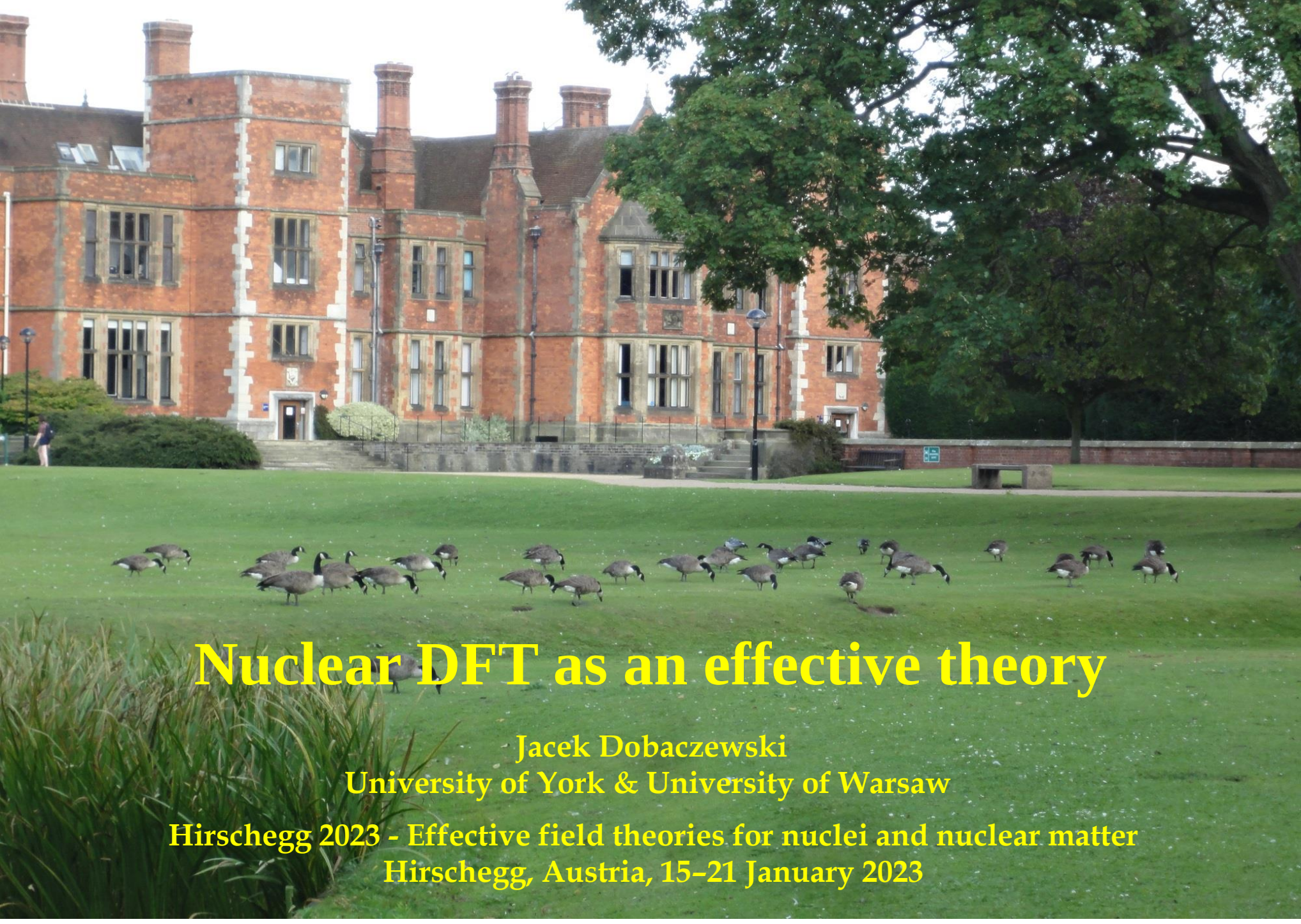

Nuclear DFT as an effective theory

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Hirschegg 2023 - Effective field theories for nuclei and nuclear matter
Hirschegg, Austria, 15–21 January 2023

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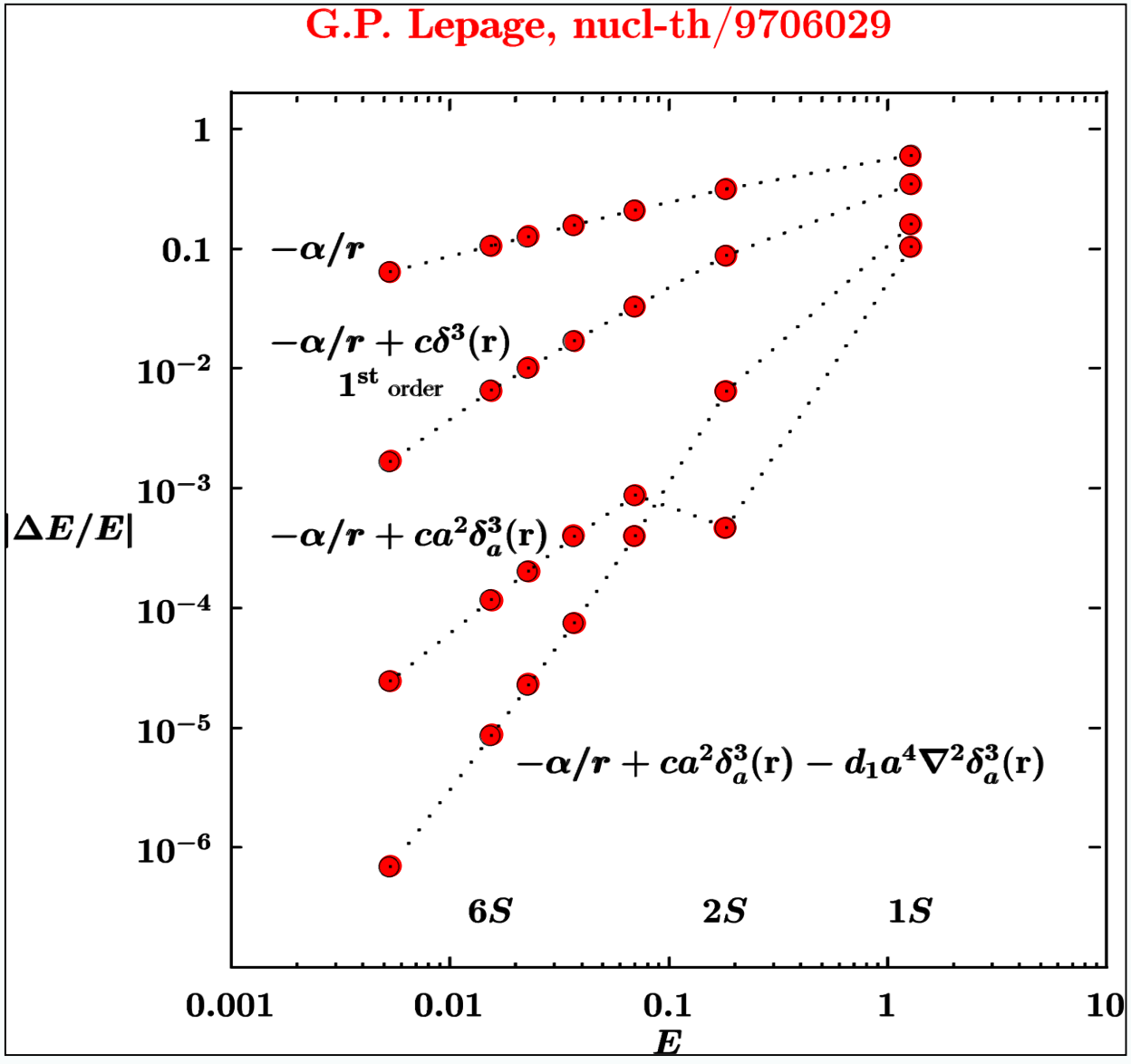
In collaboration with

- Jérémy Bonnard, Markus Kortelainen, Gauthier Danneaux
- Gianluca Salvioni, Carlo Barbieri, Gillis Carlsson, Andrea Idini, Alessandro Pastore
- Karim Bennaceur, Francesco Raimondi

Outline

1. Effective theory by Lepage
2. Introduction to DFT
3. LDA vs. generator functionals
4. *Ab-initio*-derived Skyrme functional
5. Regularized finite-range pseudopotentials as functional generators
6. Gogny-equivalent regularized N^nLO density functional
7. Density-independent N^2LO density functional
8. Density-dependent N^3LO density functional
9. Conclusions

Hydrogen atom perturbed near the center



Relative errors in the S-wave binding energies are plotted versus:
(i) the binding energy for the Coulomb theory
(ii) the Coulomb theory augmented with a delta function in first-order perturbation theory
(iii) the non-perturbative effective theory through a^2, and
(iv) the effective theory through a^4.

