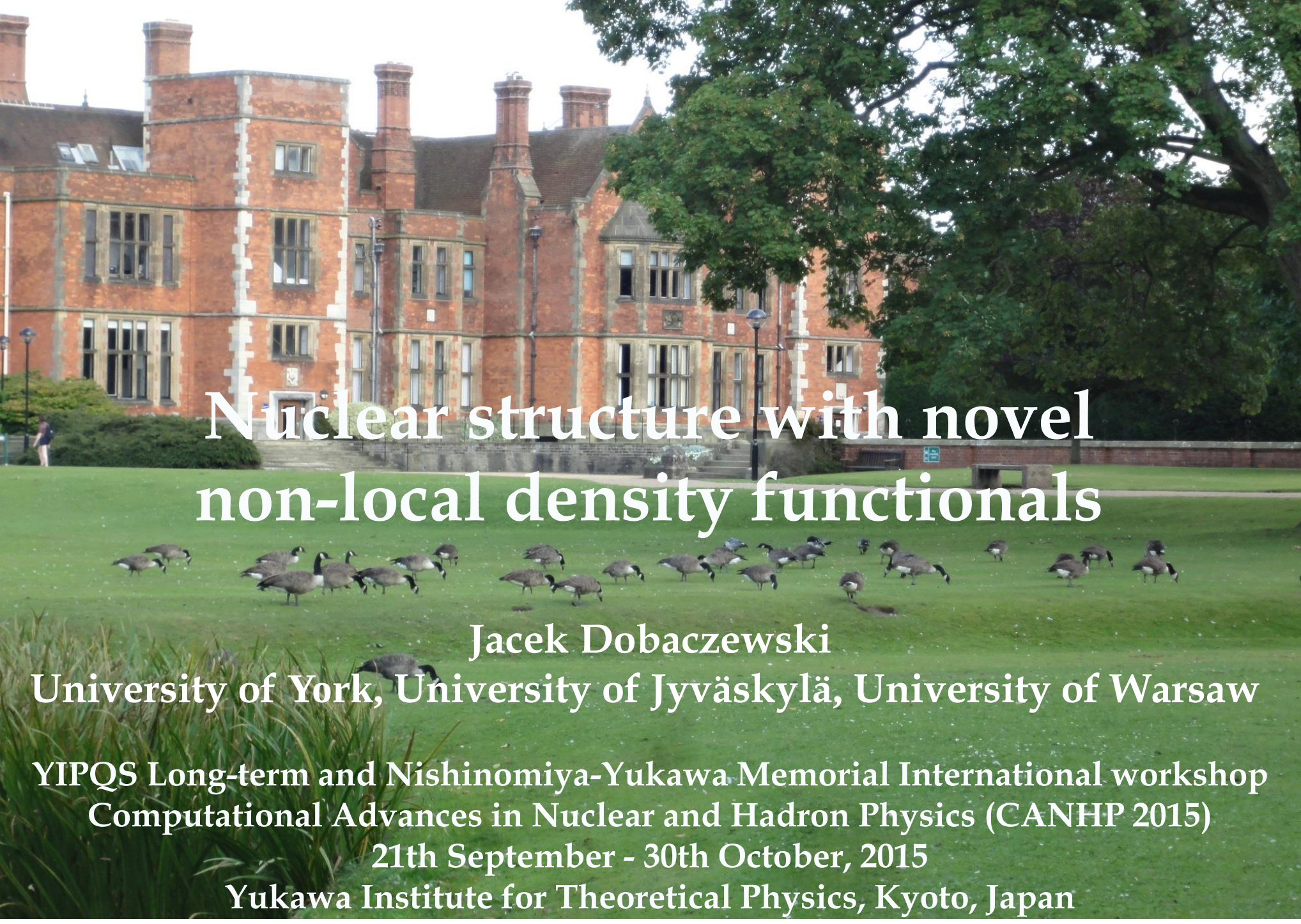


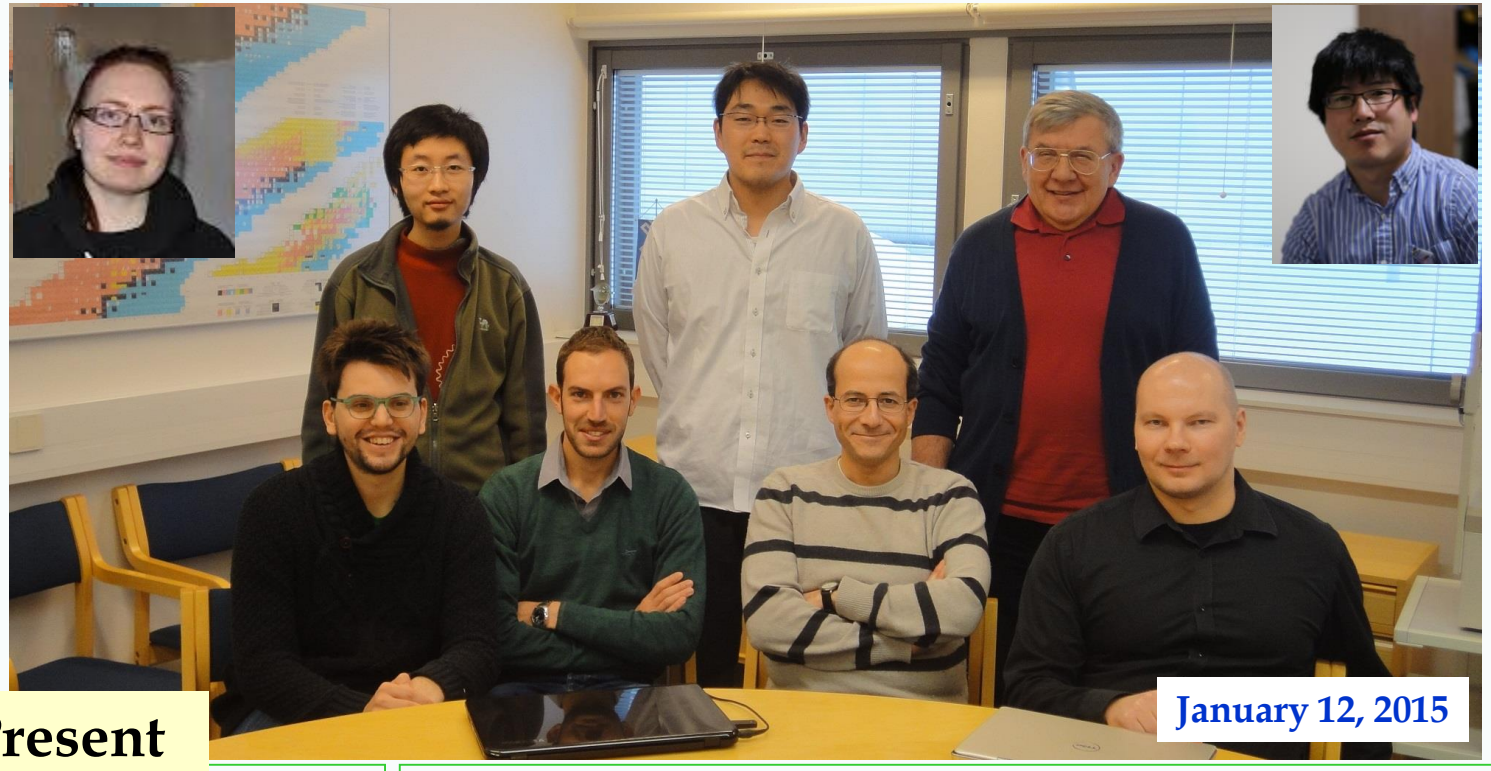
Nuclear structure with novel non-local density functionals

Jacek Dobaczewski

University of York, University of Jyväskylä, University of Warsaw

YIPQS Long-term and Nishinomiya-Yukawa Memorial International workshop
Computational Advances in Nuclear and Hadron Physics (CANHP 2015)
21th September - 30th October, 2015
Yukawa Institute for Theoretical Physics, Kyoto, Japan

FIDIPRO project 2007-2017



January 12, 2015

Present

Karim Bennaceur
Yuan Gao
Tiia Haverinen
Andrea Idini
Markus Kortelainen
Tomohiro Oishi
Gianluca Salvioni
Yue Shi

Past

Jussi Toivanen
Kazuhito Mizuyama
Gillis Carlsson
Rayner Rodriguez-Guzman
Marcin Borucki
Pekka Toivanen
Francesco Raimondi
Alessandro Pastore
Nicolas Michel
Petr Veselý
Yue Shi
Vaia Prassa
Xiaobao Wang
Lingfei Yu
Maciej Konieczka

Outline

1. Introduction: nuclear EDF
2. Precision frontier
3. Novel nuclear EDFs
4. *Ab initio* derivation of model EDFs
5. Conclusions

Nuclear energy density functionals

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,

$$V(\vec{r}_1-\vec{r}_2) = \sum\nolimits_{i=1,2} e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_i^2} \times (W_i + B_iP_\sigma - H_iP_\tau - M_iP_\sigma P_\tau)$$
$$+t_3(1+P_\sigma)\delta(\vec{r}_1-\vec{r}_2)\rho^{1/3}\left[\tfrac{1}{2}(\vec{r}_1+\vec{r}_2)\right].$$

$P_\sigma=\frac{1}{2}(1+\vec{\sigma}_1\cdot\vec{\sigma}_2)$ 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*

