New developments in nuclear DFT

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Reflections on the atomic nucleus
University of Liverpool
28-30 July 2015

Outline

1. Introduction: the nuclear EDF
2. What EDF can do for us?
3. Precision frontier
4. Effective theory for low-energy nuclear structure
5. *Ab initio* derivation of model EDFs
6. Conclusions

How the nuclear EDF is built?

$$E[\rho(\vec{r}_1,\vec{r}_2)] = \int\!\!\int \mathrm{d}\vec{r}_1 \mathrm{d}\vec{r}_2\, \mathcal{H}(\rho(\vec{r}_1,\vec{r}_2))$$

↑ Energy Density Functional (EDF)

↑ Energy Density

$$\mathcal{H}(\rho(\vec{r}_1,\vec{r}_2)) = V(\vec{r}_1-\vec{r}_2)\Big[\rho(\vec{r}_1)\rho(\vec{r}_2) - \rho(\vec{r}_1,\vec{r}_2)\rho(\vec{r}_2,\vec{r}_1)\Big]$$

↑ EDF generator

↑ Direct

↑ Exchange

Standard EDF generators

- **Gogny***

$$V(\vec r_1 \vec r_2; \vec r\,'_1 \vec r\,'_2) = \delta(\vec r_1 - \vec r\,'_1)\delta(\vec r_2 - \vec r\,'_2)V(\vec r_1 - \vec r_2),$$

where,

$$V(\vec r_1 - \vec r_2) = \sum_{i=1,2} e^{-(\vec r_1 - \vec r_2)^2/\mu_i^2} \times (W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau)$$
$$\boxed{+t_3(1 + P_\sigma)\delta(\vec r_1 - \vec r_2)\rho^{1/3}\left[\tfrac{1}{2}(\vec r_1 + \vec r_2)\right]}.$$

$P_\sigma = \frac{1}{2}(1+\vec\sigma_1\cdot\vec\sigma_2)$ 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 μ_i=0.7 and 1.2 fm, W_i, B_i, H_i, M_i, and t_3 are parameters.

- **Skyrme***

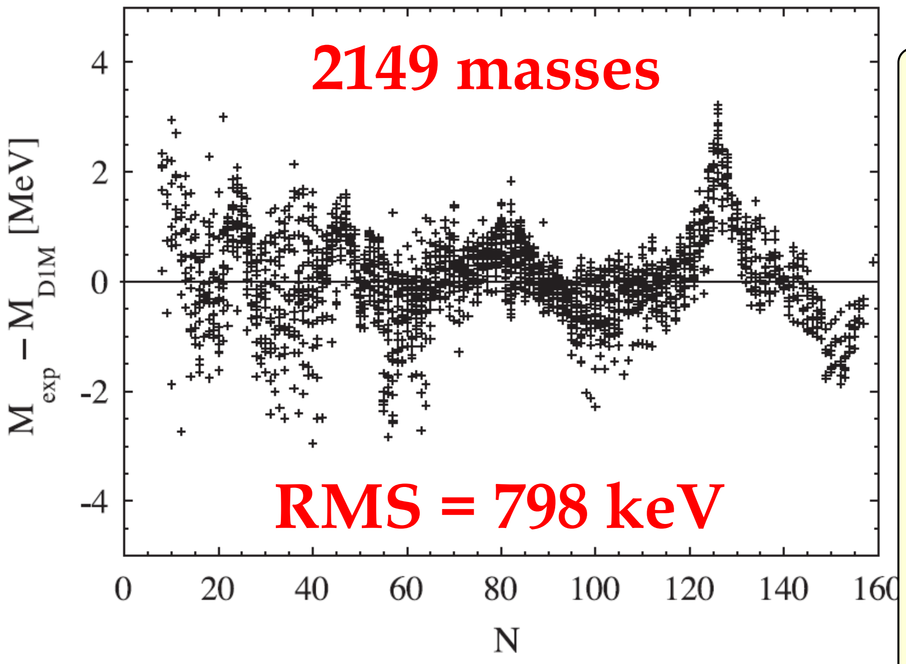
$$V(\vec r_1 \vec r_2; \vec r\,'_1 \vec r\,'_2) = \Big\{t_0(1 + x_0 P^\sigma) + \boxed{\tfrac{1}{6}t_3(1 + x_3 P^\sigma)\rho^\alpha\left(\tfrac{1}{2}(\vec r_1 + \vec r_2)\right)}$$
$$+\tfrac{1}{2}t_1(1 + x_1 P^\sigma)[\vec k'^{*2} + \vec k^2] + t_2(1 + x_2 P^\sigma)\vec k'^{*} \cdot \vec k\Big\}\,\delta(\vec r_1 - \vec r\,'_1)\delta(\vec r_2 - \vec r\,'_2)\delta(\vec r_1 - \vec r_2),$$

where the relative-momentum operators read $\hat{\vec k} = \frac{1}{2i}\left(\vec\nabla_1 - \vec\nabla_2\right)$, $\hat{\vec k}' = \frac{1}{2i}\left(\vec\nabla\,'_1 - \vec\nabla\,'_2\right)$.

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

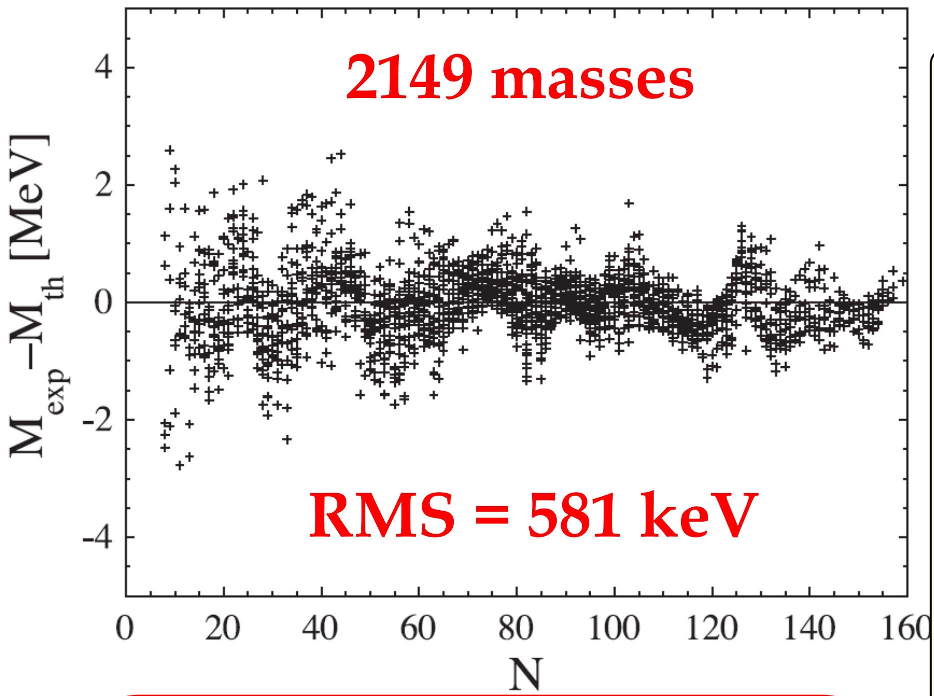
What EDF can do for us?