What is DFT?

Density Functional Theory:

A variational method that uses observables as variational parameters.

$$\delta\langle \hat{H} - \lambda \hat{Q} \rangle = 0$$

$$\Downarrow$$

$$E = E(Q)$$

for $E(\lambda) \equiv \langle \hat{H} \rangle$ and $Q(\lambda) \equiv \langle \hat{Q} \rangle$

Levy–Lieb constrained variation

Phys. Rev. A26, 1200 (1982), Int. J. Quantum Chem. 24, 243 (1983)

J. D., J. Phys.: Conf. Ser. 312, 092002 (2011)

Which DFT?

$$\delta\langle \hat{H} - \lambda \hat{Q} \rangle = 0 \Longrightarrow E = E(Q)$$

$$\delta\langle \hat{H} - \sum_k \lambda_k \hat{Q}_k \rangle = 0 \Longrightarrow E = E(Q_k)$$

$$\delta\langle \hat{H} - \int \mathrm{d}q\, \lambda(q) \hat{Q}(q) \rangle = 0 \Longrightarrow E = E[Q(q)]$$

$$\delta\langle \hat{H} - \int \mathrm{d}\vec{r}\, \lambda(\vec{r}) \hat{\rho}(\vec{r}) \rangle = 0 \Longrightarrow E = E[\rho(\vec{r})]$$

$$\text{for} \quad \hat{\rho}(\vec{r}) = \sum_{i=1}^{A} \delta(\vec{r} - \vec{r}_i)$$

$$\delta\langle \hat{H} - \int\int \mathrm{d}\vec{r}\mathrm{d}\vec{r}\,' \lambda(\vec{r},\vec{r}\,') \hat{\rho}(\vec{r},\vec{r}\,') \rangle = 0 \Longrightarrow E = E[\rho(\vec{r},\vec{r}\,')]$$

J. D., J. Phys.: Conf. Ser. 312, 092002 (2011)

LDA vs. Generator functionals

$$E^{dir} = \int d^3r \, \mathcal{H}^{dir}(\rho(r), \tilde{\rho}(r))$$
$$E^{exc} = \int d^3r \, \mathcal{H}^{exc}(\rho(r), \tilde{\rho}(r))$$
$$E^{pair} = \int d^3r \, \mathcal{H}^{pair}(\rho(r), \tilde{\rho}(r))$$

$$E^{dir} = \int d^3r_1 d^3r_2 \, \rho(r_1) \, \mathcal{O}(r_1 - r_2) \, \rho(r_2)$$
$$E^{exc} = \int d^3r_1 d^3r_2 \, \rho(r_1, r_2) \, \mathcal{O}(r_1 - r_2) \, \rho(r_2, r_1)$$
$$E^{pair} = \int d^3r_1 d^3r_2 \, \tilde{\rho}(r_1) \, \mathcal{O}(r_1 - r_2) \, \tilde{\rho}(r_2)$$

	LDA	Generator
E	✚	✚
(Q)RPA, ATDHF(B)	✚	✚
AMP, PNP, GCM	✘	✚
1B spectroscopic observables	✚	✚
MB spectroscopic observables	✘	✚
Odd & odd-odd nuclei	✘	✚

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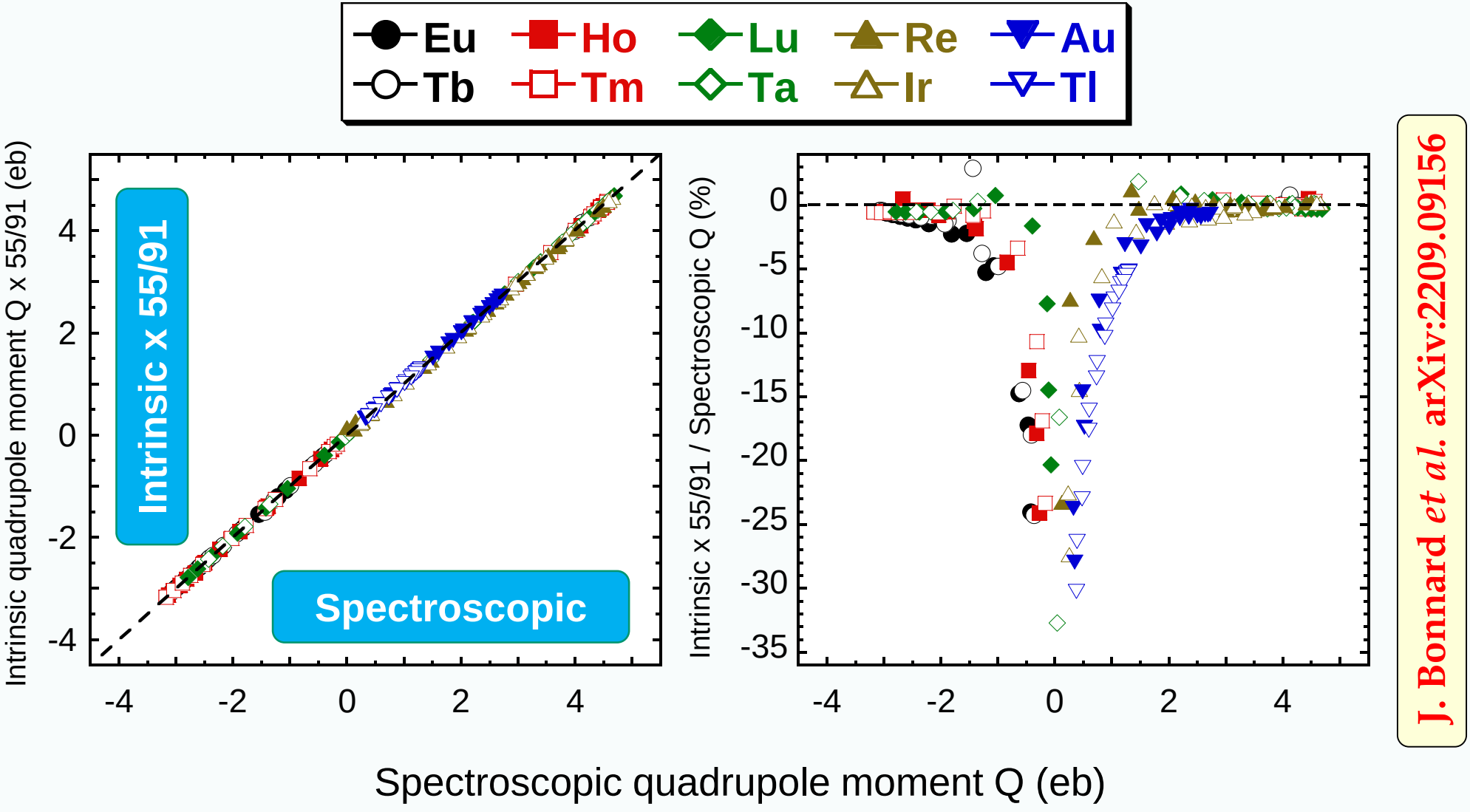
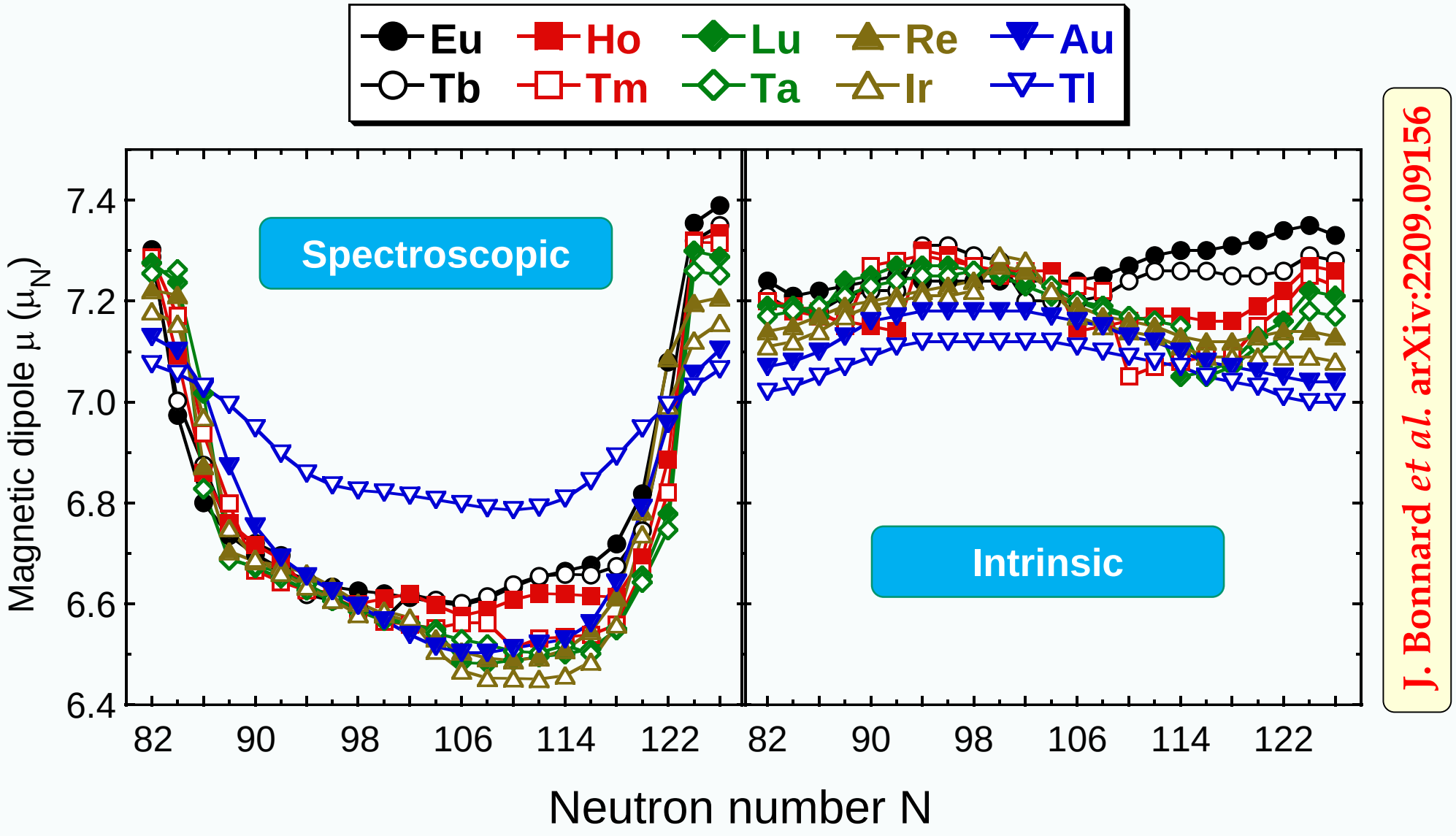
Heavy deformed π11/2⁻ odd-Z nuclei