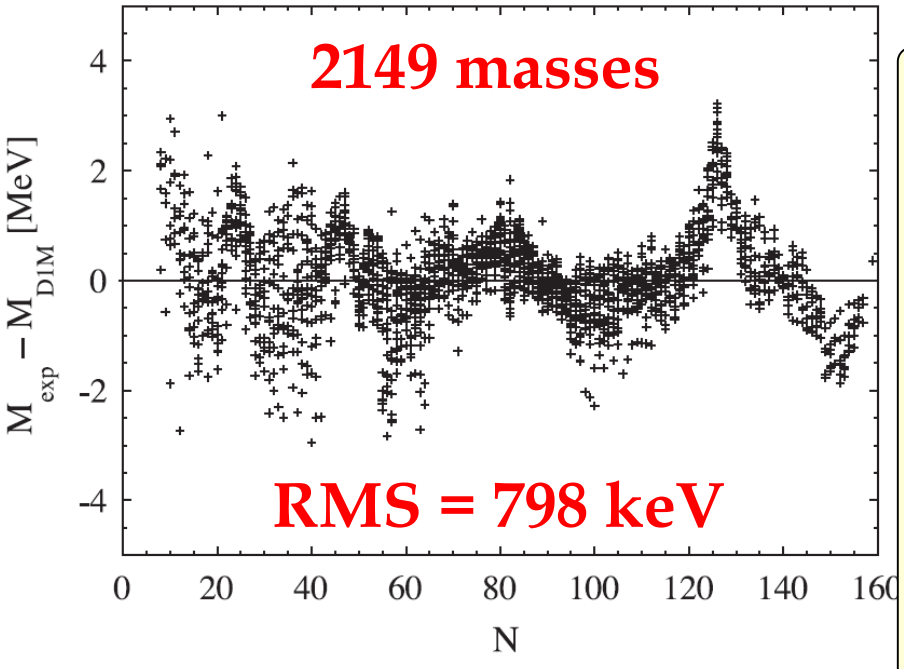
$$V(\vec{r}_1\vec{r}_2;\vec{r}\,'_1\vec{r}\,'_2) = \Big\{t_0(1+x_0P^\sigma) + \tfrac{1}{6}t_3(1+x_3P^\sigma)\rho^\alpha\left(\tfrac{1}{2}(\vec{r}_1+\vec{r}_2)\right)$$
$$+\tfrac{1}{2}t_1(1+x_1P^\sigma)[\vec{k}'^{*2}+\vec{k}^2] + t_2(1+x_2P^\sigma)\vec{k}'^{*}\cdot\vec{k}\Big\}\,\delta(\vec{r}_1-\vec{r}\,'_1)\delta(\vec{r}_2-\vec{r}\,'_2)\delta(\vec{r}_1-\vec{r}_2),$$

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.

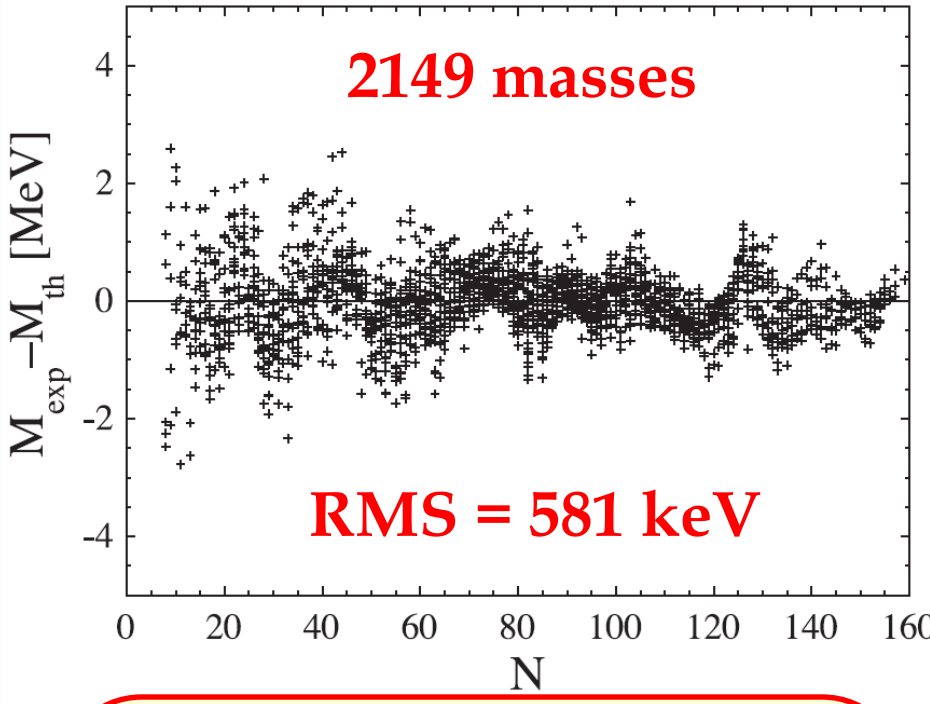
Precision frontier

Nuclear binding energies (masses)



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

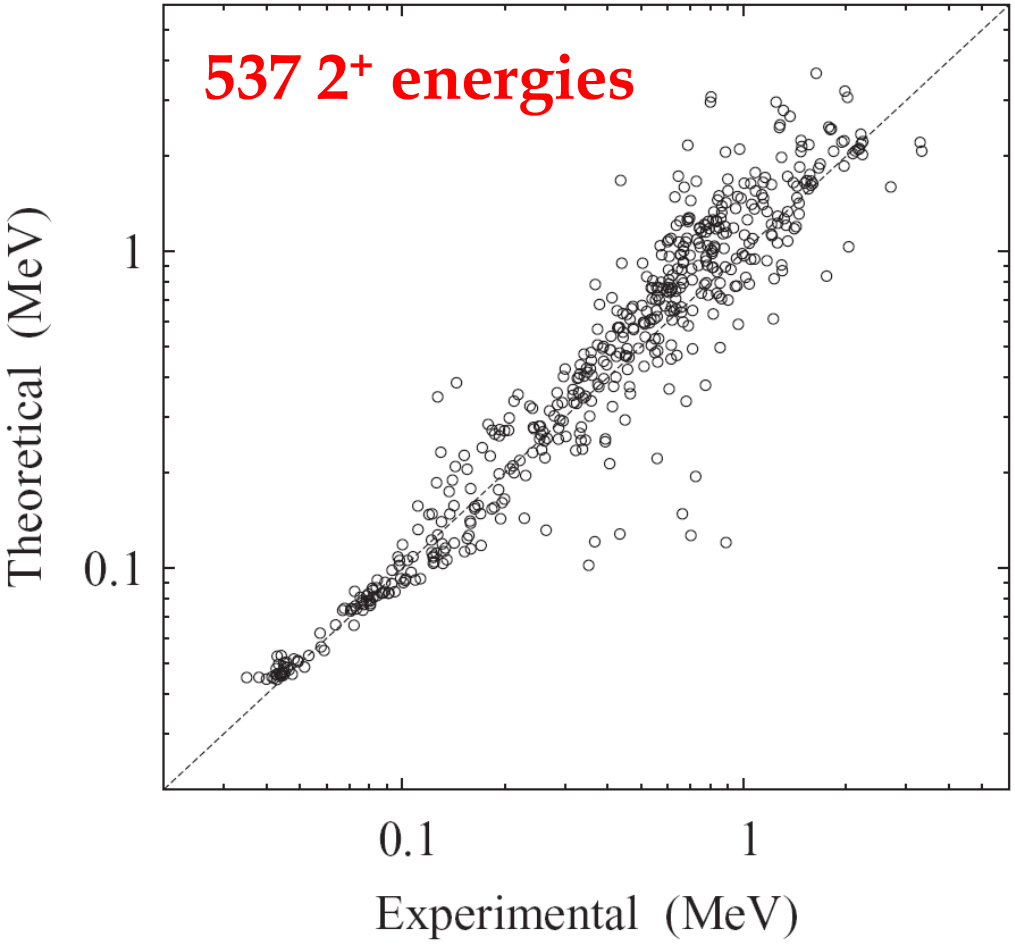
The first Gogny HFB mass model. An explicit and self-consistent account of all the quadrupole correlation energies are included within the 5D collective Hamiltonian approach.



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

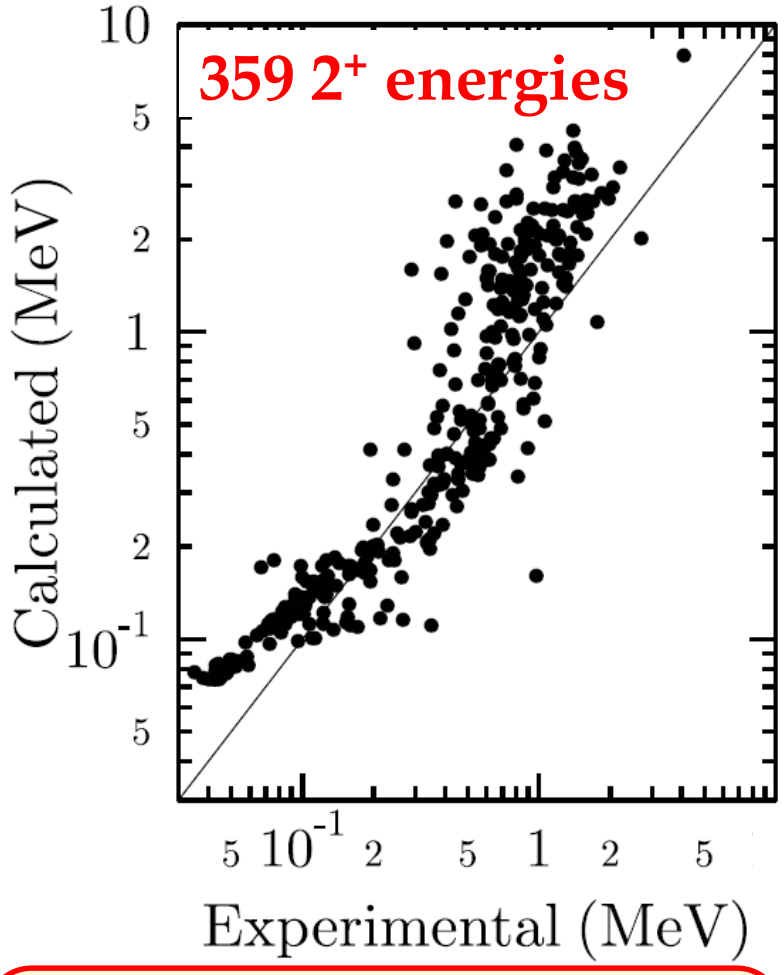
The new Skyrme HFB nuclear-mass model, in which the contact-pairing force is constructed from microscopic pairing gaps of symmetric nuclear matter and neutron matter.