Nuclear binding energies (masses)



S. Goriely *et al.*, Phys. Rev. Lett. 102, 242501 (2009)

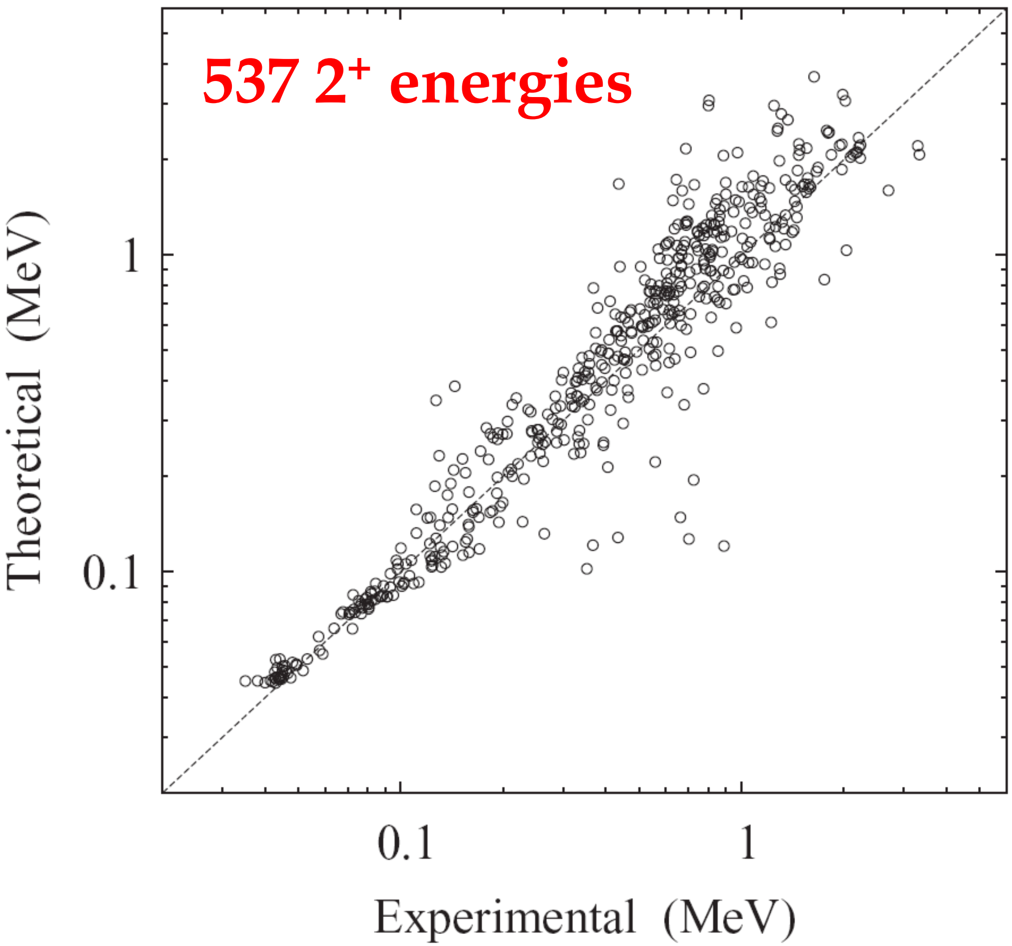
The first Gogny HFB mass model. An explicit and self-consistent account of all the quadrupole correlation energies are included within the 5D collective Hamiltonian approach.



S. Goriely *et al.*, Phys. Rev. Lett. 102, 152503 (2009)

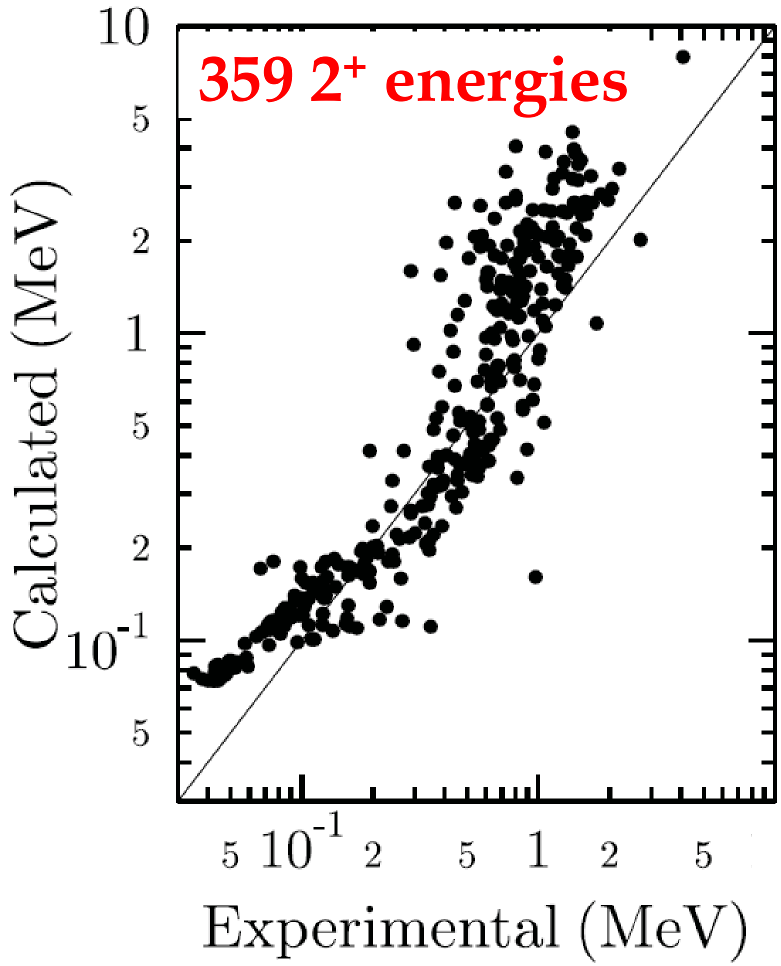
The new Skyrme HFB nuclear-mass model, in which the contact-pairing force is constructed from microscopic pairing gaps of symmetric nuclear matter and neutron matter.

First 2⁺ excitations of even-even nuclei



J.-P. Delaroche *et al.*, Phys. Rev. C81, 014303 (2010)

Gogny HFB calculations plus the 5D collective Hamiltonian approach.