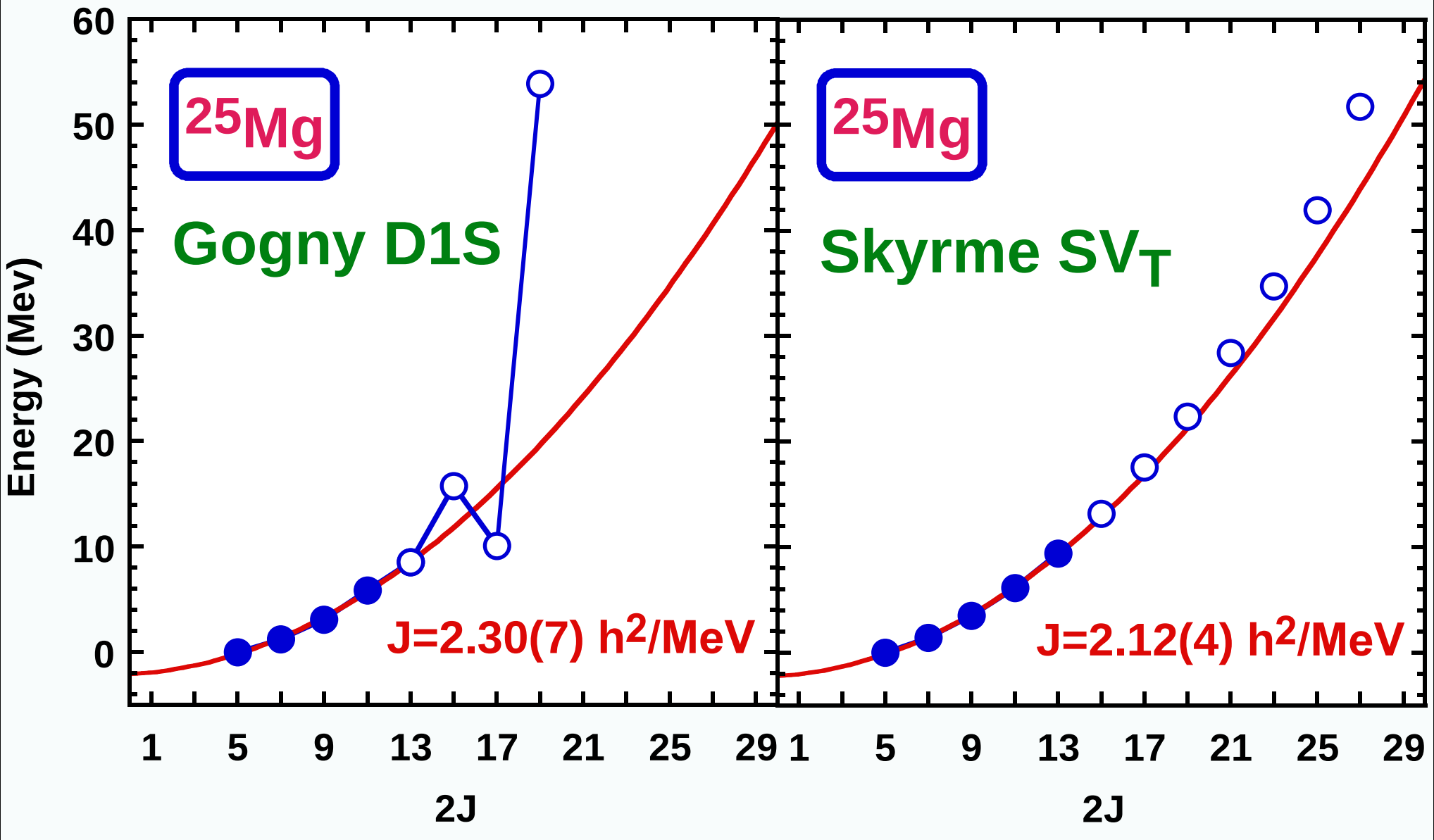


Heavy deformed π11/2⁻ odd-Z nuclei



J. Bonnard *et al.* arXiv:2209.09156

AMP rotational band



Ab-initio-derived Skyrme functional

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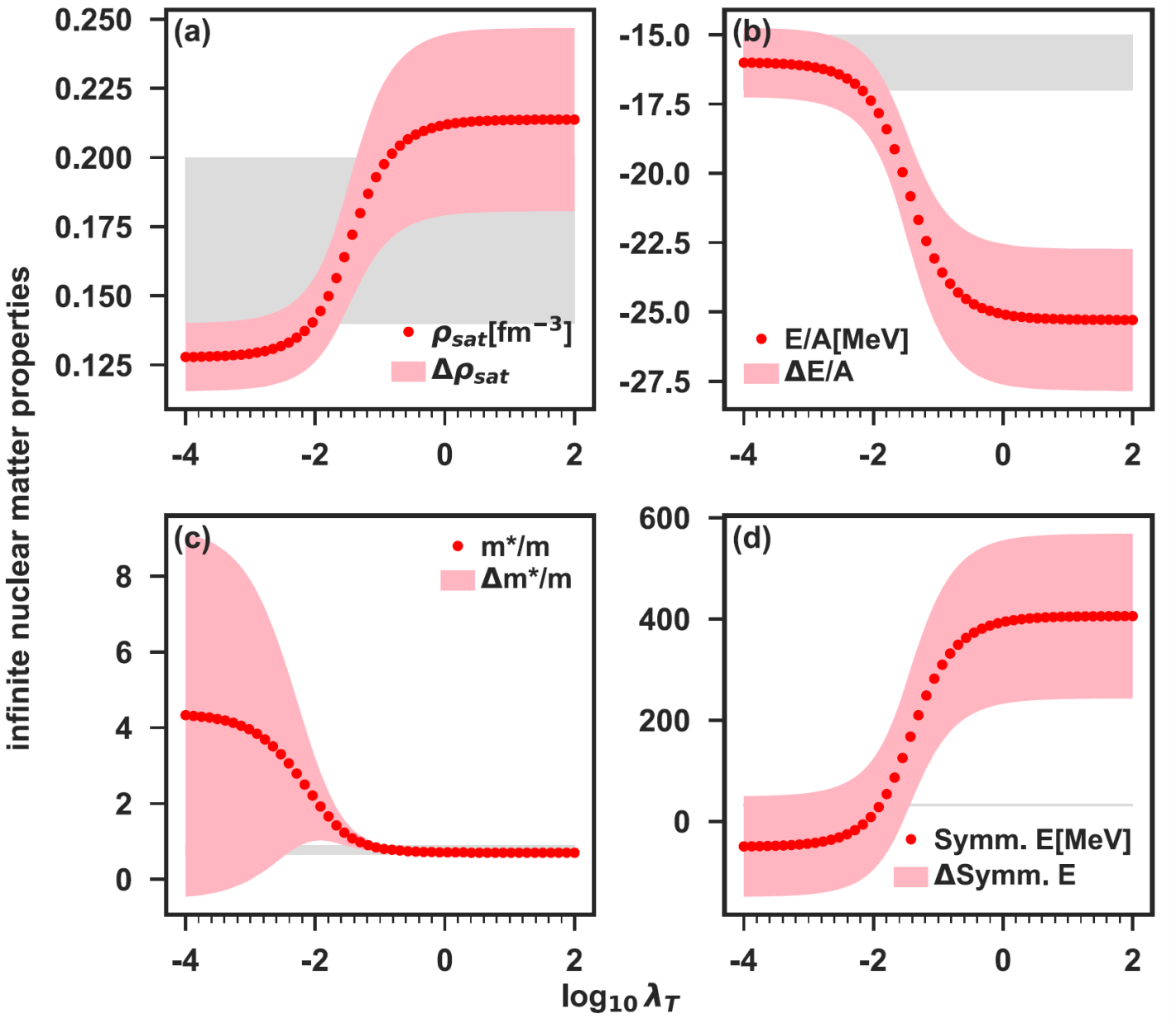
Ab-initio-derived Skyrme functional