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.



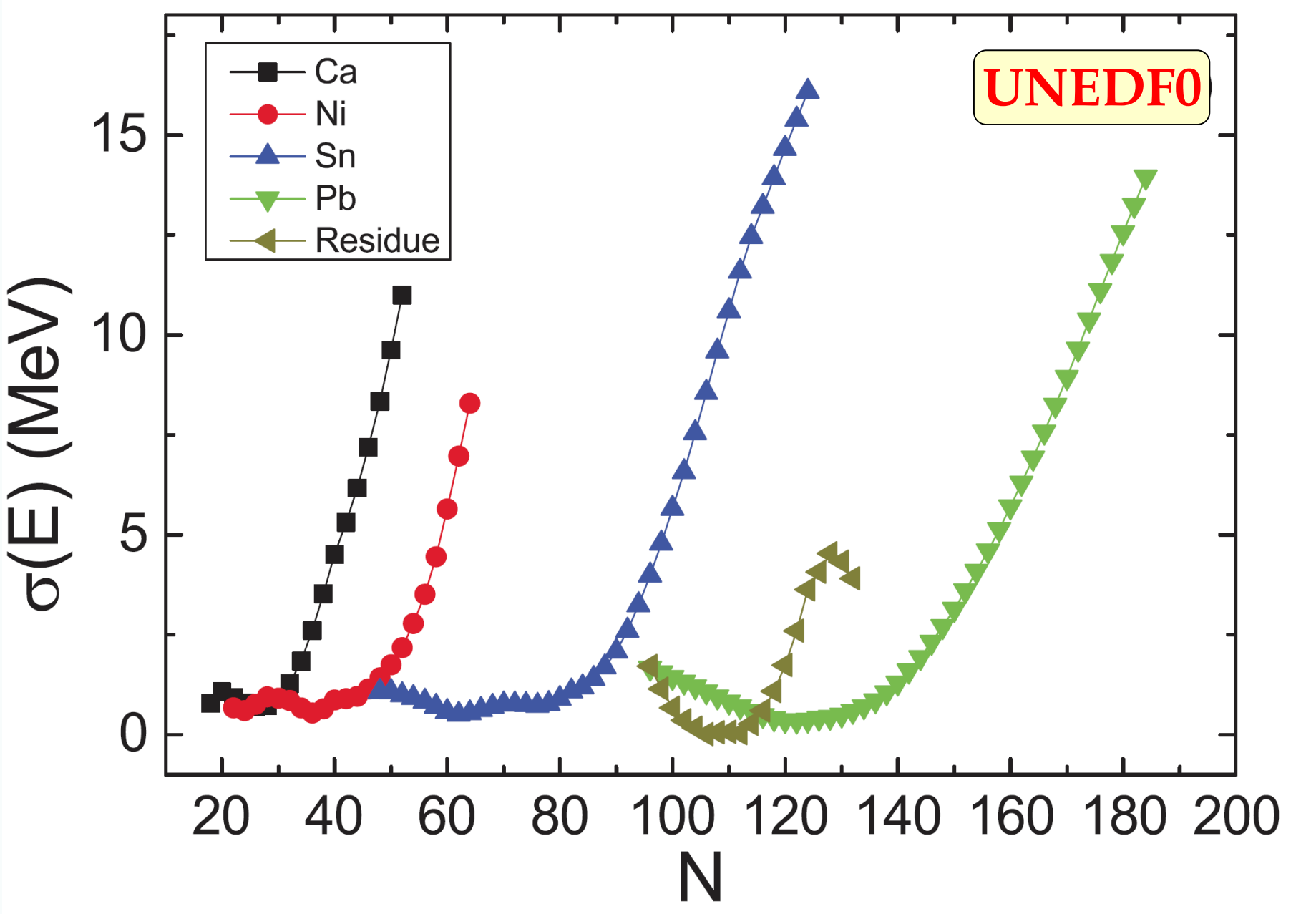
B. Sabbey *et al.*, Phys. Rev. C75, 044305 (2007)

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

1) **"Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful"**
G.E.P. Box and N.R. Draper
Empirical Model Building and Response Surfaces
(John Wiley & Sons, New York, 1987)

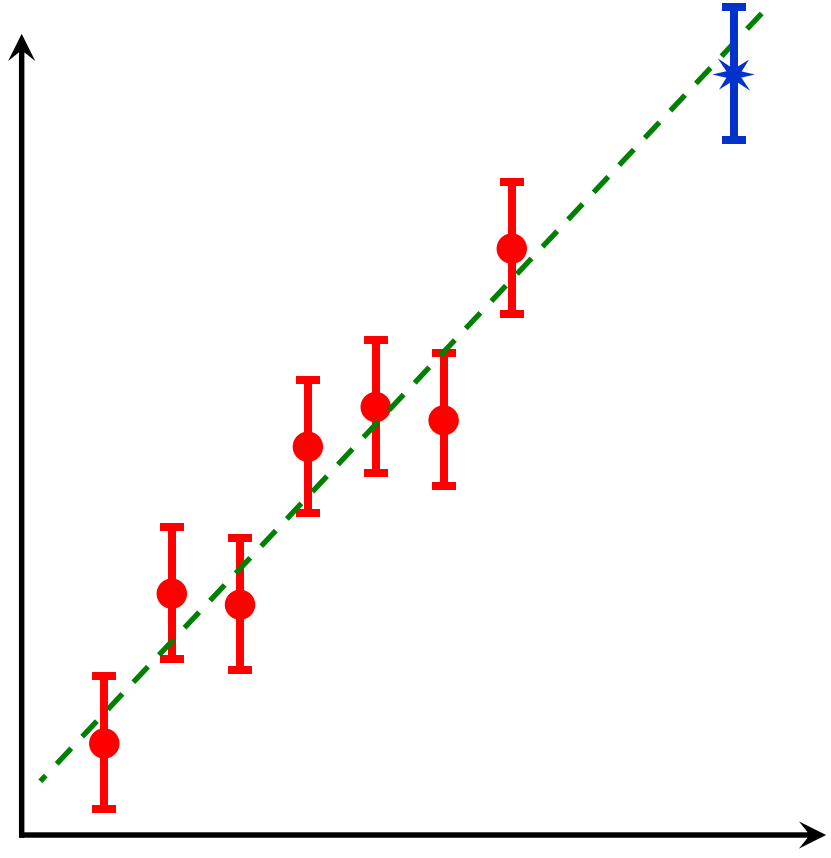
- **Error Estimates of Theoretical Models: a Guide:**
  J. Dobaczewski, W. Nazarewicz, P.-G. Reinhard,
  J. Phys. G: Nucl. Part. Phys. 41 (2014) 074001
- **Enhancing the interaction between nuclear experiment and theory through information and statistics**
  D.G. Ireland and W. Nazarewicz
  J. Phys. G: Nucl. Part. Phys. 42 (2015) 030301

