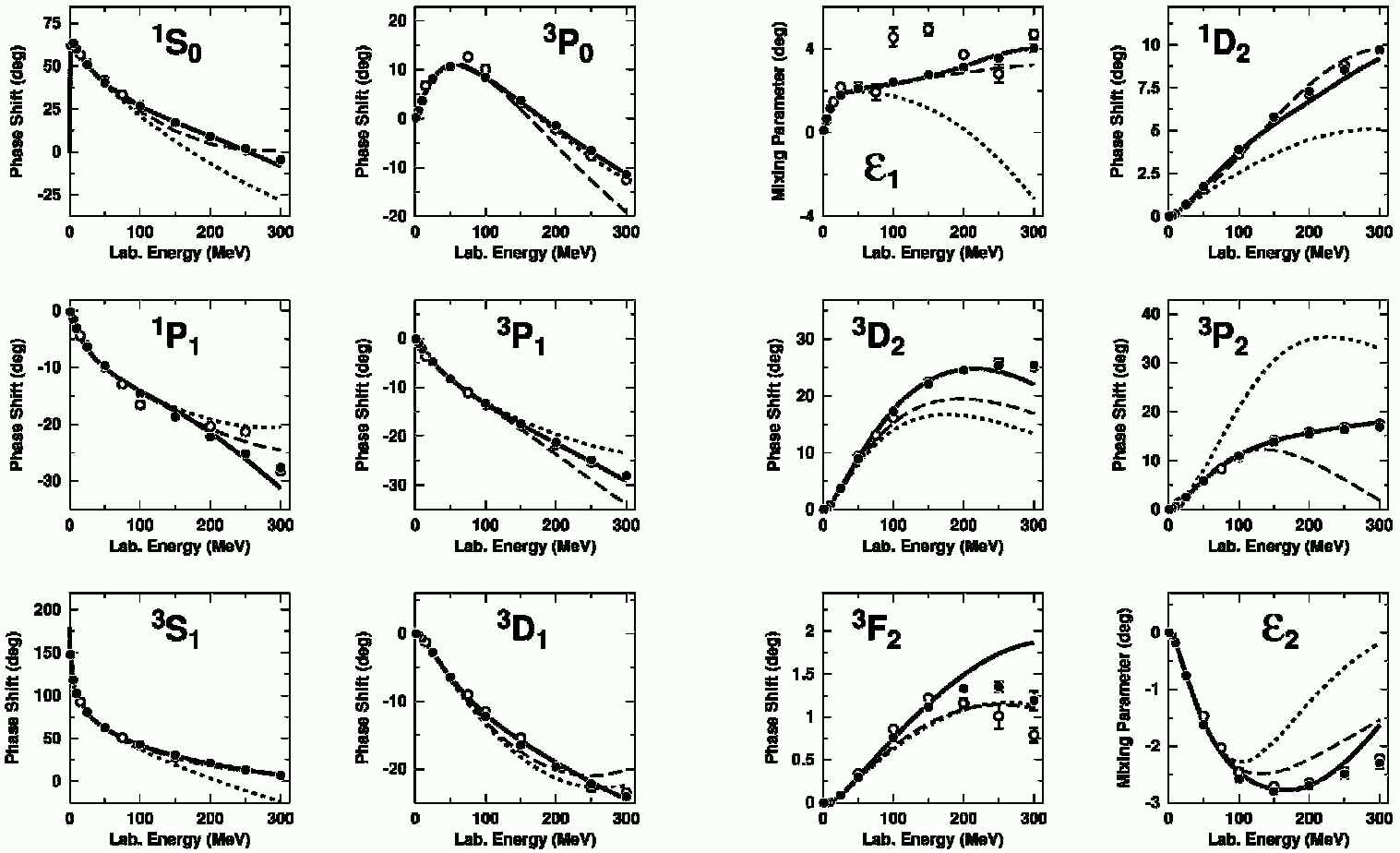
N^{3}LO in the chiral perturbation effective field theory

Table 1: Contact-gradient expansion for relative-coordinate two-particle matrix elements. Here $\vec{D}^2_M = (\vec{\nabla} \otimes \vec{\nabla})_{2M}$, $\vec{D}^0_0 = [(\sigma(1) \otimes \sigma(2))_2 \otimes D^2]_{00}$, $\vec{F}^3_M = (\vec{\nabla} \otimes \vec{D}^2)_{3M}$, $\vec{F}^1_M = [(\sigma(1) \otimes \sigma(2))_2 \otimes F^3]_{1M}$, $\vec{G}^4_M = (\vec{D}^2 \otimes \vec{D}^2)_{4M}$, $\vec{G}^2_M = [(\sigma(1) \otimes \sigma(2))_2 \otimes G^4]_{2M}$, and the scalar product of tensor operators is defined as $A^J \cdot B^J = \sum_{M=-J}^{M=J} (-1)^M A^J_M B^J_{-M}$.