G Salvioni *et al.* J. Phys. G: Nucl. Part. Phys. 47 (2020) 085107

Regularized finite-range pseudopotentials as functional generators

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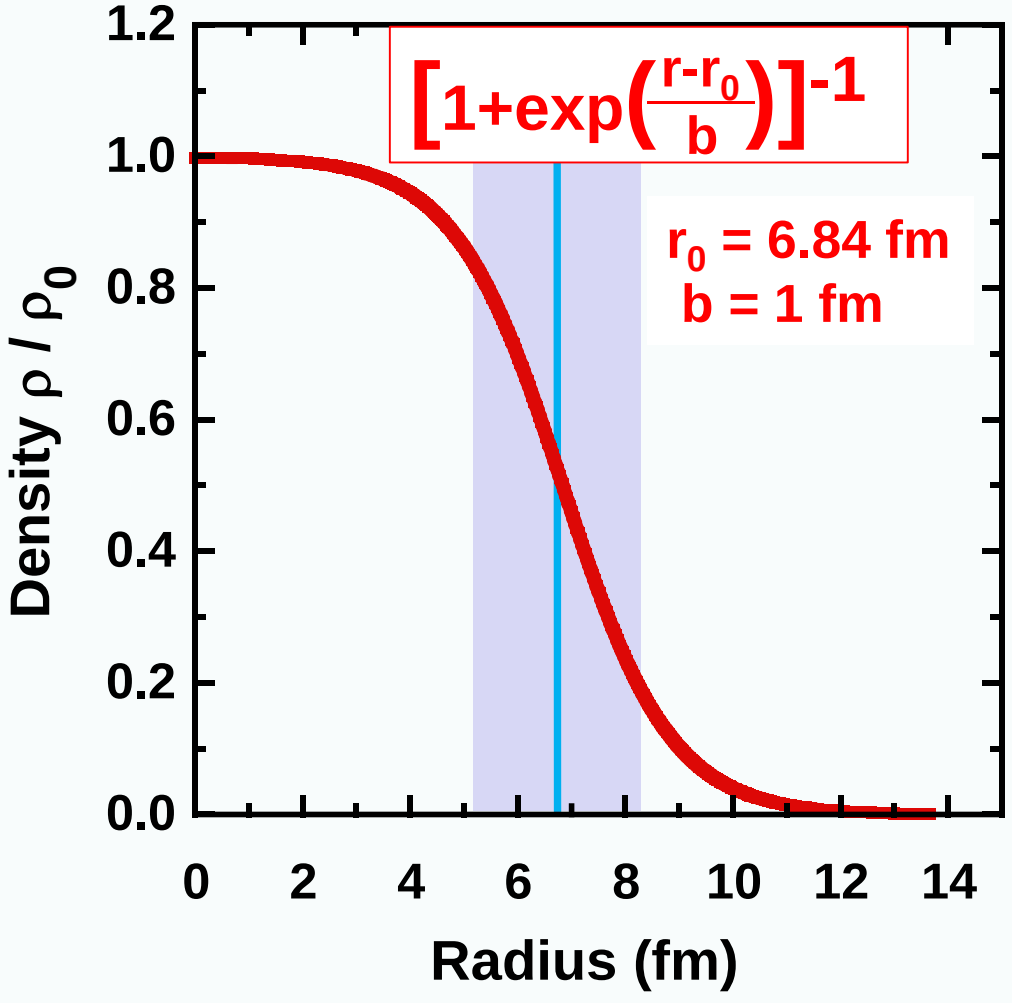
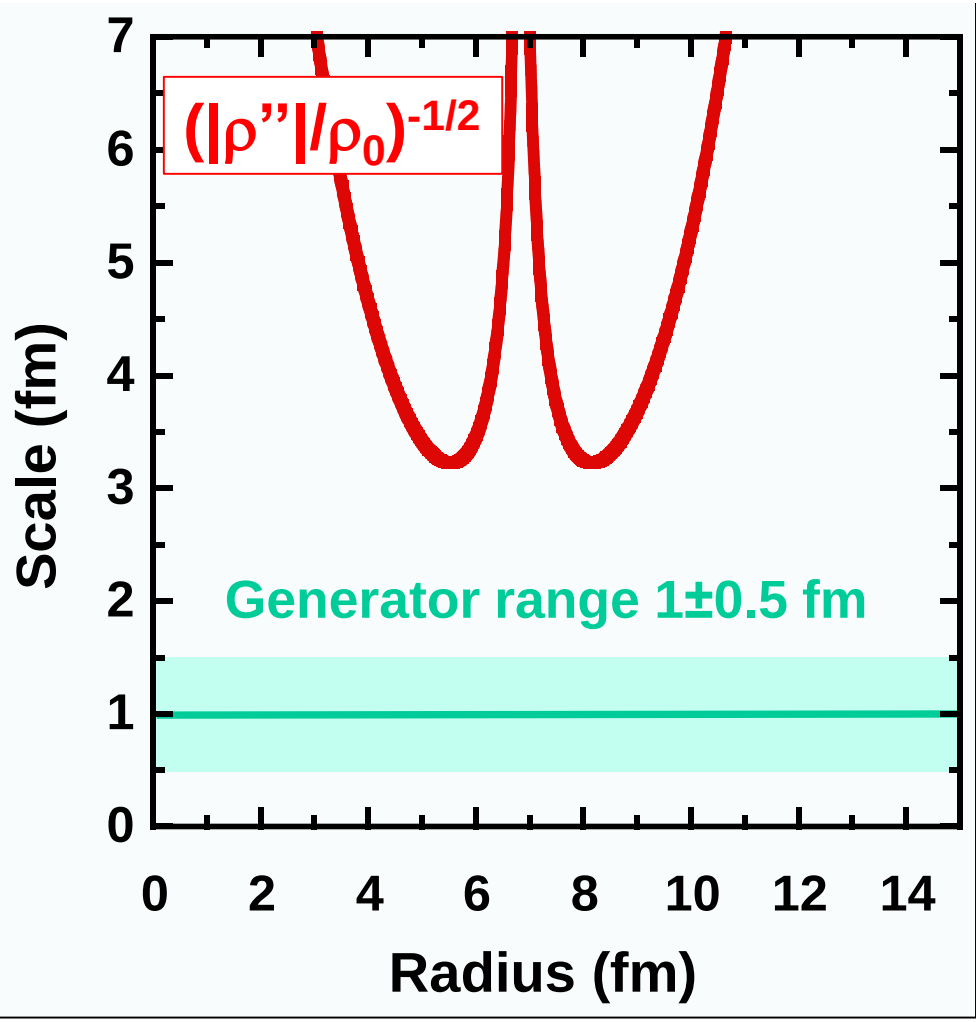
$$V^{dir}(\mathrm{r}_1) = \int \mathrm{d}^3\mathrm{r}_2\, \mathcal{O}(\mathrm{r}_1 - \mathrm{r}_2)\ \rho(\mathrm{r}_2) = \int \mathrm{d}^3\mathrm{r}\, \mathcal{O}(\mathrm{r})\ \rho(\mathrm{R}+\mathrm{r})$$
$$= \int \mathrm{d}^3\mathrm{r}\, \mathcal{O}(\mathrm{r})\Big(\rho(\mathrm{R}) + \tfrac{1}{2}\rho''(\mathrm{R})\mathrm{r}^2) + \ldots\Big) = \mathcal{O}_0\rho(\mathrm{R}) + \tfrac{1}{2}\mathcal{O}_2\rho''(\mathrm{R}) + \ldots$$