Propagation of uncertainties

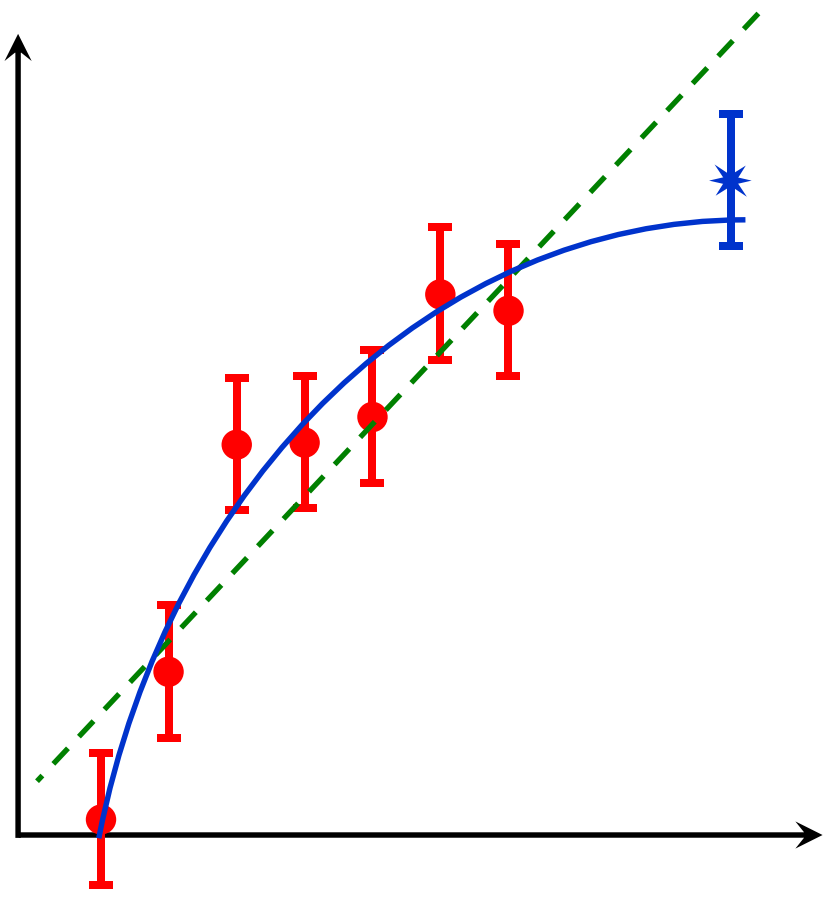


Y. Gao, *et al.*, Phys. Rev C 87, 034324 (2013)

Exact model



Inaccurate model



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

Exact model

Novel nuclear EDFs and higher-order gradients

Pseudopotentials, the terminology

Proc. Rehovoth Conf. Nucl. Structure

1957

SHORT CONTRIBUTION

A NUCLEAR PSEUDO-POTENTIAL

BY

T. H. R. SKYRME

Atomic Energy Research Establishment, Harwell, Didcot, Berks.

In the course of some work on problems of collective motion we have needed some expression for the effective internucleon potential (to be used in calculations of the shell-model type) which would (i) reproduce roughly the observed sizes and binding energies of nuclei. (ii) lead to a reasonable system of low-lying levels, and (iii) be simple enough to use in calculations with deformed oscillator wave-functions.

Pseudopotentials, a primer

Pseudopotentials in the one-body LOCAL Schrödinger equation:

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V_0(\vec{r}) + \vec{V}_1(\vec{r})\cdot\vec{\nabla} - \vec{\nabla}\cdot\vec{V}_1(\vec{r}) + V_2(\vec{r})\Delta + \Delta V_2(\vec{r})$$

can be EQUIVALENT or NON-EQUIVALENT to potentials, for example:

$$\vec{V}_1(\vec{r})\cdot\vec{\nabla} - \vec{\nabla}\cdot\vec{V}_1(\vec{r}) \equiv -\Big(\vec{\nabla}\cdot\vec{V}_1\Big)(\vec{r}).$$

Pseudopotentials in the one-body NONLOCAL Schrödinger equation, e.g.,

$$(\hat{V}\psi)(\vec{r}) = \int \mathrm{d}^3\vec{r}\,' V(\vec{r},\vec{r}\,')\Delta'\psi(\vec{r}\,') = \int \mathrm{d}^3\vec{r}\,'\Big(\Delta' V(\vec{r},\vec{r}\,')\Big)\psi(\vec{r}\,')$$

are ALWAYS EQUIVALENT to potentials. This freedom can be used to represent in terms of derivatives the nonlocality of the potential, namely,

$$V(\vec{r},\vec{r}\,') \equiv V(\vec{R},\vec{\eta}) = \int \mathrm{d}^3\vec{k}\,\exp(i\vec{k}\cdot\vec{\eta})V(\vec{R},\vec{k}),$$

which for the Taylor expansion in $\vec{k}$, $V(\vec{R},\vec{k}) = \sum_n \frac{\vec{k}^n}{n!}V_n(\vec{R})$, gives:

$$V(\vec{r},\vec{r}\,') = \sum_n V_n(\vec{R})\frac{(-i\vec{\nabla}_\eta)^n}{n!}\int \mathrm{d}^3\vec{k}\,\exp(i\vec{k}\cdot\vec{\eta}) = \sum_n V_n(\vec{R})\frac{(\hat{\vec{k}})^n}{n!}\delta(\vec{r}-\vec{r}\,').$$

Zero-range pseudopotentials

In the central-like form, the pseudopotential is a sum of terms,

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

Each term in the sum is accompanied by the corresponding strength parameter $C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}$, and explicitly reads,

$$\begin{aligned}\hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S} = \quad & \tfrac{1}{2} i^{v_{12}} \left(\left[\left[K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}} \right]_S \hat{S}_{v_{12}S} \right]_0 + (-1)^{v_{12}+S} \left[\left[K'_{\tilde{n}\tilde{L}} K_{\tilde{n}'\tilde{L}'} \right]_S \hat{S}_{v_{12}S} \right]_0 \right) \\ & \times \left(1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau \right) \hat{\delta}_{12}(r'_1 r'_2; r_1 r_2).\end{aligned}$$

$K_{\tilde{n}\tilde{L}}$ are the spherical tensor derivatives of order $\tilde{n}$ and rank $\tilde{L}$ are built of $k = (\nabla_1 - \nabla_2)/2i$, The two-body spin operators $\hat{S}_{v_{12}S}$ are defined as,

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

where $v_{12} = v_1 + v_2$ and $\sigma^{(i)}_{v\mu}$ are the spherical-tensor components of the rank-v Pauli matrices. The Dirac delta function,

$$\hat{\delta}_{12}(\vec{r}'_1 \vec{r}'_2, \vec{r}_1 \vec{r}_2) = \delta(\vec{r}'_1 - \vec{r}_1)\delta(\vec{r}'_2 - \vec{r}_2)\delta(\vec{r}_1 - \vec{r}_2),$$

ensures the locality and zero-range character of the pseudopotential.

F. Raimondi *et al.*, Phys. Rev. C 83, 054311 (2011)

Quasilocal EDF up to N^{3}LO

Local (primary) densities are defined by four quantum numbers $nLvJ$ as

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

where the nth-order and rank-L relative derivative operators K_{nL} act on the scalar ($v=0$) or vector ($v=1$) isoscalar ($t=0$) or isovector ($t=1$) nonlocal densities.

We act on each of the local primary densities with mth-order and rank-I derivative operator D_{mI}, and then couple ranks I and J to the total rank J', which gives the local secondary densities, $\left[D_{mI}\rho^t_{nLvJ}(\vec{r})\right]_{J'}$. From primary and secondary densities we build terms of the EDF:

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

Then, the total energy density reads

$$\mathcal{H}(\vec{r}) = \sum_{\substack{n'L'v'J',t \\ mI,nLvJ,J'}} C^{n'L'v'J',t}_{mI,nLvJ}\, T^{n'L'v'J',t}_{mI,nLvJ}(\vec{r}),$$

where $C^{n'L'v'J',t}_{mI,nLvJ}$ are coupling constants and the summation again runs over all allowed indices.