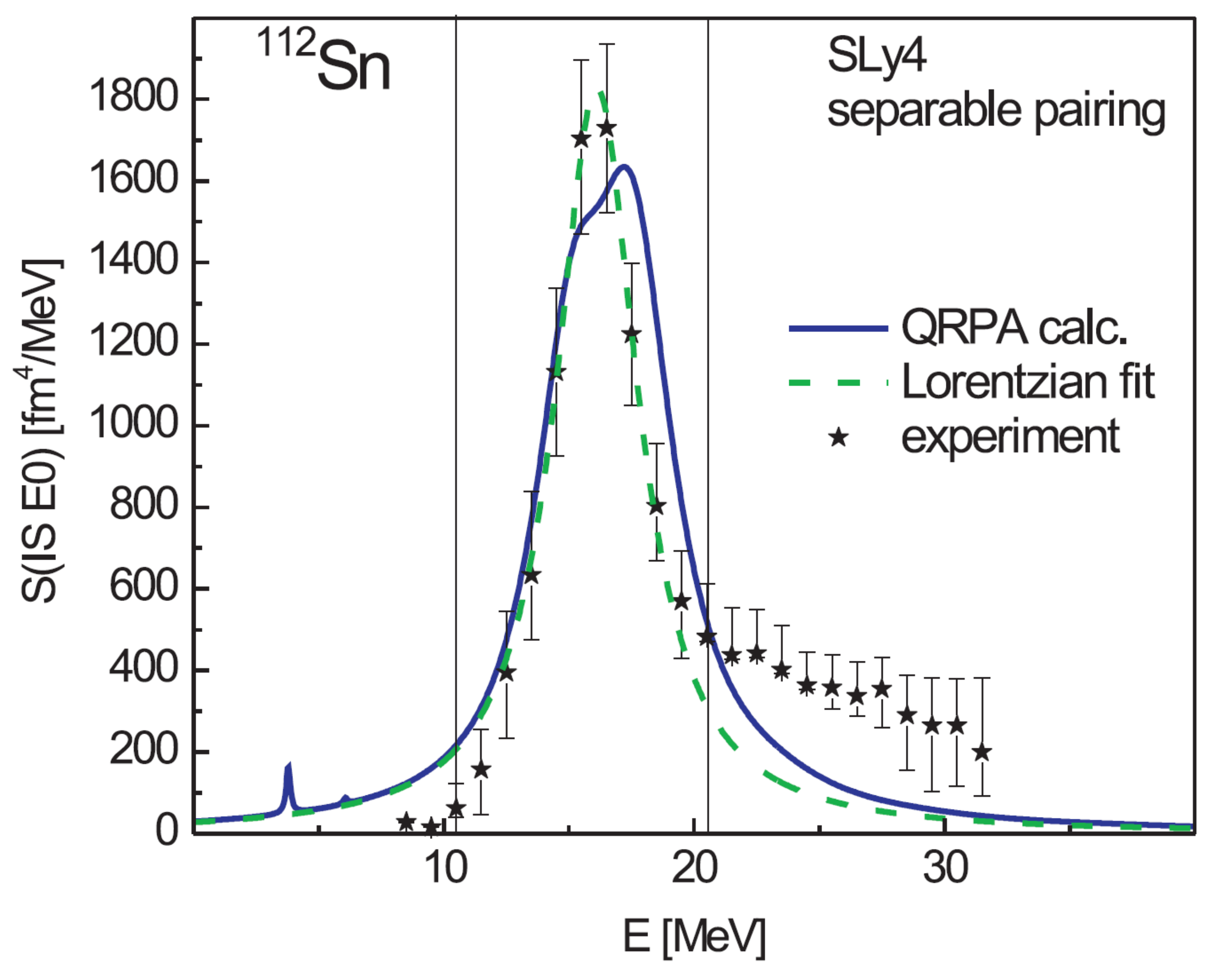


B. Sabbey *et al.*, Phys. Rev. C75, 044305 (2007)

Skyrme HF+BCS calculations plus the particle-number and angular-momentum projection and shape mixing.

Giant monopole resonances

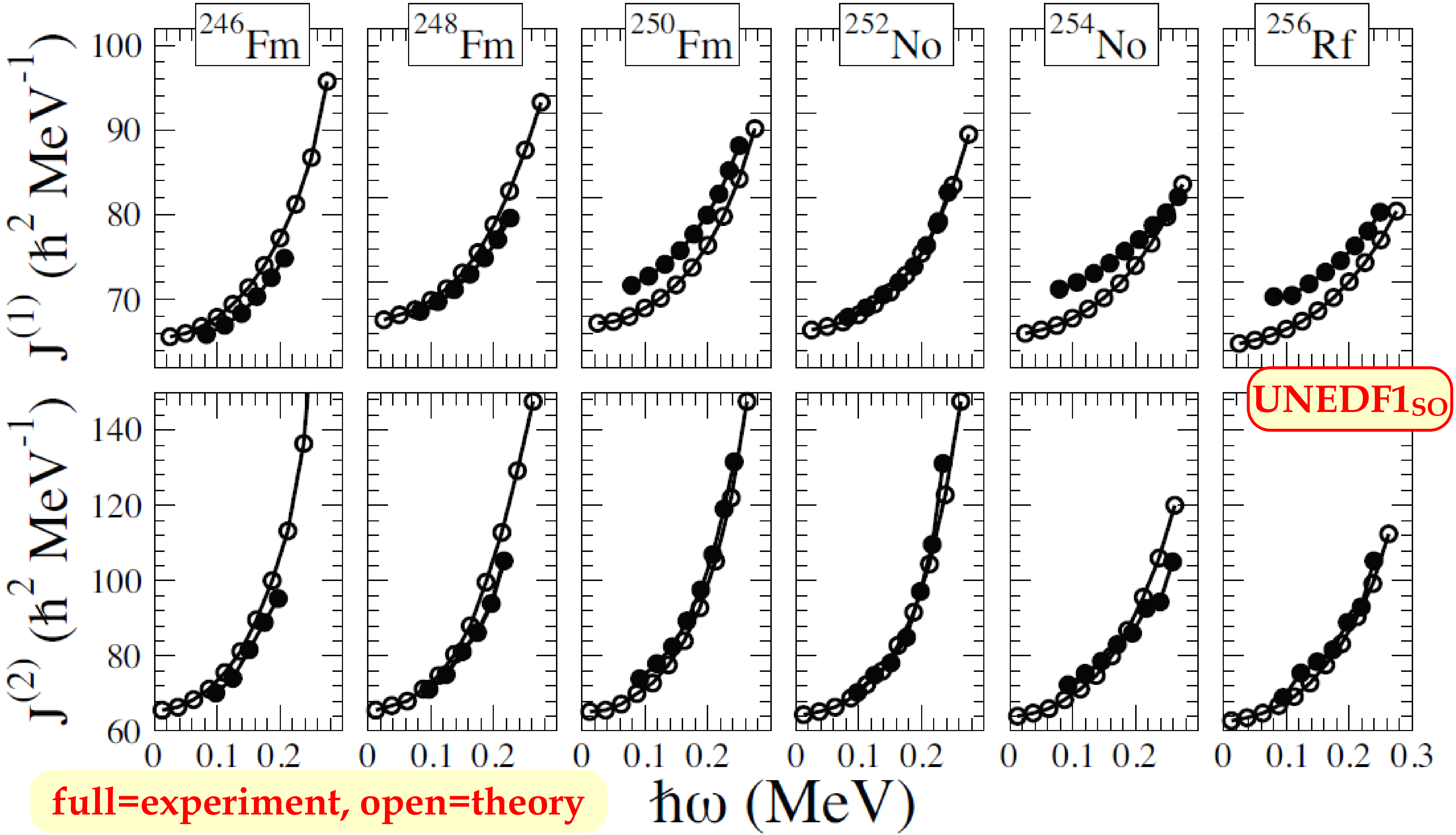
P. Veselý, *et al.*, C 86, 024303 (2012)



Experimental data from:
T. Li, U. Garg, Y. Liu, et al.,Phys. Rev. Lett. 99, 162503 (2007);
Phys. Rev. C 81, 034309 (2010))

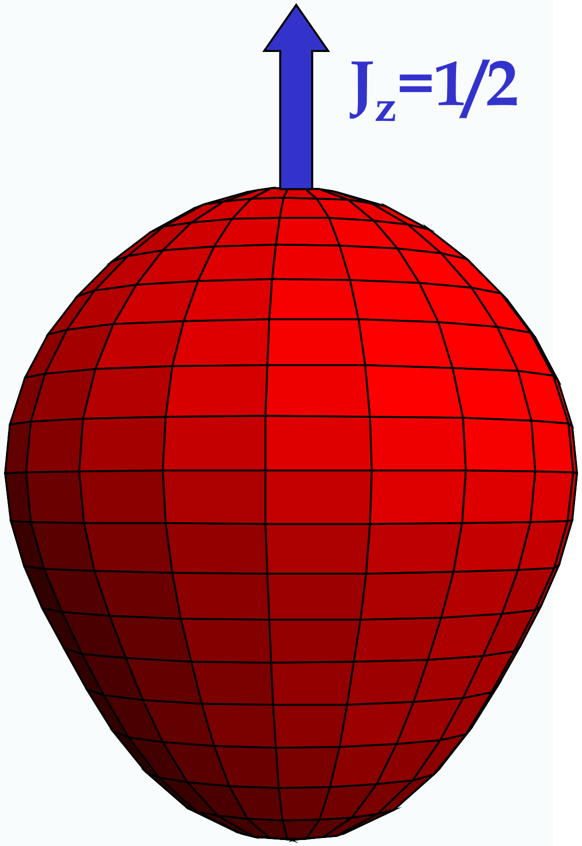
Spectroscopy in the nobelium region

Y. Shi, J.D., P.T. Greenleees, Phys. Rev. C89, 034309 (2014)



Skyrme-Hartree-Fock
J. Dobaczewski, J. Engel,
Phys. Rev. Lett. 94, 232502 (2005)

Experiment
R.G. Helmer *et al.*, Nucl. Phys. A474 (1987) 77



$$\beta_{10} = 0.023$$
$$\beta_{20} = 0.161$$
$$\beta_{30} = -0.128$$
$$\beta_{40} = 0.091$$