Regularized finite-range pseudopotentials

We regularize the zero-range delta interaction using the Gaussian function,

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

Then, the resulting central two-body regularized pseudopotential reads,

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

where $\vec{k} = \frac{1}{2i}(\vec{\nabla}_1 - \vec{\nabla}_2)$ and $\vec{k}' = \frac{1}{2i}(\vec{\nabla}'_1 - \vec{\nabla}'_2)$ are the standard relative-momentum operators, and the Wigner, Bartlett, Heisenberg, and Majorana terms are given by the standard spin and isospin exchange operators, $\hat{P}_1 \equiv 1$, $\hat{P}_2 \equiv \hat{P}_\sigma$, $\hat{P}_3 \equiv -\hat{P}_\tau$, $\hat{P}_4 \equiv -\hat{P}_\sigma\hat{P}_\tau$.

To give a specific example, up to the second-order, that is, up to the next-to-leading-order (NLO) expansion, operators $\hat{O}_i(\vec{k}\,',\vec{k})$ read

$$\hat{O}_i(\vec{k}\,',\vec{k}) = T_0^{(i)} + \frac{1}{2}T_1^{(i)}\left(\vec{k}'^{*2} + \vec{k}^2\right) + T_2^{(i)}\vec{k}'^{*}\cdot\vec{k},$$

where $T_k^{(i)}$ are the channel-dependent coupling constants.

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

Regularized finite-range pseudopotentials, the general case

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

$$\hat{O}_i(\vec{k}\,',\vec{k}) \;=\; \sum\nolimits_{nj} T_j^{(ni)}\hat{O}_j^{(n)}(\vec{k}\,',\vec{k})$$

Differential operators $\hat{O}_j^{(n)}(k',k)$ are scalar polynomial functions of two vectors, so owing to the Generalized Cayley-Hamilton theorem, they must be polynomials of three elementary scalars: k^2, k'^2, and $k'\cdot k$, or

$$\hat{T}_1 \;=\; \tfrac{1}{2}(k'^{*2}+k^2), \quad \hat{T}_2 = k'^{*}\cdot k, \quad \hat{T}_3 = \tfrac{1}{2}(k'^{*2}-k^2),$$

with the condition that only even powers of $\hat{T}_3$ can appear. In terms of $\hat{T}_1$, $\hat{T}_2$, and $\hat{T}_3$, we now can define the following differential operators:

$$\begin{aligned}
\text{LO:}\quad & \hat{O}_1^{(0)}(k',k) \;=\; \hat{1}, \\
\text{NLO:}\quad & \hat{O}_1^{(2)}(k',k) \;=\; \hat{T}_1, \quad \hat{O}_2^{(2)}(k',k) = \hat{T}_2, \\
\text{N2LO:}\quad & \hat{O}_1^{(4)}(k',k) \;=\; \hat{T}_1^2+\hat{T}_2^2, \quad \hat{O}_2^{(4)}(k',k) = 2\hat{T}_1\hat{T}_2, \\
& \hat{O}_3^{(4)}(k',k) \;=\; \hat{T}_1^2-\hat{T}_2^2, \quad \hat{O}_4^{(4)}(k',k) = \hat{T}_3^2.
\end{aligned}$$

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

Gogny-equivalent regularized N^{n}LO density functional

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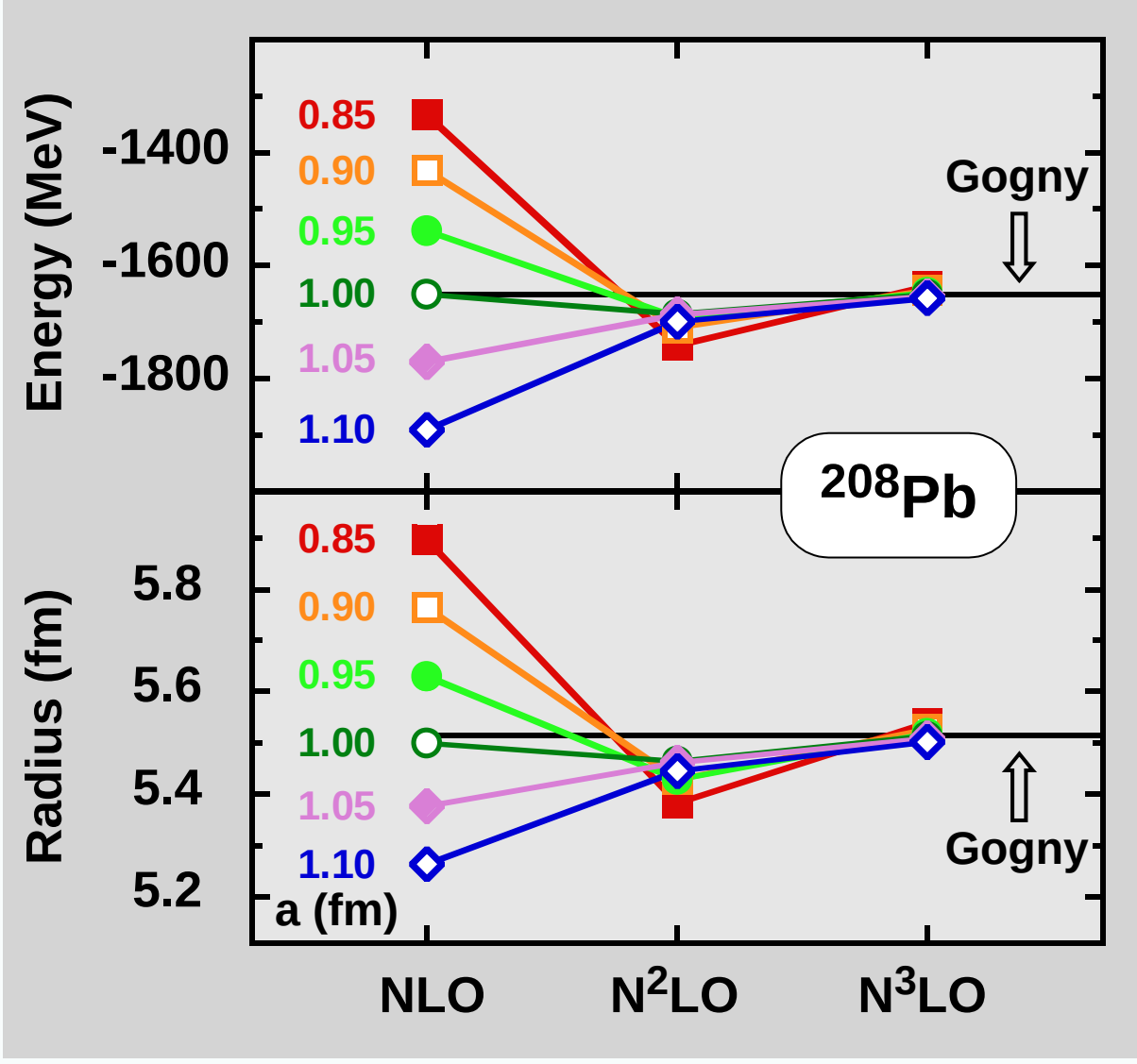
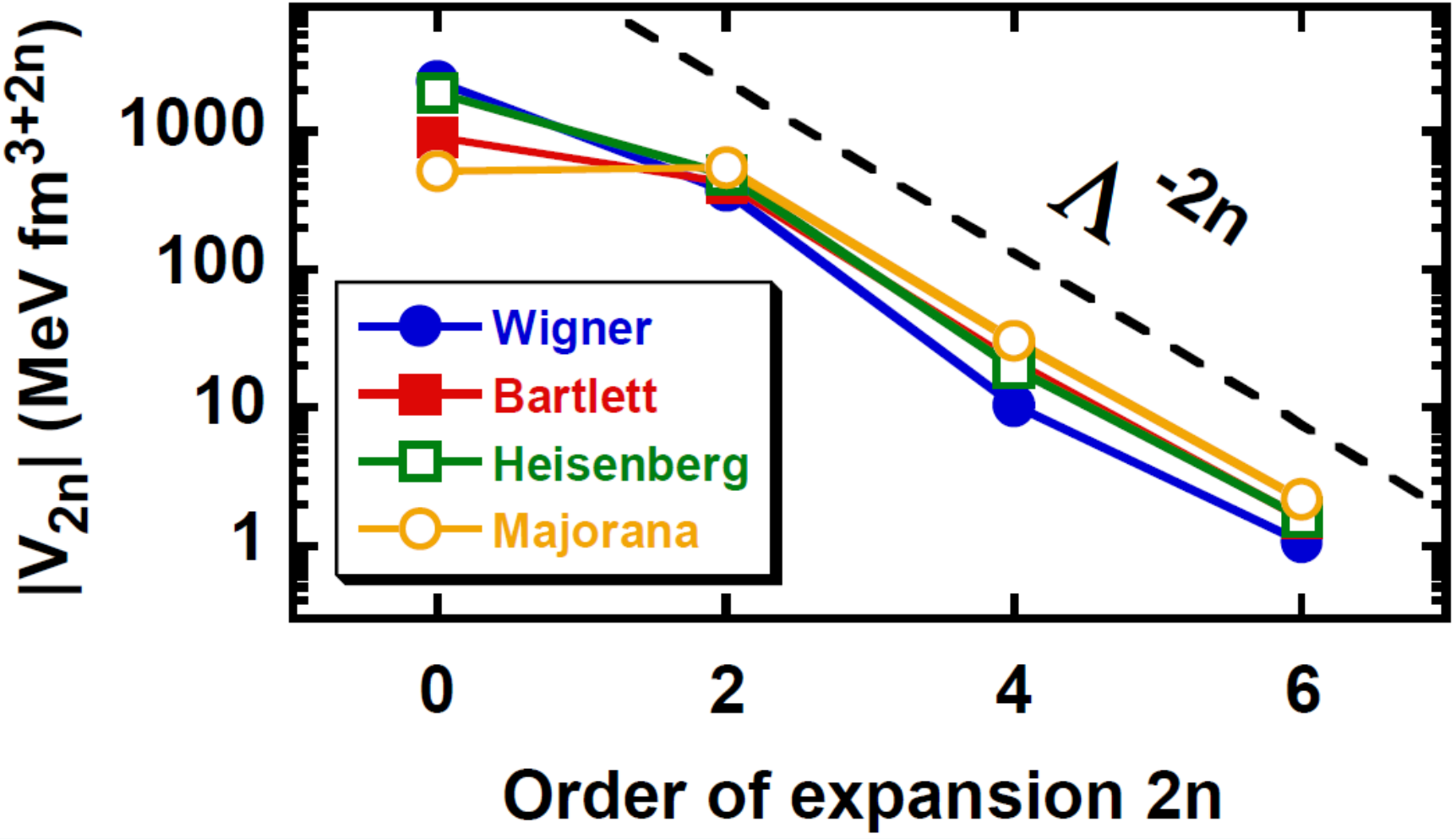
Regularized pseudopotentials vs. Gogny