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

Two-body N^{3}LO zero range, density dependent

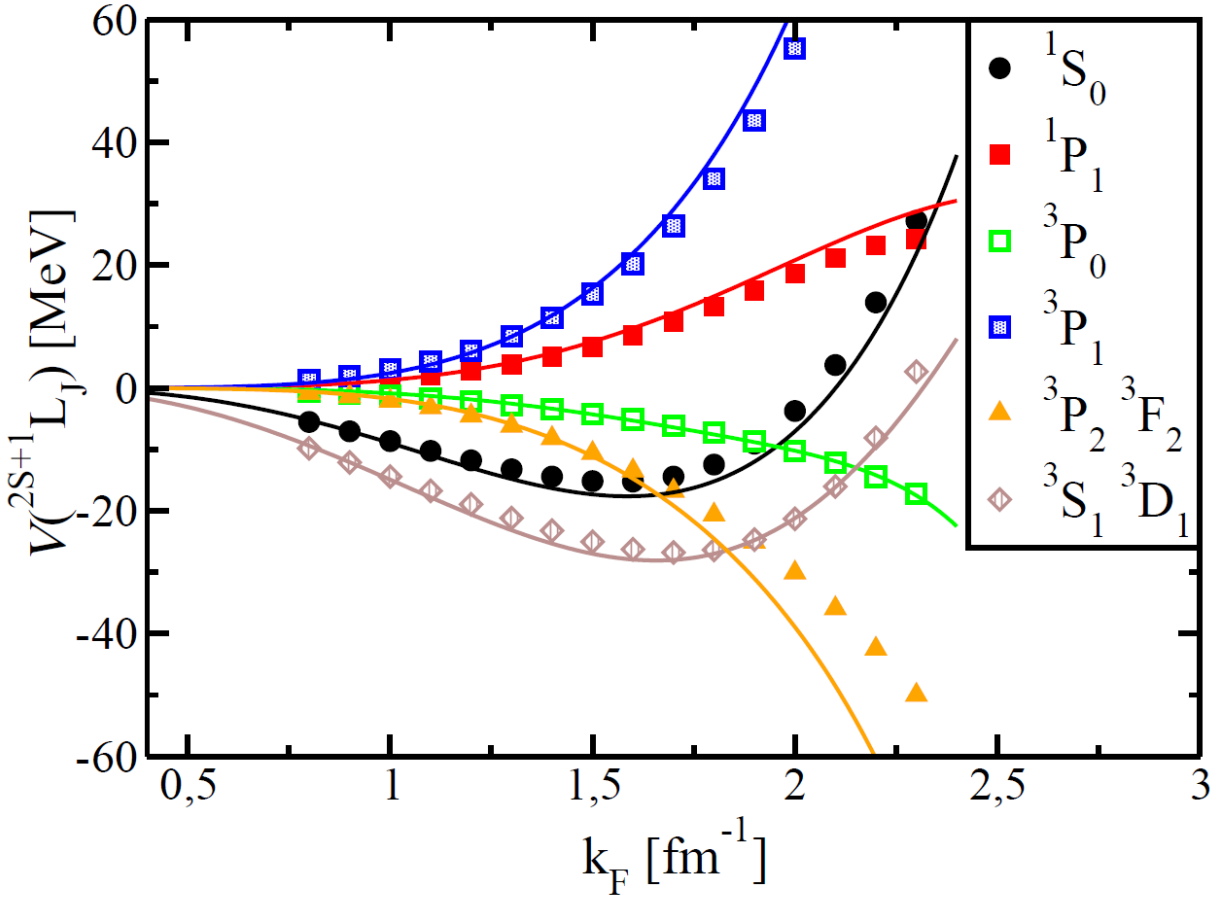
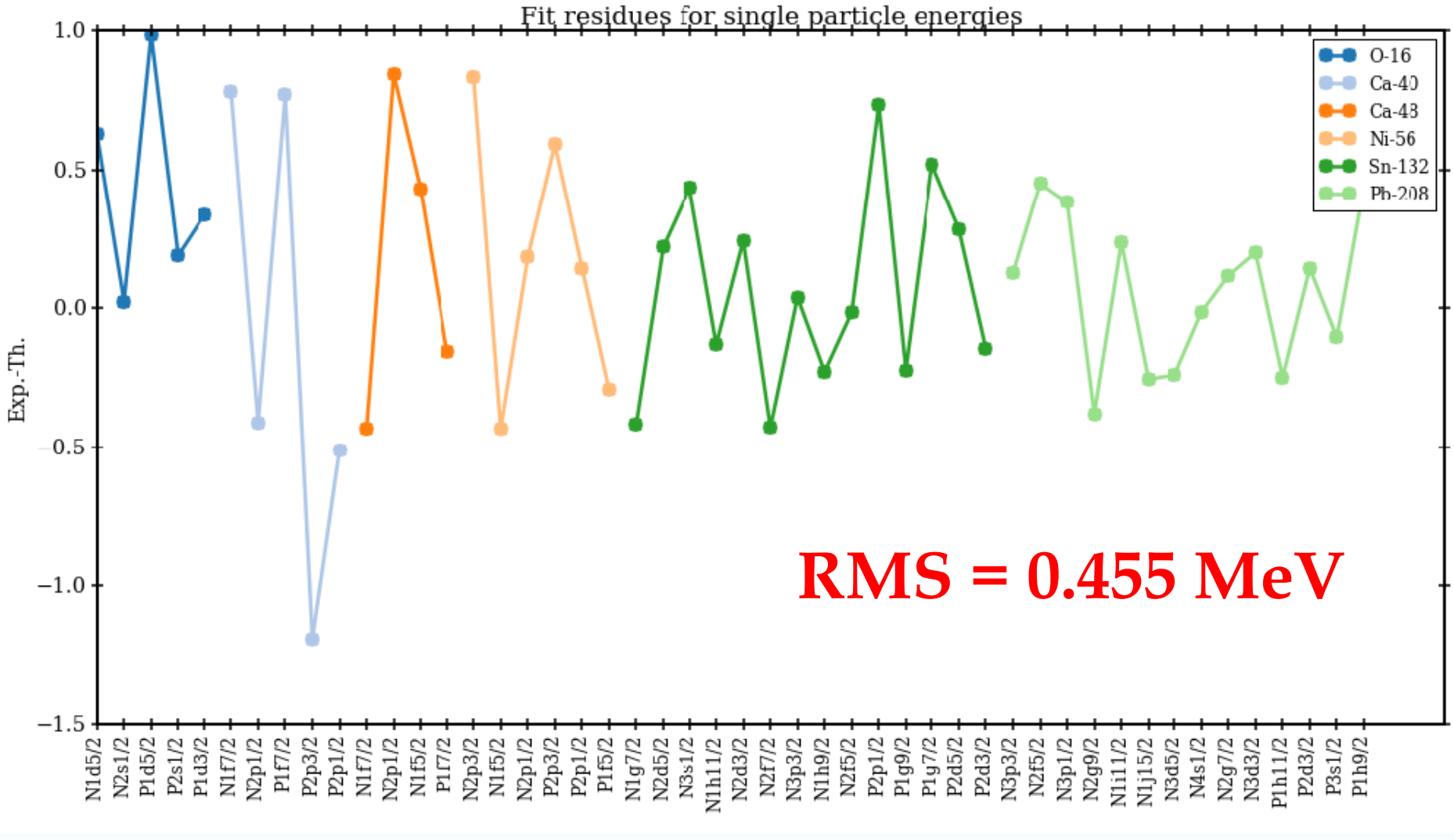


FIG. 2: (Color online) Comparing the partial waves $\mathcal{V}(^{2S+1}L_J)$. The dots are the BHF results, and the lines are the results of our fit with VLyB3.

D. Davesne *et al.*, Phys. Rev. C91, 064303 (2015)

Fits of N3LO zero-range pseudopotential



RMS = 0.455 MeV

B. Szpak, *et al.*, to be published

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 equivalent to local potentials

Let us first assume that the differential operators $\hat{O}_i(\vec{k}\,', \vec{k})$ depend only on the sum of relative momenta, that is,

$$\hat{O}_i(\vec{k}\,', \vec{k}) = \hat{O}_i\left(\vec{k} + \vec{k}'\right) = \hat{O}_i\left(\vec{k} - \vec{k}'^{\,*}\right), \text{ which requires that } T_2^{(i)} = -T_1^{(i)}.$$

Such particular differential operators commute with the locality deltas $\delta(\vec{r}\,'_1 - \vec{r}_1)\delta(\vec{r}\,'_2 - \vec{r}_2)$, and thus can be applied directly onto the regularized delta $g_a(\vec{r}_1 - \vec{r}_2)$. In such a case, the pseudopotential reduces to a simple local potential

$$V(\vec{r}) = \sum_{i=1}^{4} \hat{P}_i V_i(\vec{r}), = \sum_{i=1}^{4} \hat{P}_i \hat{O}_i(\vec{k}) g_a(\vec{r}),$$

Moreover, since $\hat{O}_i(\vec{k})$ are scalar differential operators, the potentials must have forms of power series of Laplacians Δ in $\vec{r}$, that is,

$$V_i(\vec{r}) = \sum_{n=0}^{n_{max}} V_{2n}^{(i)} \Delta^n g_a(\vec{r}),$$

where $V_{2n}^{(i)}$ are the coupling constants at order $2n$.

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

Local regularized pseudopotentials vs. Gogny

Below we determine coupling constants $V_{2n}^{(i)}$ by requiring that the lowest moments of the regularized and Gogny potentials are equal, that is,

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

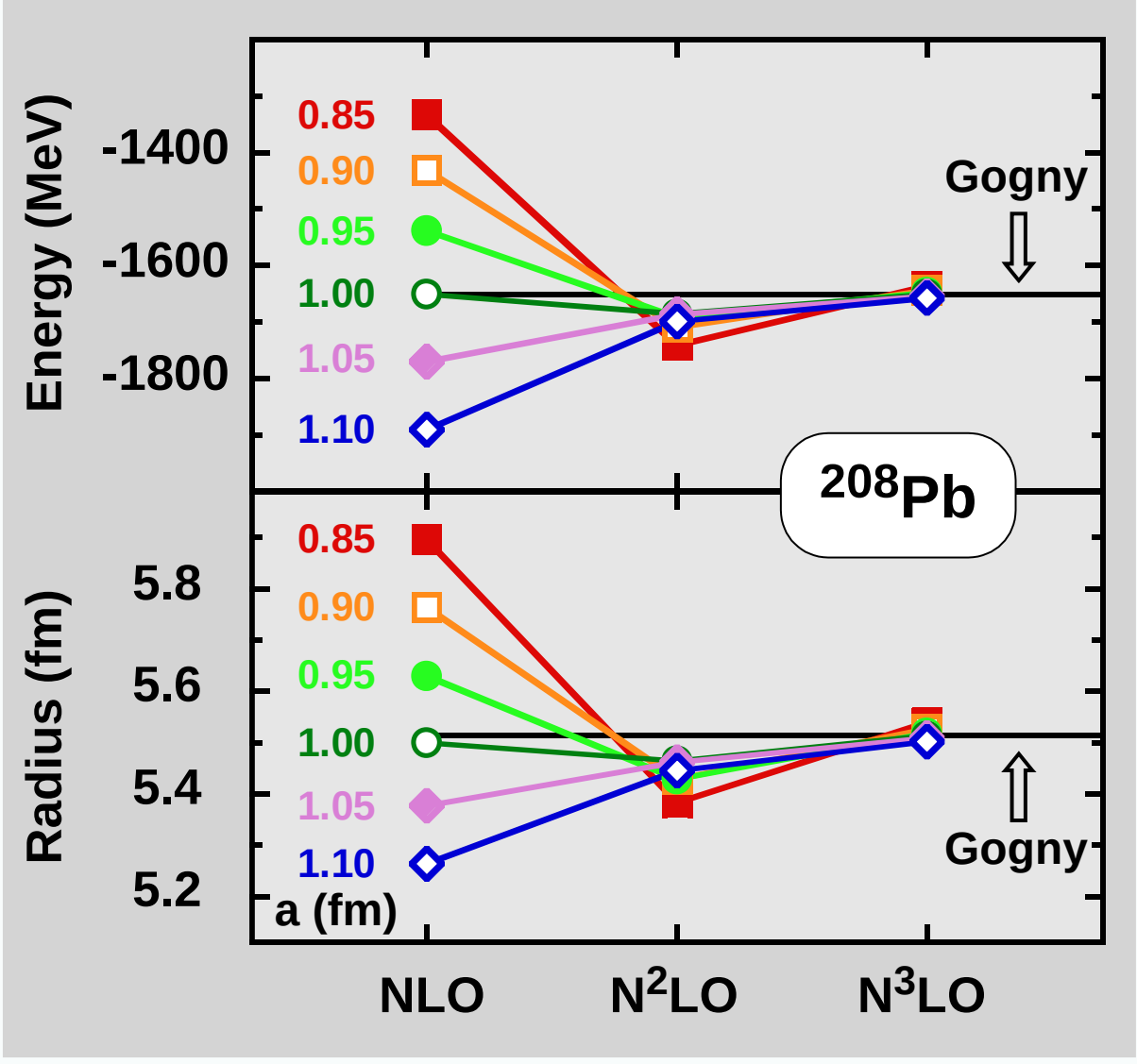
for $m = 0, 1, \ldots, n_{max}$. This conditions gives the coupling constants of the regularized potential in simple analytical forms,