Transitions	LO	NLO	NNLO	N^{3}LO
$^3S_1 \leftrightarrow {}^3S_1$ or $^1S_0 \leftrightarrow {}^1S_0$	$\delta(\mathrm{r}$	$\overleftarrow{\nabla^2}\,\delta(\mathrm{r}) + \delta(\mathrm{r})\,\overrightarrow{\nabla^2}$	$\overleftarrow{\nabla^2}\,\delta(\mathrm{r})\,\overrightarrow{\nabla^2}$ $\overleftarrow{\nabla^4}\,\delta(\mathrm{r}) + \delta(\mathrm{r})\,\overrightarrow{\nabla^4}$	$\overleftarrow{\nabla^4}\,\delta(\mathrm{r})\,\overrightarrow{\nabla^2} + \overleftarrow{\nabla^2}\,\delta(\mathrm{r})\,\overrightarrow{\nabla^4}$ $\overleftarrow{\nabla^6}\,\delta(\mathrm{r}) + \delta(\mathrm{r})\,\overrightarrow{\nabla^6})$
$^3S_1 \leftrightarrow {}^3D_1$		$\delta(\mathrm{r})\,\overrightarrow{D^0} + \overleftarrow{D^0}\,\delta(\mathrm{r})$	$\overleftarrow{\nabla^2}\,\delta(\mathrm{r})\,\overrightarrow{D^0} + \overleftarrow{D^0}\,\delta(\mathrm{r})\,\overrightarrow{\nabla^2}$ $\delta(\mathrm{r})\,\overrightarrow{\nabla^2 D^0} + \overleftarrow{D^0 \nabla^2}\,\delta(\mathrm{r})$	$(\overleftarrow{\nabla^4}\,\delta(\mathrm{r})\,\overrightarrow{D^0} + \overleftarrow{D^0}\,\delta(\mathrm{r})\,\overrightarrow{\nabla^4}$ $(\overleftarrow{\nabla^2}\,\delta(\mathrm{r})\,\overrightarrow{\nabla^2 D^0} + \overleftarrow{D^0 \nabla^2}\,\delta(\mathrm{r})\,\overrightarrow{\nabla^2}$ $(\delta(\mathrm{r})\,\overrightarrow{\nabla^4 D^0} + \overleftarrow{D^0 \nabla^4}\,\delta(\mathrm{r})$
$^1D_2 \leftrightarrow {}^1D_2$ or $^3D_J \leftrightarrow {}^3D_J$			$\overleftarrow{D^2}\cdot\delta(\mathrm{r})\,\overrightarrow{D^2}$	$\overleftarrow{D^2 \nabla^2}\cdot\delta(\mathrm{r})\,\overrightarrow{D^2} + \overleftarrow{D^2}\cdot\delta(\mathrm{r})\,\overrightarrow{\nabla^2 D^2}$
$^3D_3 \leftrightarrow {}^3G_3$				$(\overleftarrow{D^2}\cdot\delta(\mathrm{r})\,\overrightarrow{G^2} + \overleftarrow{G^2}\cdot\delta(\mathrm{r})\,\overrightarrow{D^2}$
$^1P_1 \leftrightarrow {}^1P_1$ or $^3P_J \leftrightarrow {}^3P_J$		$\overleftarrow{\nabla}\cdot\delta(\mathrm{r})\,\overrightarrow{\nabla}$	$\overleftarrow{\nabla}\overleftarrow{\nabla^2}\cdot\delta(\mathrm{r})\,\overrightarrow{\nabla}+\overleftarrow{\nabla}\cdot\delta(\mathrm{r})\,\overrightarrow{\nabla^2}\overrightarrow{\nabla}$	$\overleftarrow{\nabla}\overleftarrow{\nabla^2}\cdot\delta(\mathrm{r})\,\overrightarrow{\nabla^2}\overrightarrow{\nabla}$ $\overleftarrow{\nabla}\overleftarrow{\nabla^4}\cdot\delta(\mathrm{r})\,\overrightarrow{\nabla}+\overleftarrow{\nabla}\cdot\delta(\mathrm{r})\,\overrightarrow{\nabla^4}\overrightarrow{\nabla}$
$^3P_2 \leftrightarrow {}^3F_2$			$\overleftarrow{\nabla}\cdot\delta(\mathrm{r})\,\overrightarrow{F^1} + \overleftarrow{F^1}\cdot\delta(\mathrm{r})\,\overrightarrow{\nabla}$	$\overleftarrow{\nabla}\overleftarrow{\nabla^2}\cdot\delta(\mathrm{r})\,\overrightarrow{F^1} + \overleftarrow{F^1}\cdot\delta(\mathrm{r})\,\overrightarrow{\nabla^2}\overrightarrow{\nabla})$ $\overleftarrow{\nabla}\cdot\delta(\mathrm{r})\,\overrightarrow{\nabla^2 F^1} + \overleftarrow{F^1 \nabla^2}\cdot\delta(\mathrm{r})\,\overrightarrow{\nabla}$
$^1F_3 \leftrightarrow {}^1F_3$ or $^3F_J \leftrightarrow {}^3F_J$				$\overleftarrow{F^3}\cdot\delta(\mathrm{r})\,\overrightarrow{F^3}$