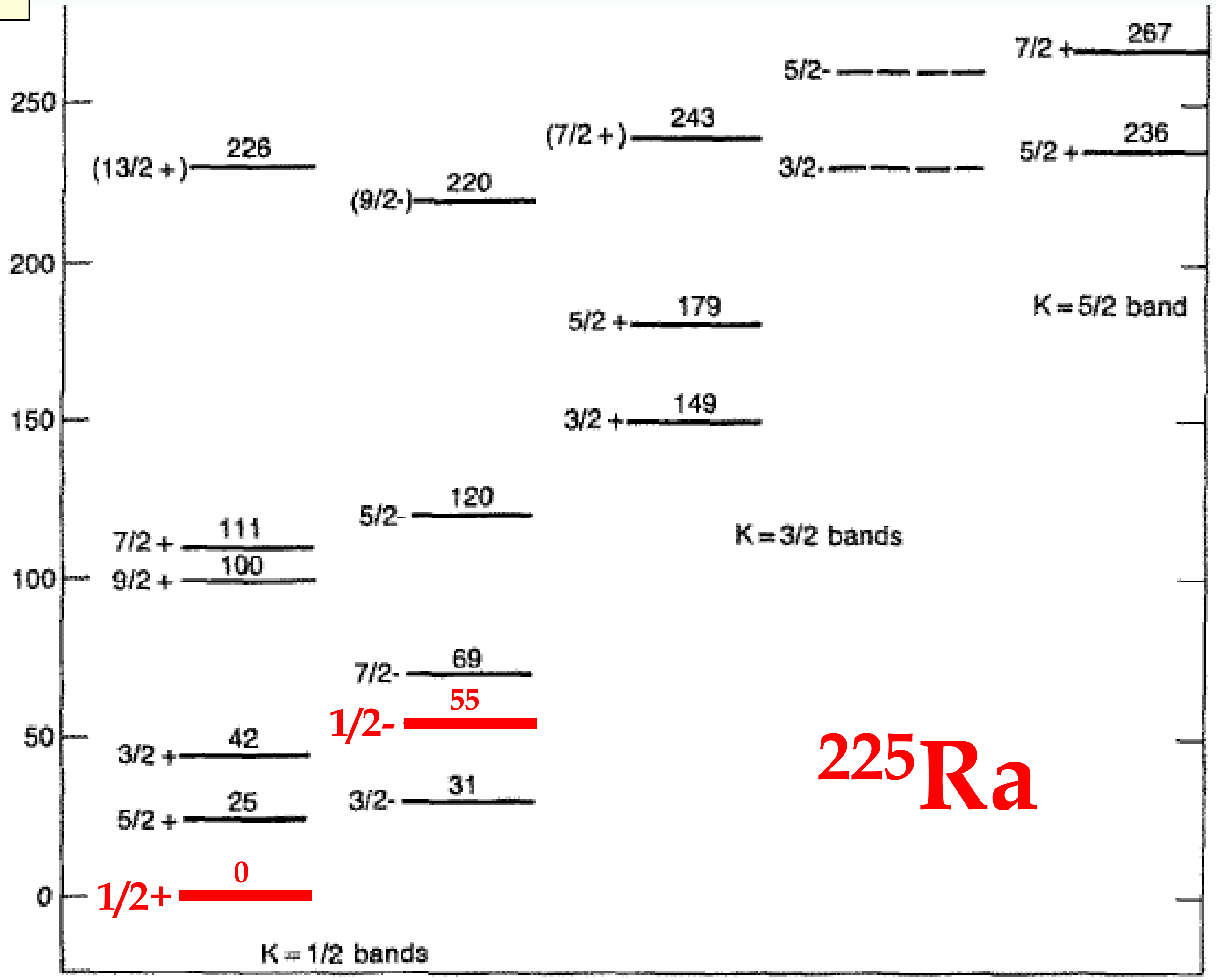
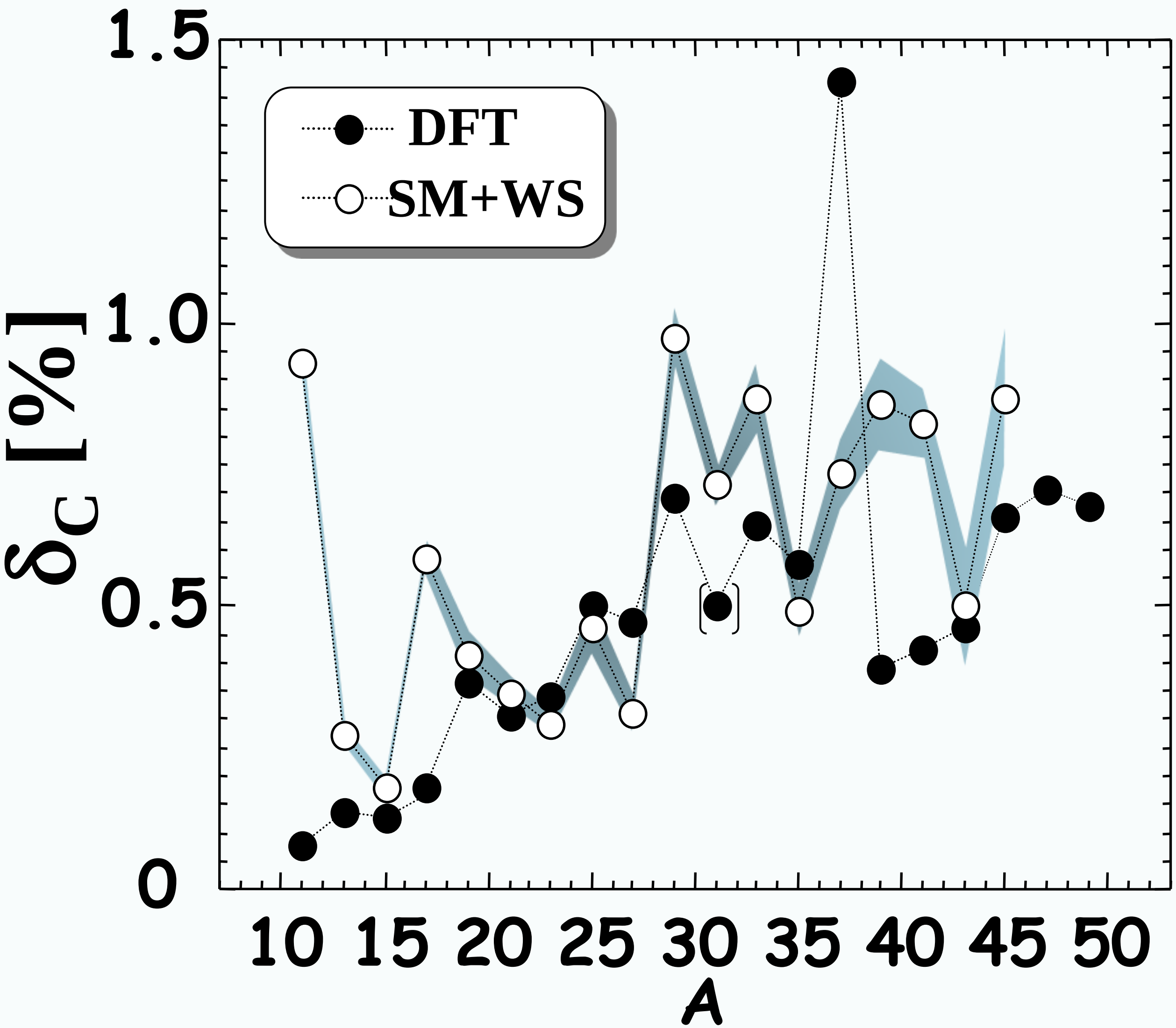


Fig. 5. Proposed grouping of the low-lying states of ^{225}Ra into rotational bands. The two members of the $K^\pi = \frac{3}{2}^-$ band have been reported in a study of the ^{225}Fr decay [20]; they are not observed in the present study.