$$\begin{aligned} V_{2n}^{(i)} &= \sum_{m=0}^{n} \left(-\frac{a^2}{4}\right)^{n-m} \frac{M_{2m}^{(i)}}{(n-m)!(2m+1)!} \\ &= \frac{1}{4^n n!} \sum_{k=1,2} G_k^{(i)} \left(a_k^2 - a^2\right)^n, \end{aligned}$$

where $G_k^{(i)}$ and a_k are the parameters of the Gogny interaction.

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

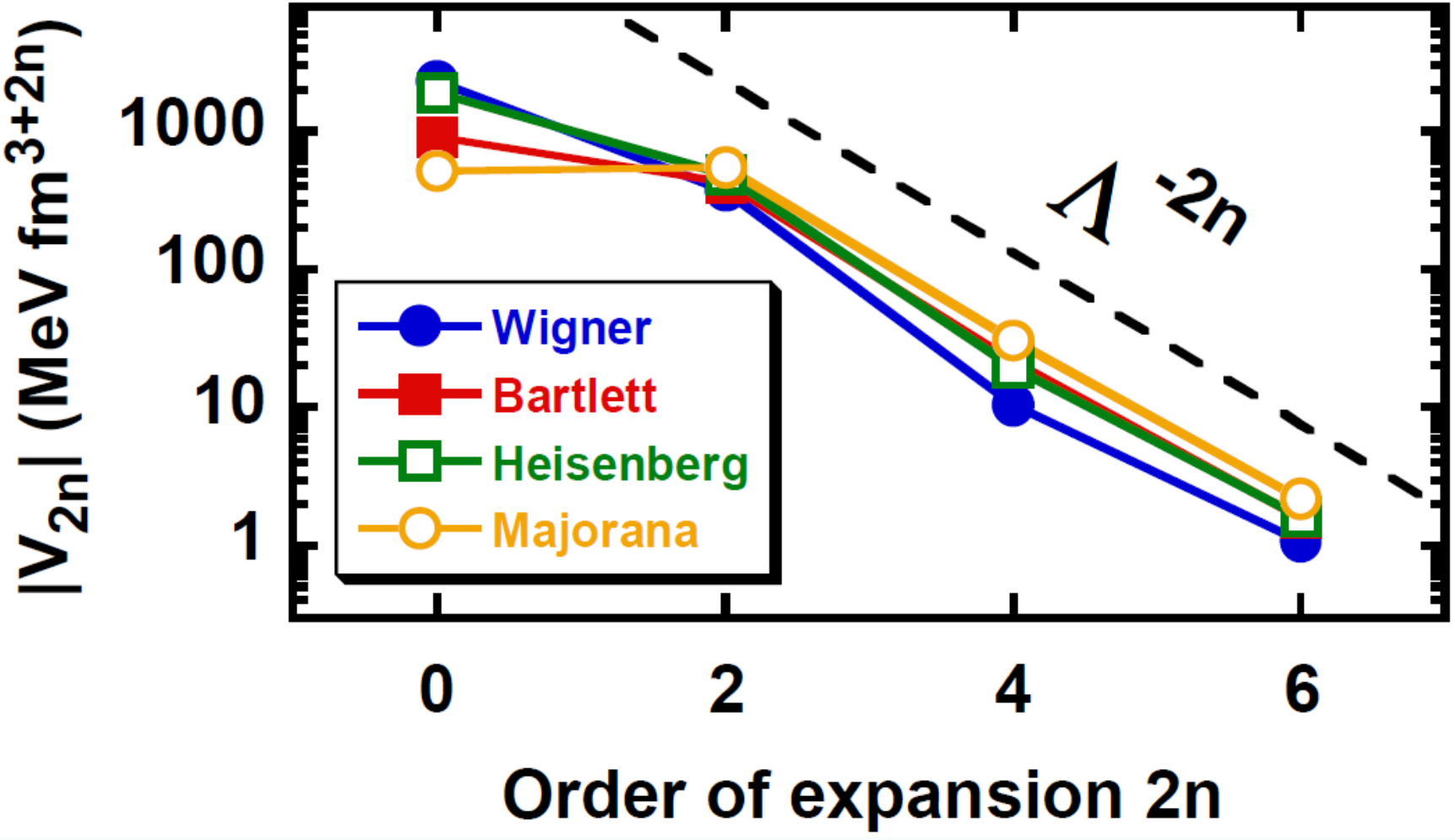
Regularized pseudopotentials vs. Gogny



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

Coupling constants of the regularized pseudopotentials

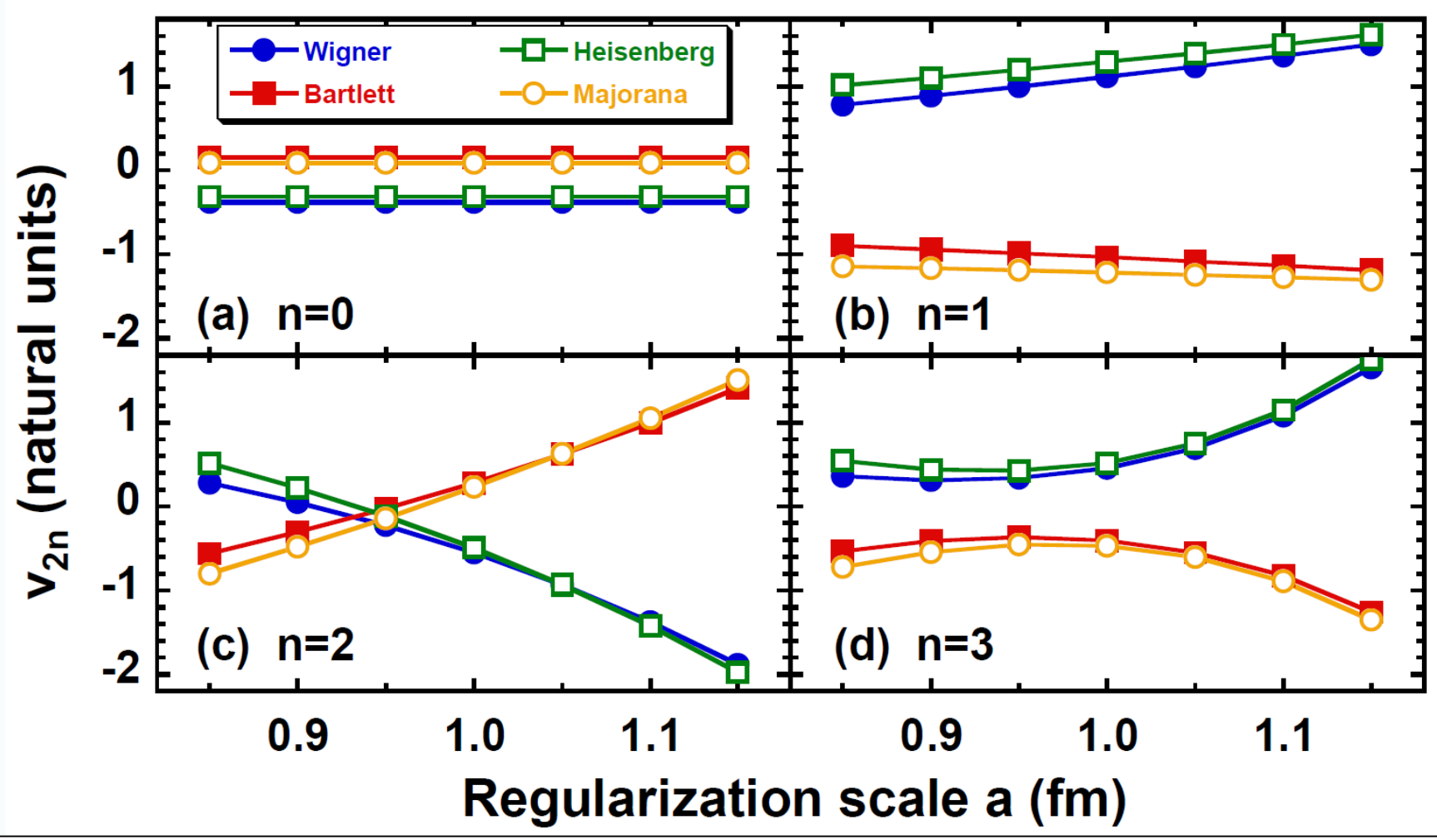
$\Lambda \approx 700$ MeV/$\hbar c \approx 3.8$ fm^{-1}