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

Coupling constants of the regularized pseudopotentials

$\Lambda \approx 700$ MeV/$\eta c \approx 3.8$ fm^{-1}



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

Density-independent N²LO density functional with pairing

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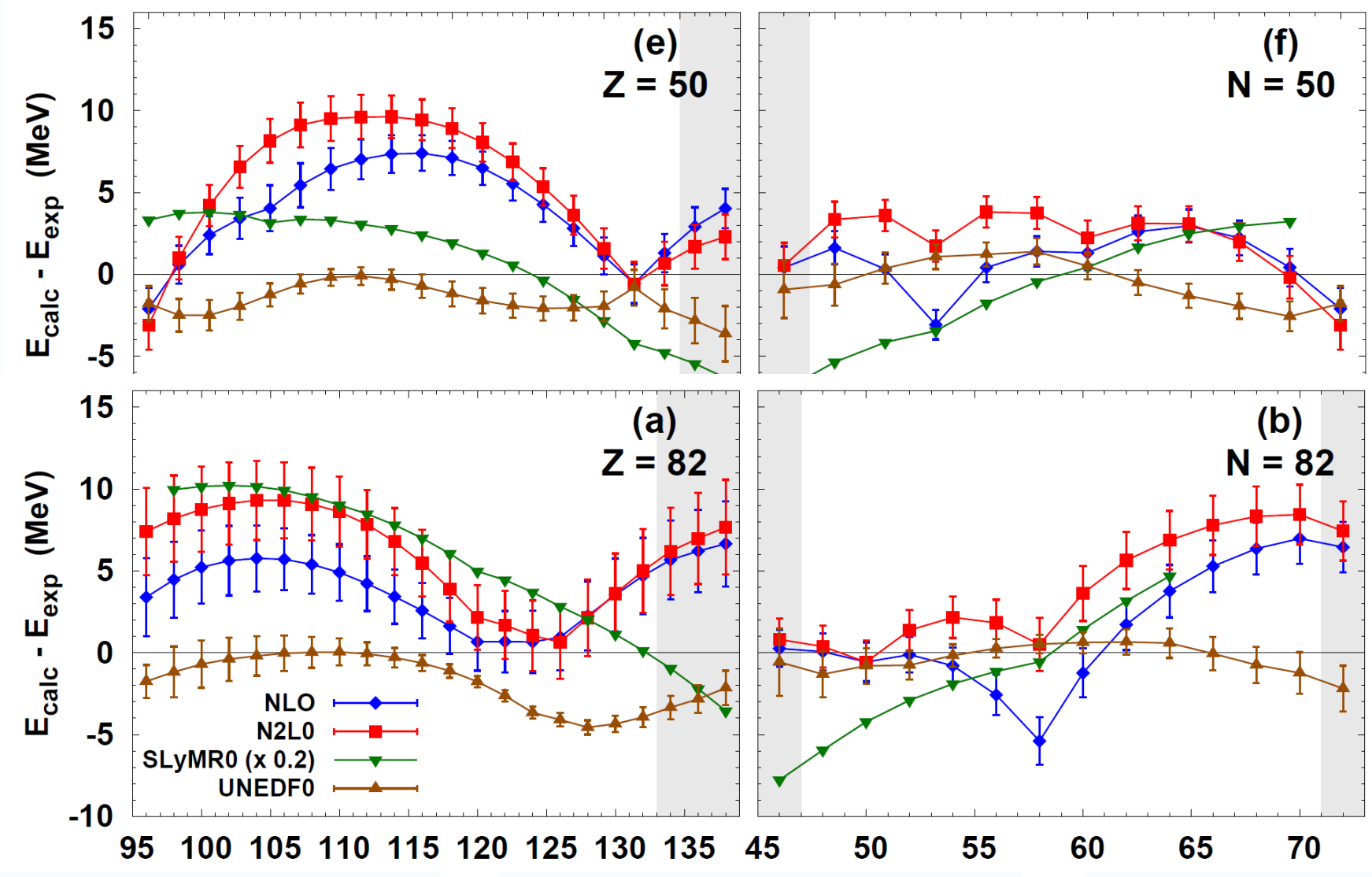
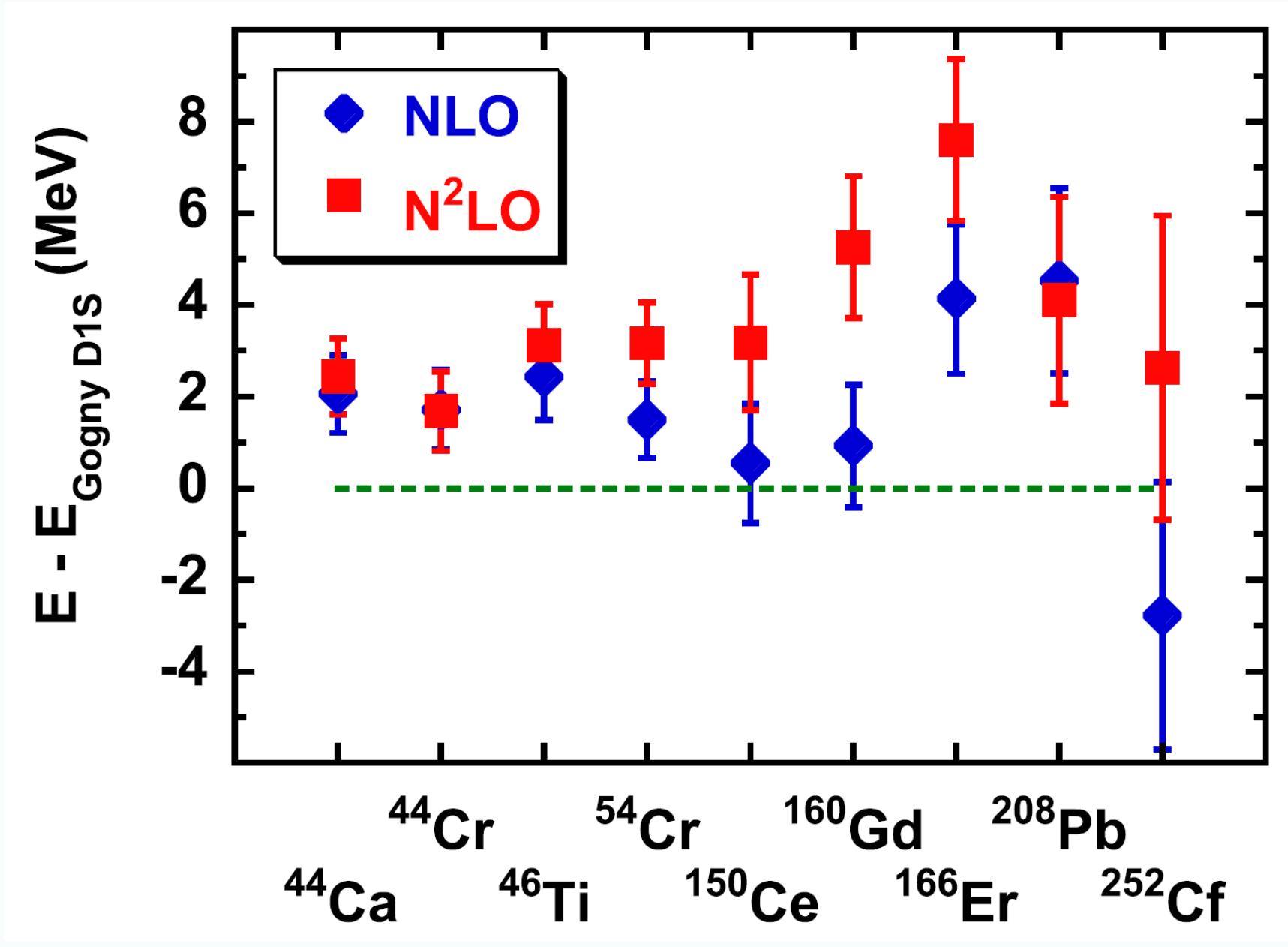
Ground-state energies at a = 1.15 fm