ISB corrections to the Fermi transitions in T=1/2 mirrors

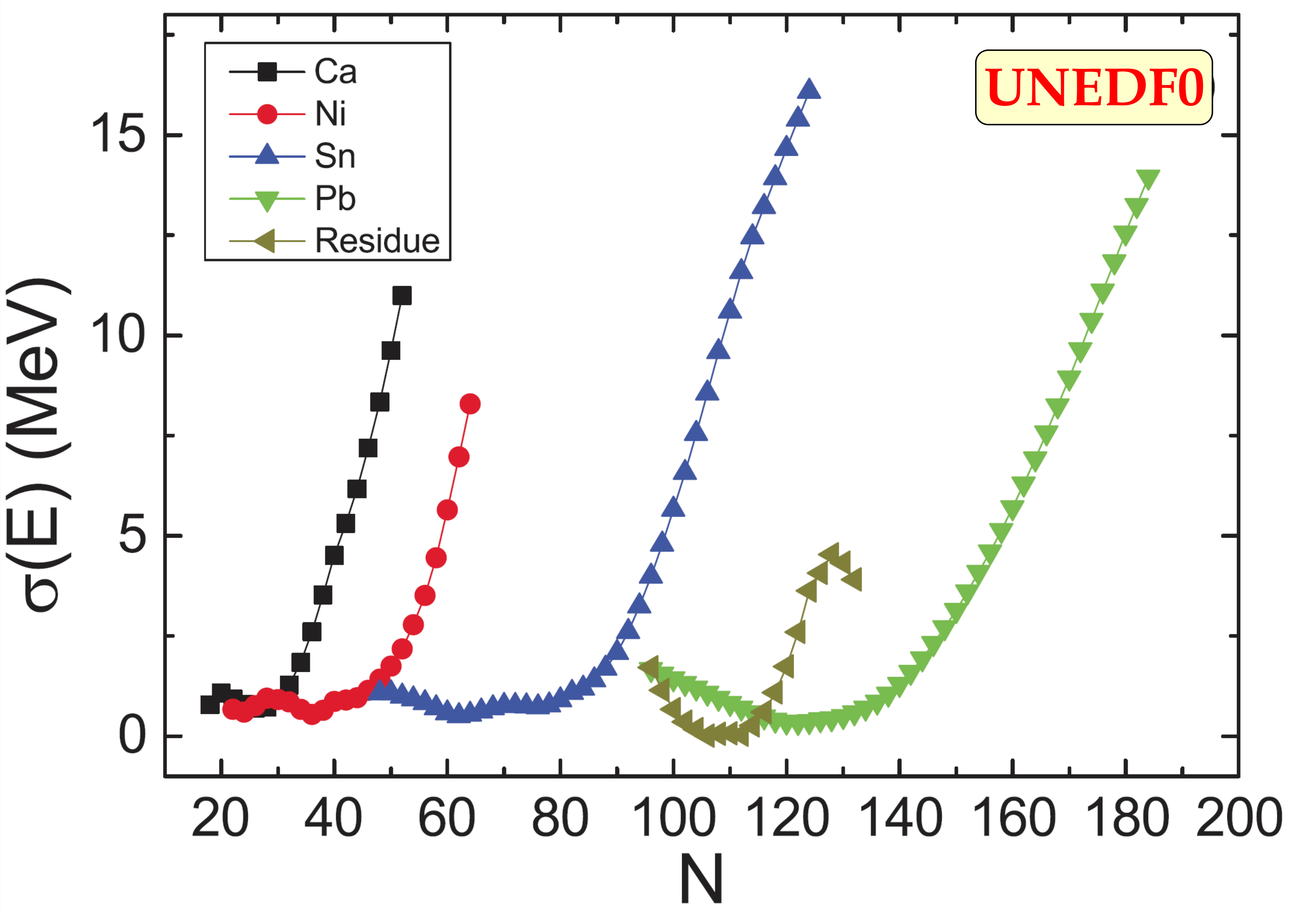


DFT results from:
W. Satuła, J. Dobaczewski, W. Nazarewicz, and M. Rafalski, Phys. Rev. C86, 054314(2012).

SM+WS results from:
N. Severijns, M. Tandecki, T. Phalet, and I. S. Towner, Phys. Rev. C **78**, 055501 (2008).