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

Coupling constants of the regularized pseudopotentials in natural units

$$v_{2n} = f^2 \Lambda^{2n} V_{2n} \text{ for } f = 35 \text{ MeV}/(\hbar c)^{3/2}$$



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)

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)

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

Finite range:

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

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

Numbers of terms of the finite-range pseudopotential at different orders up to N^{3}LO. 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^{3}LO	52	14	34	100

Nonlocal energy density functionals

We performed derivations of average energies separately for all terms of the regularized finite-range pseudopotential. The final result of this derivation is given by linear combinations of terms of the EDF appearing on the rhs of the following expression,

$$\langle C^{\tilde{n}'\tilde{L}',\tilde{t}}_{\tilde{n}\tilde{L},v_{12}\tilde{S}} \hat{V}^{\tilde{n}'\tilde{L}',\tilde{t}}_{\tilde{n}\tilde{L},v_{12}\tilde{S}} \rangle = \sum C^{a',\alpha',t,\mathcal{L}}_{a,\alpha,Q} T^{a',\alpha',t,\mathcal{L}}_{a,\alpha,Q}.$$

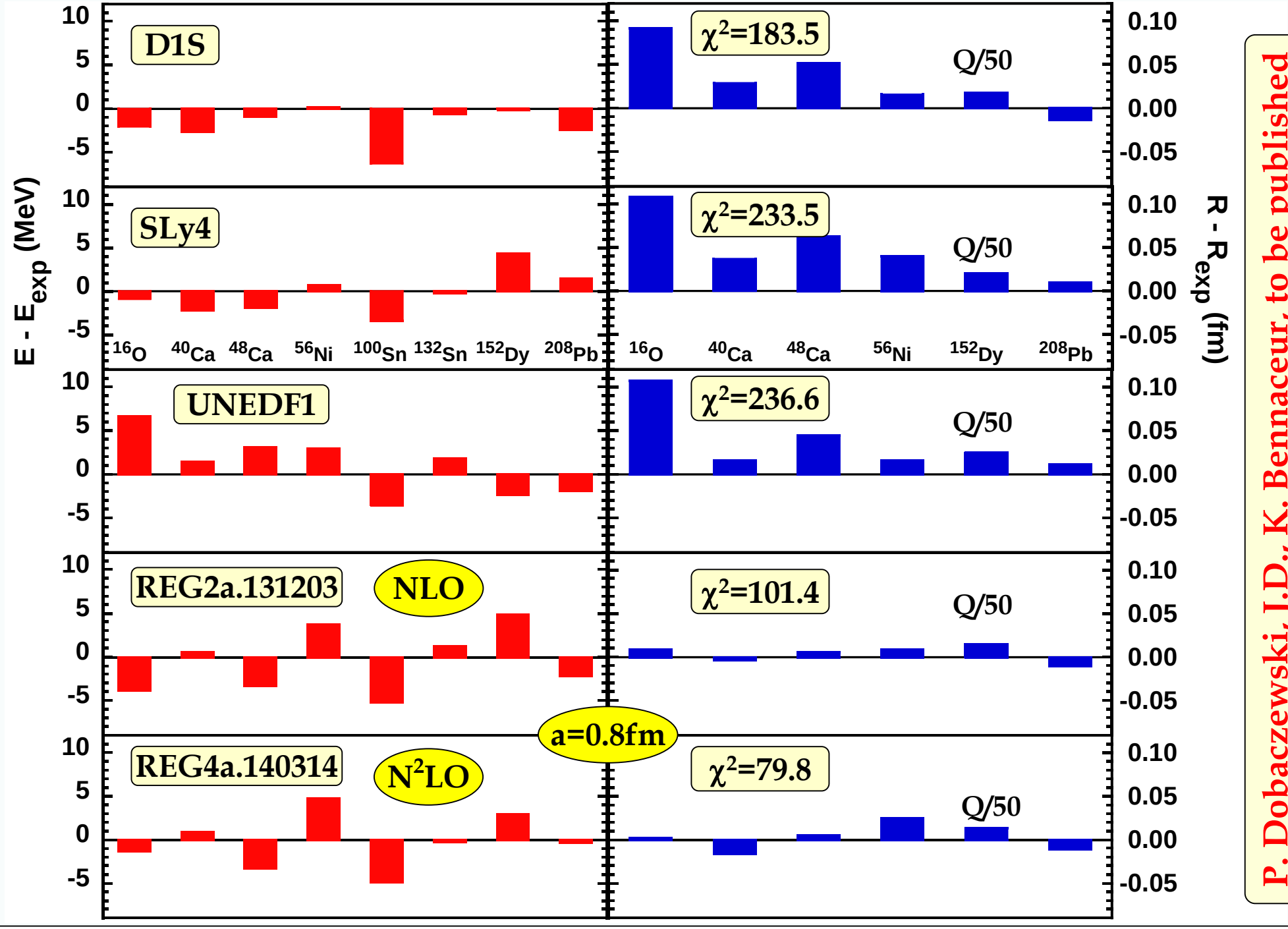
In this expression, $C^{a',\alpha',t,\mathcal{L}}_{a,\alpha,Q}$ and $T^{a',\alpha',t,\mathcal{L}}_{a,\alpha,Q}$ denote, respectively, the coupling constants and terms of the EDF according to the compact notation, where the Greek indices $\alpha = \{n_\alpha S_\alpha v_\alpha J_\alpha\}$ and Roman indices $a = \{m_a I_a\}$ combine all the quantum numbers of the local densities $\rho_\alpha(r)$ and derivative operators D_a in the spherical-tensor formalism, that is,

$$T^{a',\alpha',t,L}_{a,\alpha,Q} = \int \mathrm{d}r_1 \mathrm{d}r_2 \, g_a(r) \left[\left[\left[D_{a'} \rho^t_{\alpha'}(r_1) \right]_Q \left[D_a \rho^t_\alpha(r_2) \right]_Q \right]^0 \right]_0 .$$

$$T^{a',\alpha',t,N}_{a,\alpha,Q} = \int \mathrm{d}r_1 \mathrm{d}r_2 \, g_a(r) \left[\left[\left[D_{a'} \rho^t_{\alpha'}(r_1,r_2) \right]_Q \left[D_a \rho^t_\alpha(r_2,r_1) \right]_Q \right]^0 \right]_0 ,$$

They have been obtained using the integration by parts to transfer all derivatives onto the density matrices, and then employing the locality deltas to perform integrations over two out of four space coordinates.

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


D1S
χ²=183.5
Q/50
SLy4
χ²=233.5
Q/50
UNEDF1
χ²=236.6
Q/50
REG2a.131203
NLO
χ²=101.4
Q/50
a=0.8fm
REG4a.140314
N²LO
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
P. Dobaczewski, J.D., K. Bennaceur, to be published

Ab initio derivation of model EDFs

Jyväskylä – York – Surrey – Lyon collaboration

Ab initio derivation of model EDFs

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

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

where C^i are coupling constants and $V_i[\rho]$ 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,

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

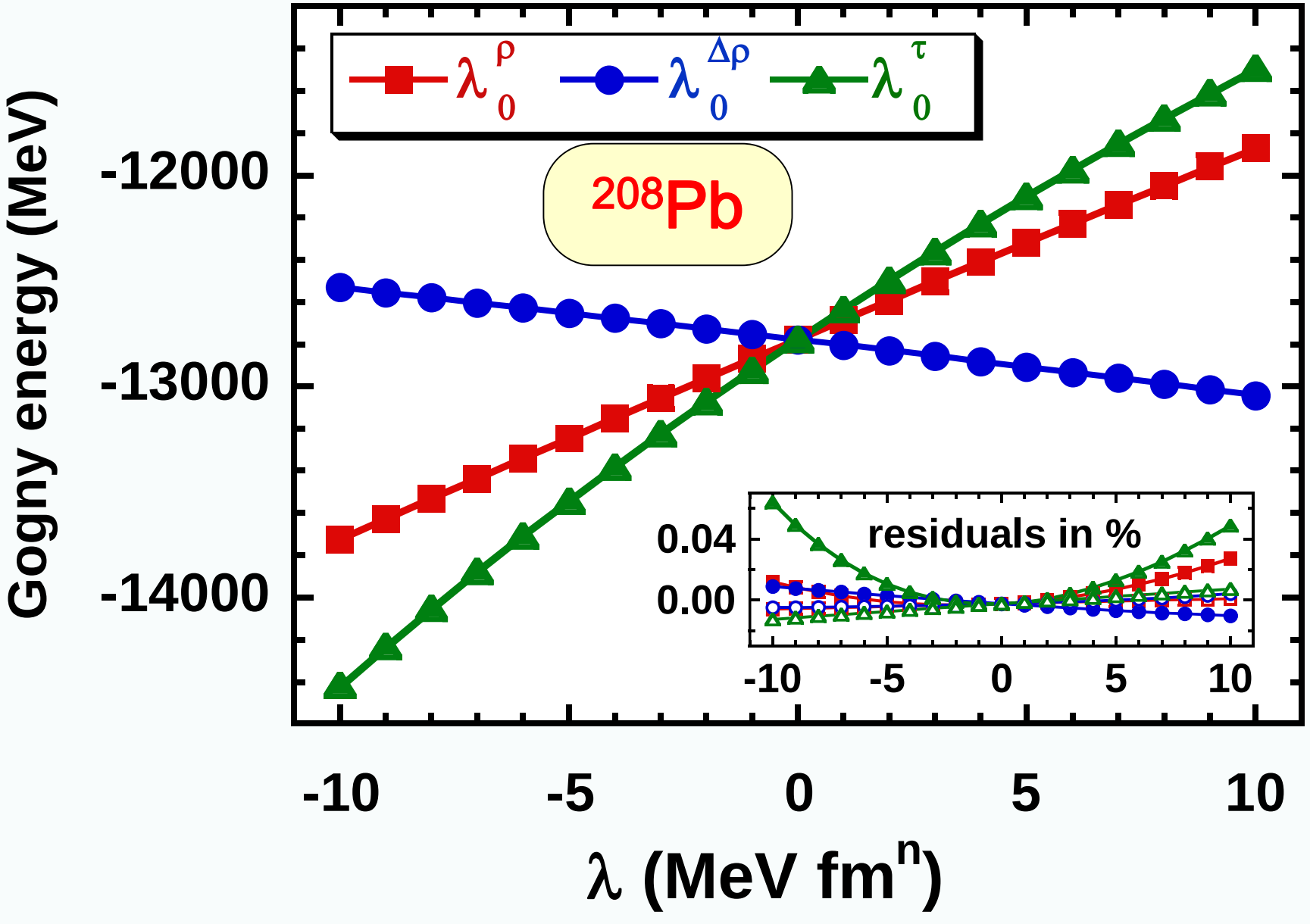
for a suitable set of values of a finite number of Lagrange multipliers λ^i, which is perfectly manageable a task.