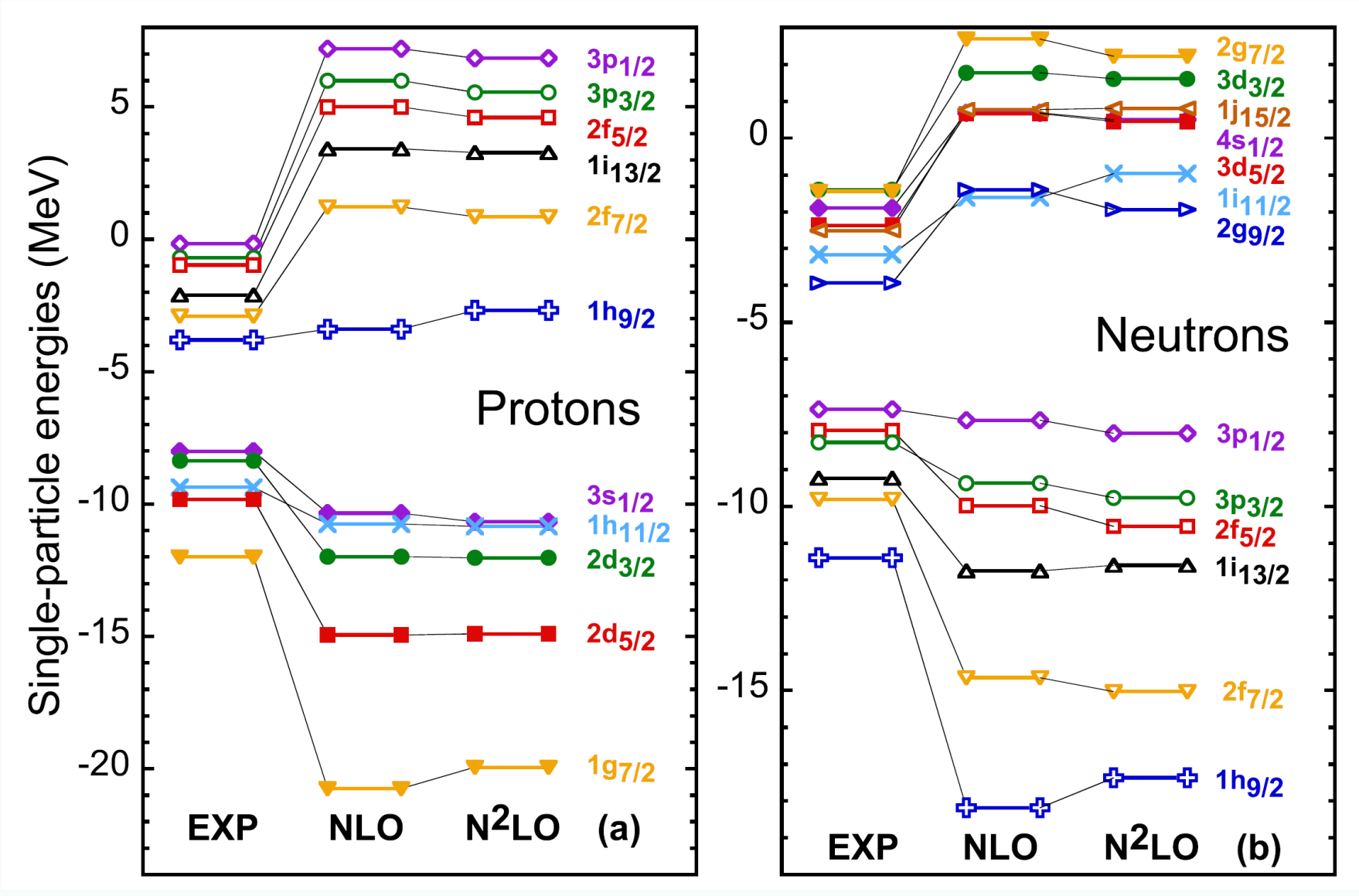
K. Bennaceur et al., arXiv:1701.08062

Ground-state energies at a = 1.15 fm



K. Bennaceur *et al.*, J. Phys. G: Nucl. Part. Phys. 44 (2017) 045106

Single-particle energies in ^{208}Pb



K. Bennaceur *et al.*, J. Phys. G: Nucl. Part. Phys. 44 (2017) 045106

Density-dependent N^{3}LO density functional with pairing

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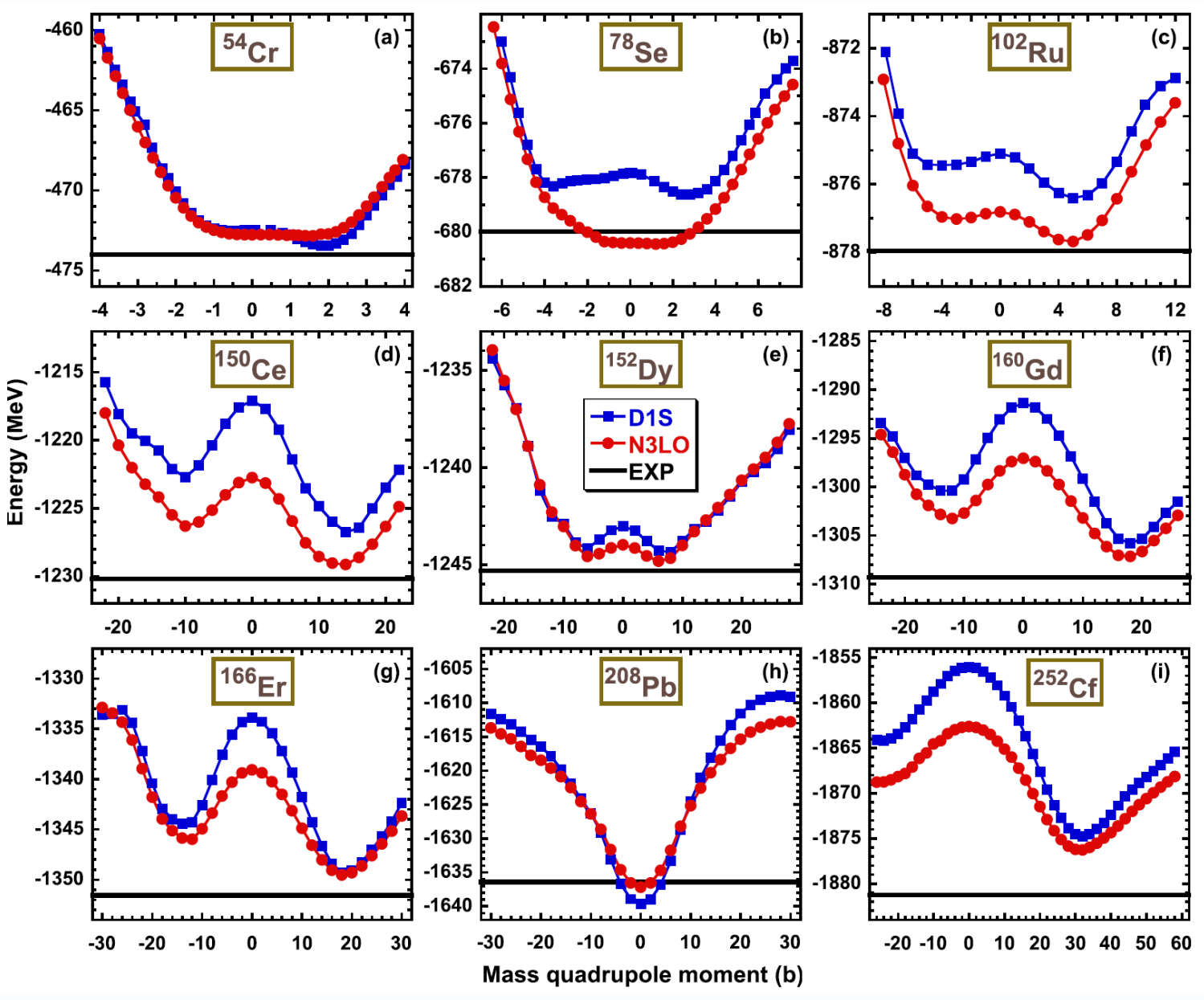
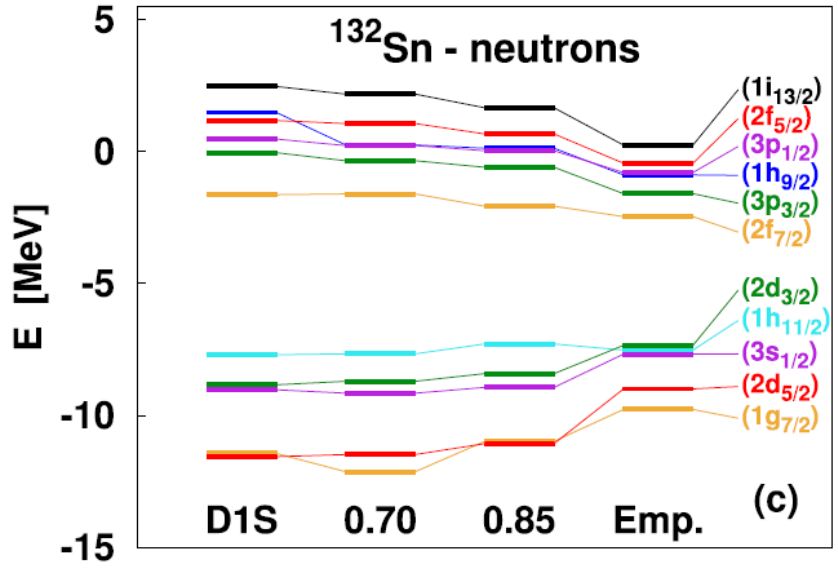
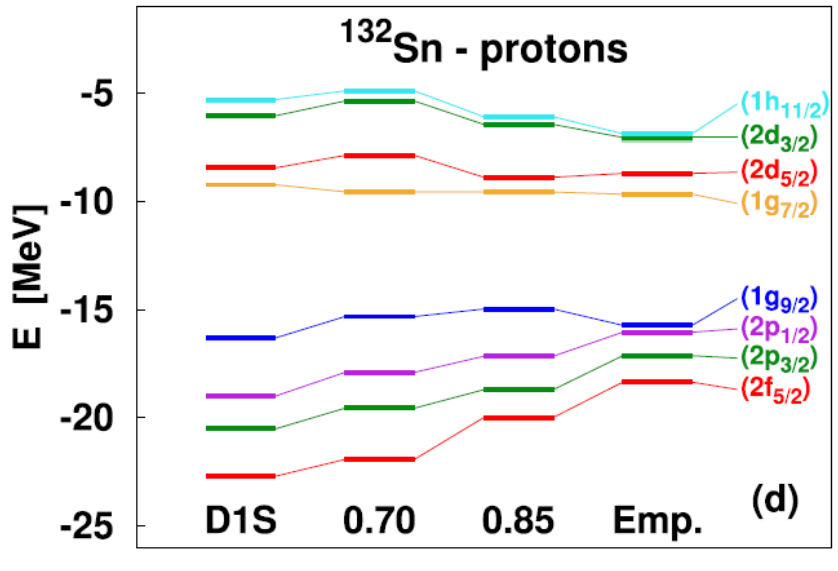
Deformation energies at m*/m = 0.85

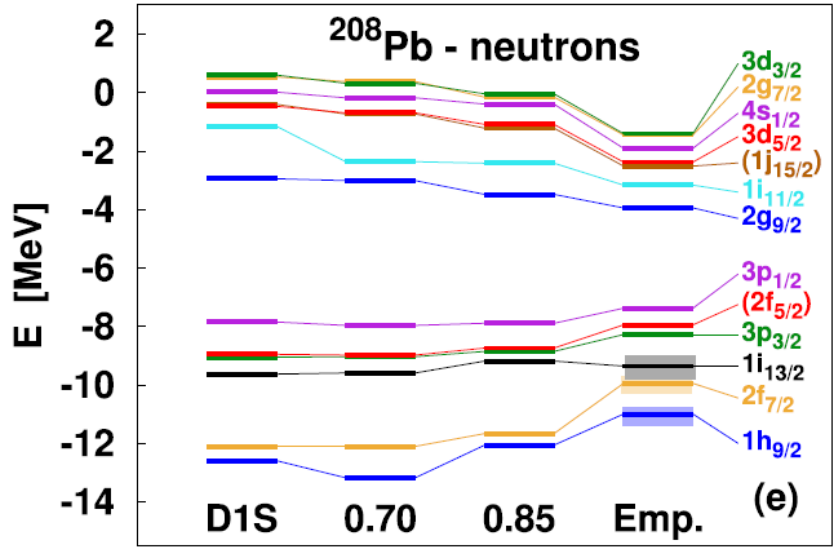


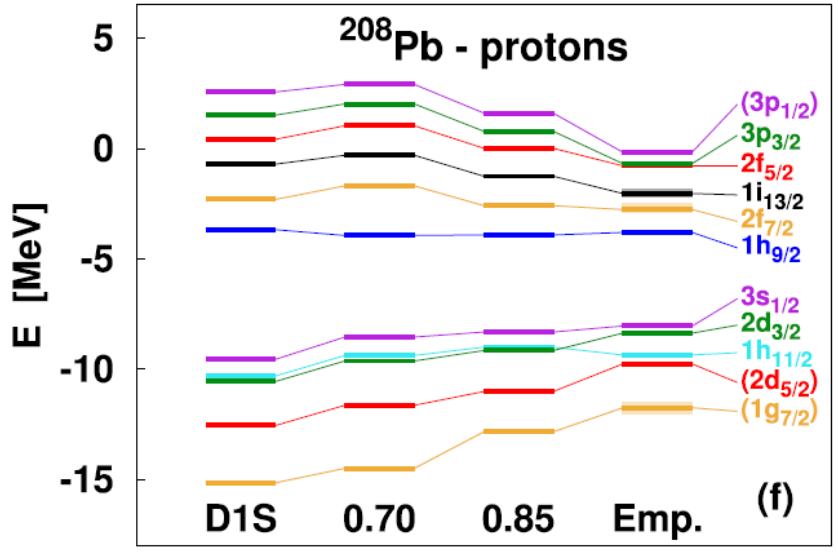
K. Bennaceur *et al.*, J. Phys. G: Nucl. Part. Phys. 47 (2020) 105101

Single-particle energies at m*/m = 0.70 & 0.85









K. Bennaceur *et al.*, J. Phys. G: Nucl. Part. Phys. 47 (2020) 105101

Conclusions

1. Nuclear density functionals are presently used in two forms:
   - Local-Density-Approximation (LDA) form does not allow for meaningful symmetry-restoration or multi-reference applications..
   - Generator-based form does.
   - In practice, hybrid forms are used.
2. Most current ab initio derivations of nuclear density functionals lead to an LDA form.
3. The separation of scales between the variability of density and range of the generators allows us to apply the ideas of effective theory to nuclear DFT.
4. A series of regularized higher-order pseudopotentials realises the effective-theory expansion..
5. Three-body generators are mandatory, see Bennaceur's talk on semi-contact interaction.

Thank you

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