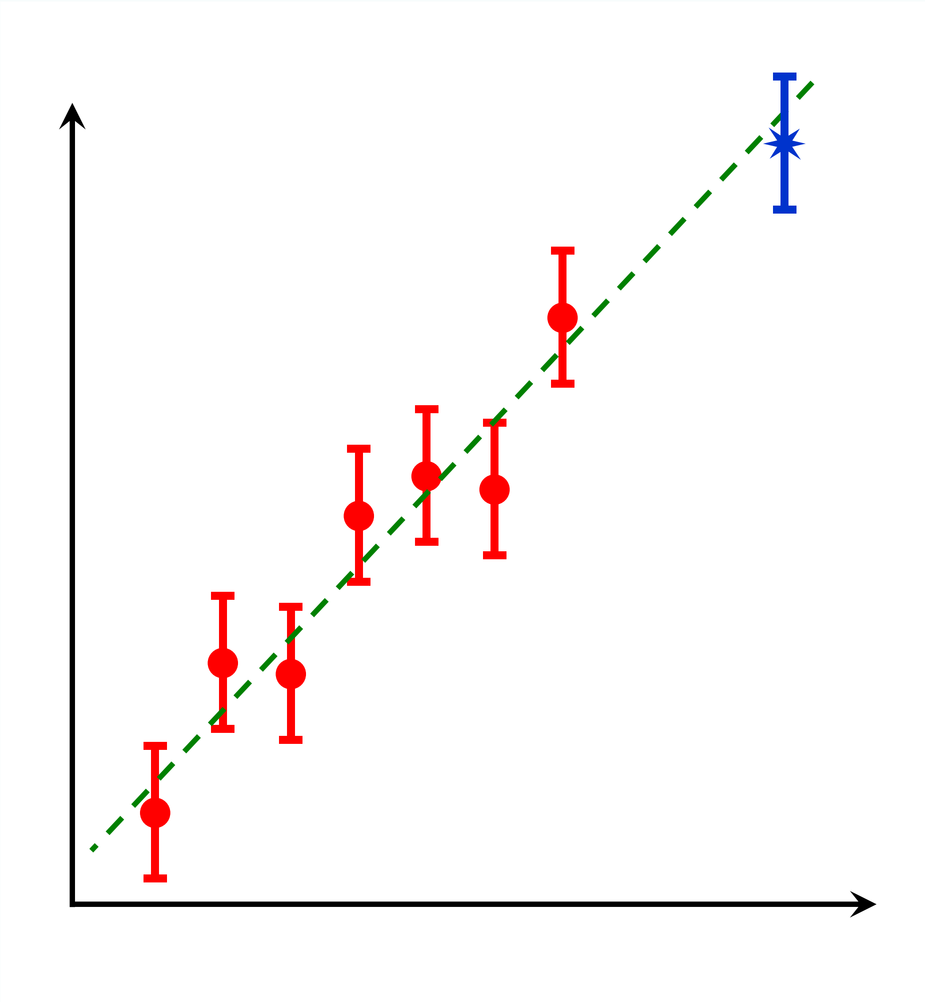
Precision frontier

Propagation of uncertainties

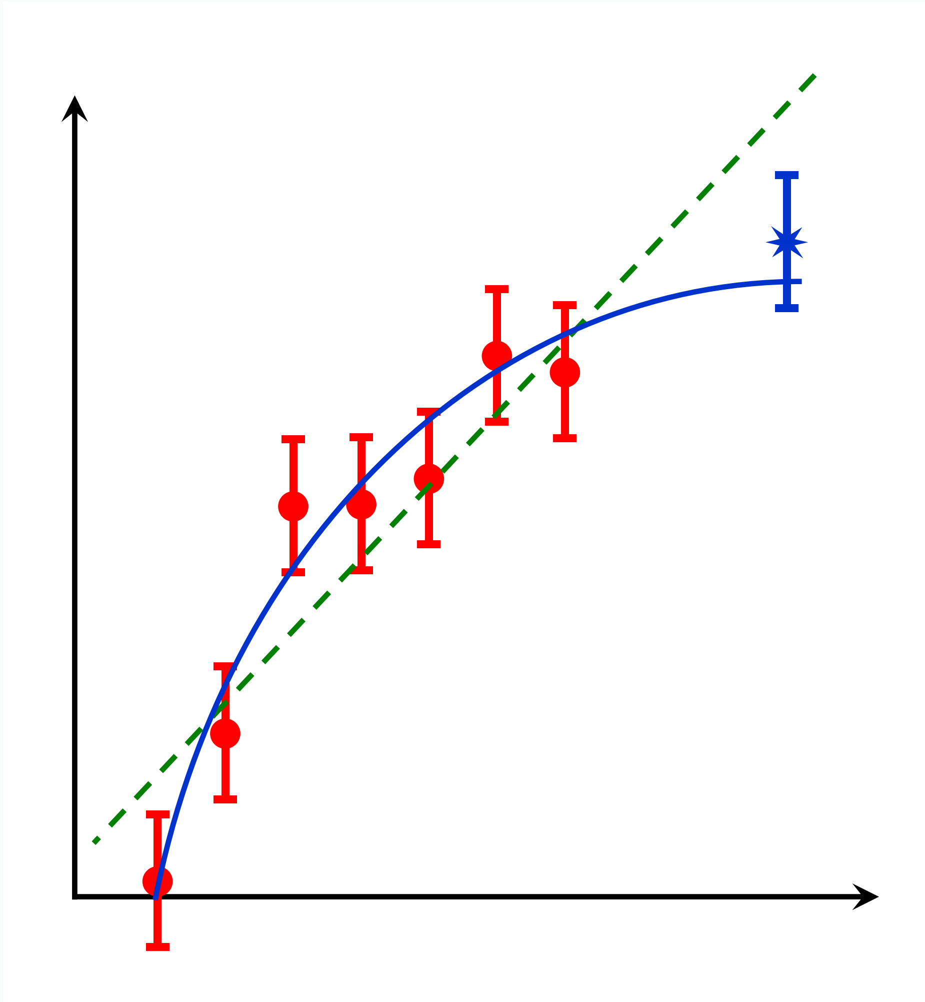


Y. Gao, *et al.*, Phys. Rev C 87, 034324 (2013)

Exact model



Inaccurate model



J. Tovanen, *et al.*, Phys. Rev. C 78, 034306 (2008)

Exact model

Effective theory for low-energy nuclear structure

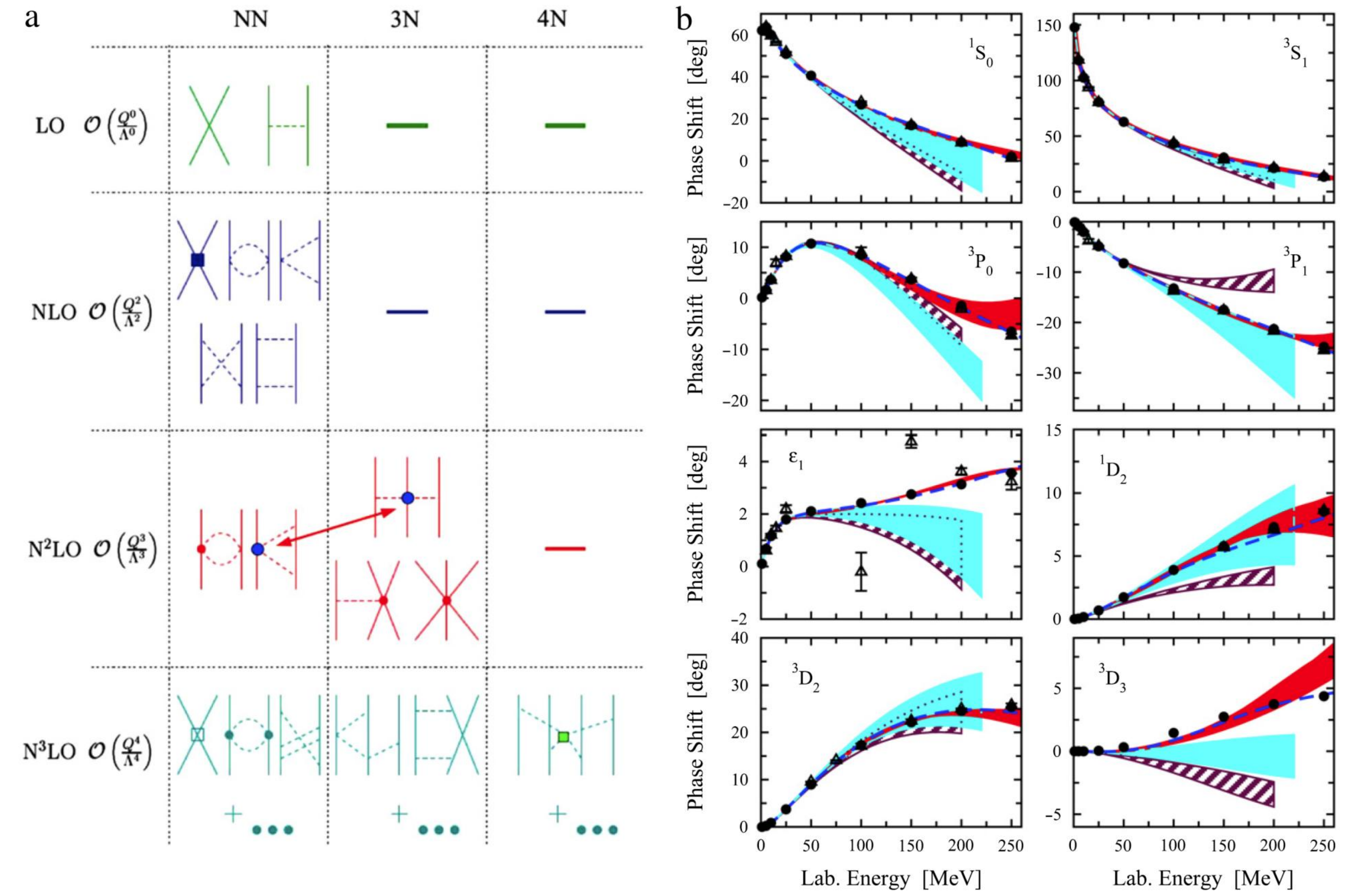


Fig. 4. (a) Chiral EFT for nuclear forces. (b) Improvement in neutron–proton phase shifts shown by shaded bands from cutoff variation at NLO (dashed), N^{2}LO (light), and N^{3}LO (dark) compared to extractions from experiment (points) [31]. The dashed line is from the N^{3}LO potential of Ref. [20].

S.K. Bogner et al., Prog. Part. Nucl. Phys. 65 (2010) 94

Zero-range vs. regularized finite-range pseudopotentials and functionals

Zero range:

B.G. Carlsson et *al.*, Phys. Rev. C 78, 044326 (2008)
F. Raimondi et al., Phys. Rev. C 83, 054311 (2011)

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

Finite range:

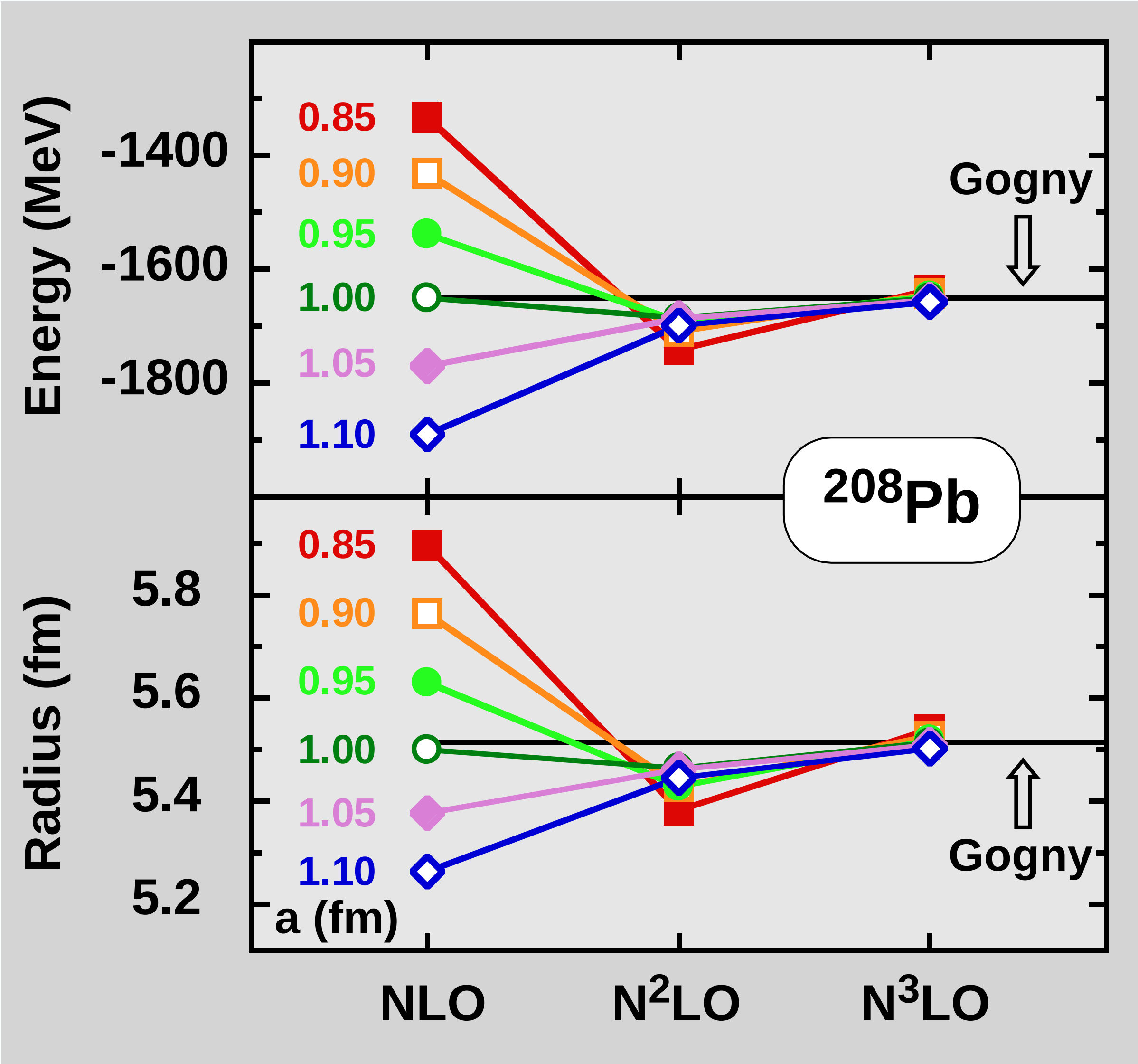
F. Raimondi et *al.*, J. Phys. G 41, 055112 (2014)

$$\hat{V}^{\tilde{n}'\tilde{L}',\bar{t}}_{\tilde{n}\tilde{L},v_{12}S} = \frac{1}{2} i^{v_{12}} \left(\left[\left[K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}} \right]_S \hat{S}_{v_{12}S} \right]_0 + (-1)^{v_{12}+S} \left[\left[K'_{\tilde{n}\tilde{L}} K_{\tilde{n}'\tilde{L}'} \right]_S \hat{S}_{v_{12}S} \right]_0 \right) \times \left(\hat{P}^\tau \right)^{\bar{t}} \left(1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau \right) \delta(\vec{r}\,'_1 - \vec{r}_1) \delta(\vec{r}\,'_2 - \vec{r}_2) g_a(\vec{r}_1 - \vec{r}_2).$$

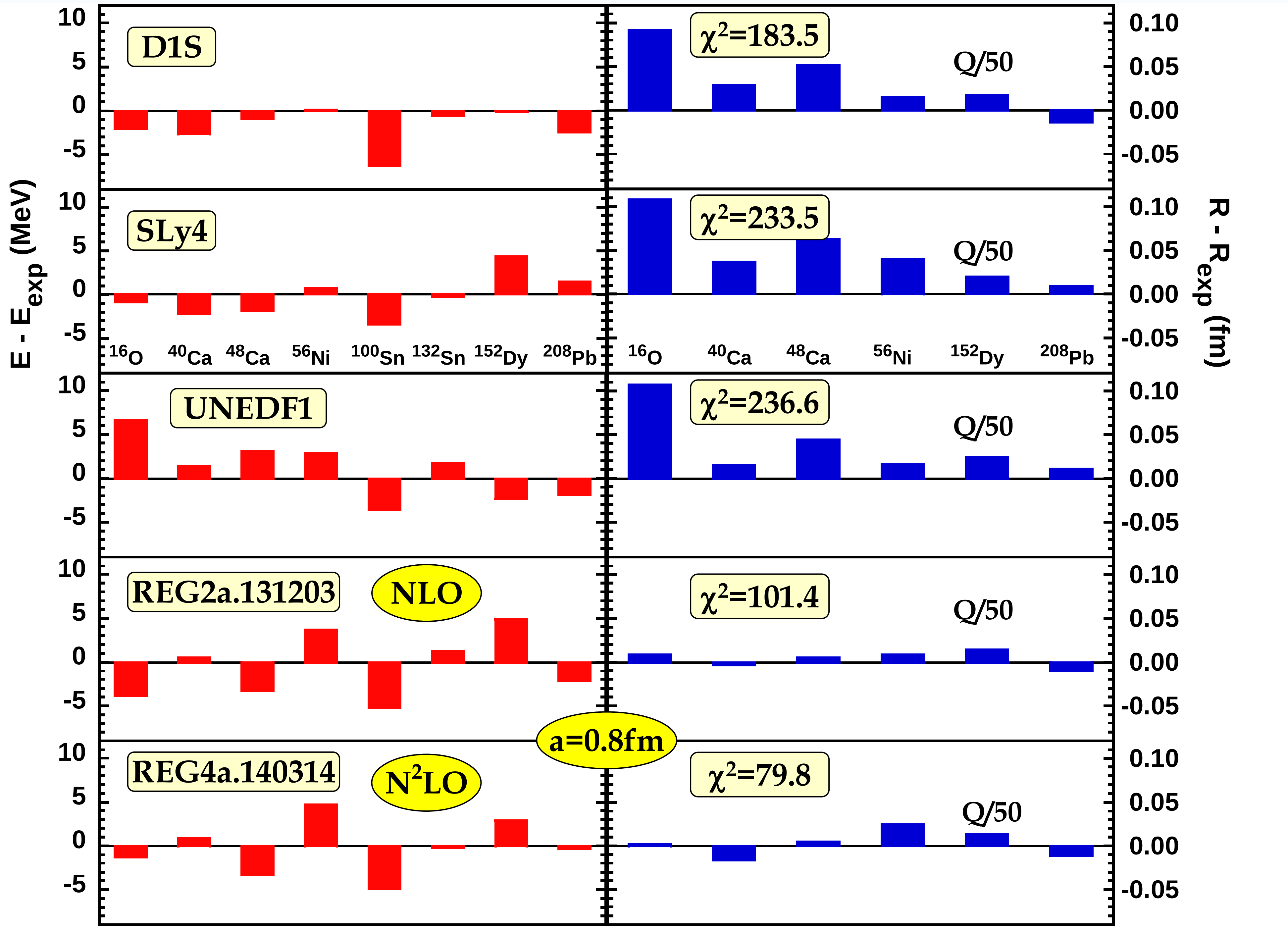
Numbers of terms of the finite-range pseudopotential at different orders up to N^3LO. In the second, third, and fourth column, numbers of central ($\tilde{S} = 0$), SO ($\tilde{S} = 1$), and tensor ($\tilde{S} = 2$) terms, respectively, are displayed.

Order	$\tilde{S}=0$	$\tilde{S}=1$	$\tilde{S}=2$	Total
0	4	0	0	4
2	8	2	4	14
4	16	4	10	30
6	24	8	20	52
N^3LO	52	14	34	100

Local regularized pseudopotentials vs. Gogny



J.D, K. Bennaceur, F. Raimondi, J. Phys. G. 39, 125103 (2012)


D1S
SLy4
UNEDF1
REG2a.131203
NLO
REG4a.140314
N²LO
a=0.8fm
χ²=183.5
χ²=233.5
χ²=236.6
χ²=101.4
χ²=79.8
Q/50
E - E_exp (MeV)
R - R_exp (fm)
16O 40Ca 48Ca 56Ni 100Sn 132Sn 152Dy 208Pb
16O 40Ca 48Ca 56Ni 152Dy 208Pb

Ab initio derivation of model EDFs

Ab initio derivation of model EDFs

The goal is to provide an *ab initio* derivation within a certain class of model EDFs $\tilde{E}\left[\rho\right]$:

$$\tilde{E}\left[\rho\right] = \sum_{i=1}^{m} C^i V_i\left[\rho\right],$$

where C^i are coupling constants and $V_i\left[\rho\right]$ are the EDF generators.