W.C. Haxton, Phys. Rev. C77, 034005 (2008)

EFT phase-shift analysis



np phase parameters below 300 MeV lab. energy for partial waves with J=0,1,2. The solid line is the result at N^{3}LO. The dotted and dashed lines are the phase shifts at NLO and NNLO, respectively, as obtained by Epelbaum *et al*. The solid dots show the Nijmegen multi-energy np phase shift analysis and the open circles are the VPI single-energy np analysis SM99.

D.R. Entem and R. Machleidt, Phys.Rev. C68 (2003) 041001

II. Derivatives of higher order up to N^{3}LO

Nr	Tensor	order n	rank L
1	1	0	0
2	∇	1	1
3	Δ	2	0
4	$[\nabla\nabla]_2$	2	2
5	$\Delta\nabla$	3	1
6	$[\nabla[\nabla\nabla]_2]_3$	3	3
7	Δ^2	4	0
8	$\Delta[\nabla\nabla]_2$	4	2
9	$[\nabla[\nabla[\nabla\nabla]_2]_3]_4$	4	4
10	$\Delta^2\nabla$	5	1
11	$\Delta[\nabla[\nabla\nabla]_2]_3$	5	3
12	$[\nabla[\nabla[\nabla[\nabla\nabla]_2]_3]_4]_5$	5	5
13	Δ^3	6	0
14	$\Delta^2[\nabla\nabla]_2$	6	2
15	$\Delta[\nabla[\nabla[\nabla\nabla]_2]_3]_4$	6	4
16	$[\nabla[\nabla[\nabla[\nabla[\nabla\nabla]_2]_3]_4]_5]_6$	6	6

Total derivatives $(\vec{\nabla}^m)_I$ up to N^{3}LO

Nr	Tensor	order n	rank L
1	1	0	0
2	k	1	1
3	k^2	2	0
4	$[kk]_2$	2	2
5	k^2k	3	1
6	$[k[kk]_2]_3$	3	3
7	$(k^2)^2$	4	0
8	$k^2[kk]_2$	4	2
9	$[k[k[kk]_2]_3]_4$	4	4
10	$(k^2)^2k$	5	1
11	$k^2[k[kk]_2]_3$	5	3
12	$[k[k[k[kk]_2]_3]_4]_5$	5	5
13	$(k^2)^3$	6	0
14	$(k^2)^2[kk]_2$	6	2
15	$k^2[k[k[kk]_2]_3]_4$	6	4
16	$[k[k[k[k[kk]_2]_3]_4]_5]_6$	6	6

Relative derivatives $(\vec{k}^n)_L$ up to N^{3}LO

B.G. Carlsson *et al.*, Phys. Rev. C 78, 044326 (2008)

$$\nabla = \nabla_1 + \nabla_2, \qquad k = \frac{1}{2i}(\nabla_1 - \nabla_2)\,,$$

$$\rho_{v=0} = \rho(r_1, r_2), \qquad \rho_{v=1} = \vec{s}(r_1, r_2),$$

$$\rho_{nLvJ} = \left((\vec{k}^n)_L \rho_v\right)_J \text{(primary)}, \rho_{mInLvJQ} = \left((\vec{\nabla}^m)_I \left((\vec{k}^n)_L \rho_v\right)_J\right)_Q \text{(secondary)}$$

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Energy density functional up to N^{3}LO

order	from ρ	from $\vec{s}$	T-even	T-odd	total
0	1	1	1	1	2
1	1	3	3	1	4
2	2	4	2	4	6
3	2	6	6	2	8
4	2	5	2	5	7
5	1	4	4	1	5
6	1	2	1	2	3
total	10	25	19	16	35

Numbers of primary ($m = 0$) local-densities up to N^{3}LO.

order	T-even	T-odd	total	Galilean invariant	Gauge invariant
0	1	1	2	2	2
2	6	6	12	7	7
4	22	23	45	15	6
6	64	65	129	26	6
N^{3}LO	93	95	188	50	21

Numbers of terms in the EDF up to N^{3}LO.

B.G. Carlsson *et al.*, Phys. Rev. C 78, 044326 (2008)