Instead of probing the system with all possible one-body potentials it is enough to probe it within the finite set of the EDF generators $-\hat{V}_j$, that is, to solve the constrained variational equation,

$$\delta E' = \delta\langle\Psi|\hat{H} - \sum_{j=1}^{m} \lambda^j \hat{V}_j|\Psi\rangle = 0,$$

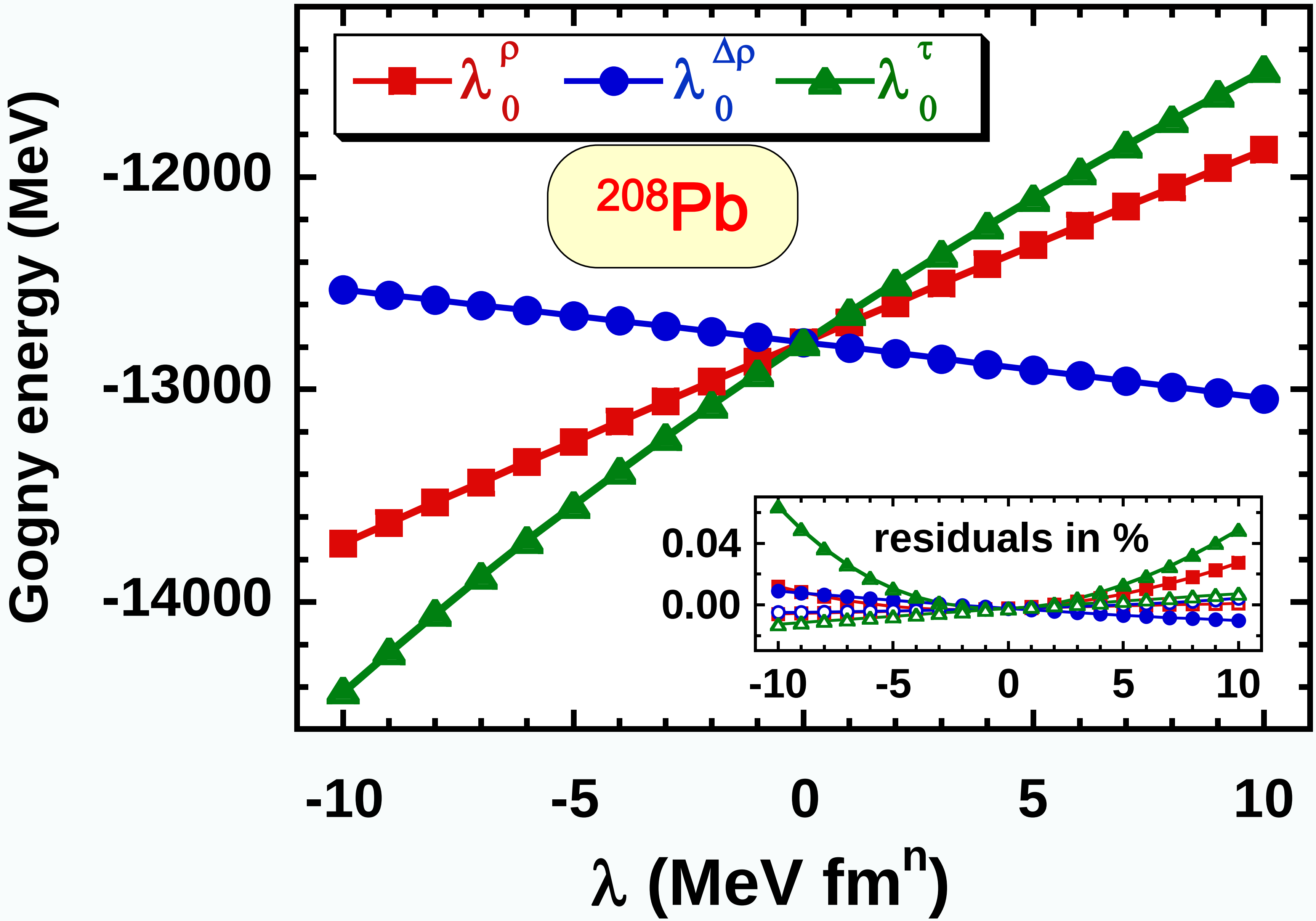
for a suitable set of values of a finite number of Lagrange multipliers λ^i, which is perfectly manageable a task.

Solution of this equation gives us the exact ground-state energies $E(\lambda^j)$ and one-body non-local densities $\rho_{\lambda^j}(r_1, r_2)$, both as functions (not functionals!) of the Lagrange multipliers λ^j. Then we adjust the EDF coupling constants C^i so as to have,

$$E(\lambda^j) = \sum_{i=1}^{m} C^i V_i\left[\rho_{\lambda^j}\right].$$

J.D., arXiv:1507.00697

Ab initio derivation of model EDFs



J.D., arXiv:1507.00697

Ab initio derivation of model EDFs

S1Se

		$t=0$	$t=1$
C_t^{ρ}	(MeV fm^3)	−605.41(16)	509(3)
$C_t^{\Delta\rho}$	(MeV fm^5)	−74.82(12)	41(2)
C_t^{τ}	(MeV fm^5)	79.73(16)	−98(2)

Table 1: Gogny-force D1S ground-state energies E_G (b) compared to energies E (c) calculated using the Skyrme EDF S1Se.

	E_G	E	δE	$\delta E/\lvert E\rvert$	$\delta E/\Delta E$
(a)	(b)	(c)	(d)	(e)	(f)
^{16}O	−129.626	−128.83(6)	0.79	0.61%	13
^{40}Ca	−344.663	−344.34(6)	0.32	0.09%	5
^{48}Ca	−416.829	−419.36(7)	−2.53	−0.61%	−37
^{56}Ni	−483.820	−485.83(7)	−2.01	−0.42%	−29
^{78}Ni	−640.598	−642.99(13)	−2.39	−0.37%	−18
^{100}Sn	−830.896	−832.60(10)	−1.70	−0.20%	−18
^{132}Sn	−1103.246	−1107.17(15)	−3.93	−0.36%	−26
^{208}Pb	−1638.330	−1641.26(16)	−2.93	−0.18%	−18
rms	n.a.	n.a.	2.34	0.40%	22

J.D., arXiv:1507.00697

Ab initio derivation of model EDFs

S1Se

		$t=0$	$t=1$
C_t^{ρ}	(MeV fm^3)	−605.41(16)	509(3)
$C_t^{\Delta\rho}$	(MeV fm^5)	−74.82(12)	41(2)
C_t^{τ}	(MeV fm^5)	79.73(16)	−98(2)

Table 2: Gogny-force D1S ground-state radii R_G (b) compared to radii R (c) calculated using the Skyrme EDF S1Se.

(a)	R_G (b)	R (c)	δR (d)	$\delta R/R$ (e)	$\delta R/\Delta R$ (f)
^{16}O	2.6689	2.6350(7)	−0.0339	−1.27%	−48
^{40}Ca	3.4117	3.3860(8)	−0.0257	−0.75%	−31
^{48}Ca	3.4423	3.4347(10)	−0.0076	−0.22%	− 8
^{56}Ni	3.6773	3.6781(11)	0.0008	0.02%	1
^{78}Ni	3.9070	3.9222(10)	0.0151	0.39%	16
^{100}Sn	4.4070	4.4118(12)	0.0048	0.11%	4
^{132}Sn	4.6530	4.6694(11)	0.0164	0.35%	15
^{208}Pb	5.4365	5.4535(12)	0.0170	0.31%	14
rms	n.a.	n.a.	0.0183	0.57%	22

J.D., arXiv:1507.00697

Conclusions

1. **Nuclear DFT provides us with one of the most spectacularly successful approaches in nuclear physics. Based on a dozen-odd parameters, nuclear DFT fairly well describes thousands of experimental data**
2. **Currently available nuclear functionals have reached their limits of applicability. To gain progress, extensions/modifications thereof are mandatory.**

Thank you