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,

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

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.

	R_G	R	δR	$\delta R/R$	$\delta R/\Delta R$
(a)	(b)	(c)	(d)	(e)	(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

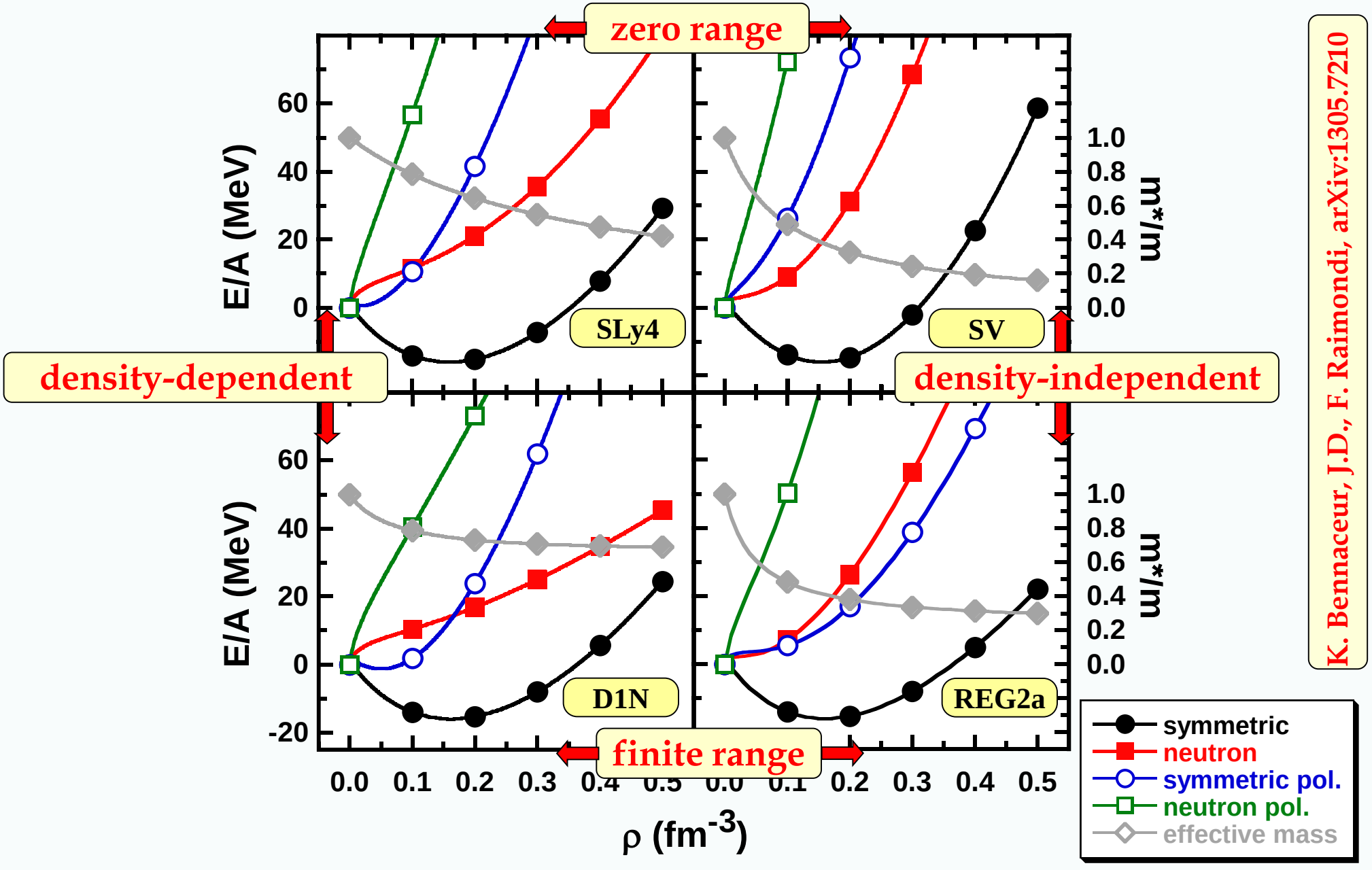
J.D., arXiv:1507.00697

Conclusions

- Currently available nuclear functionals have reached their limits of applicability.
- To gain progress, extensions/ modifications thereof are mandatory
- Higher-order derivative terms, three- or four-body generstors, finite range, *ab initio* derivations, ...

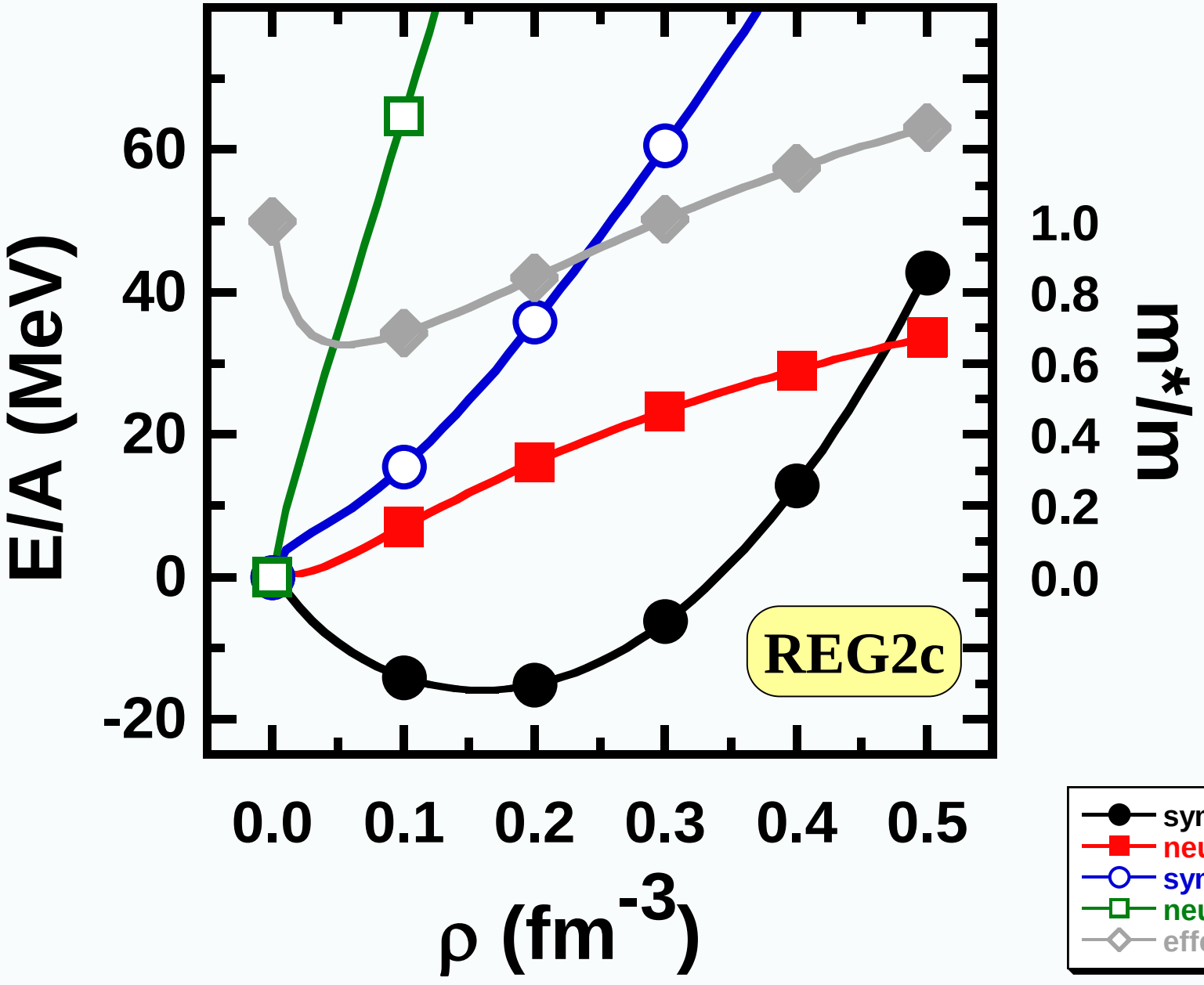
Thank you

Equations of state

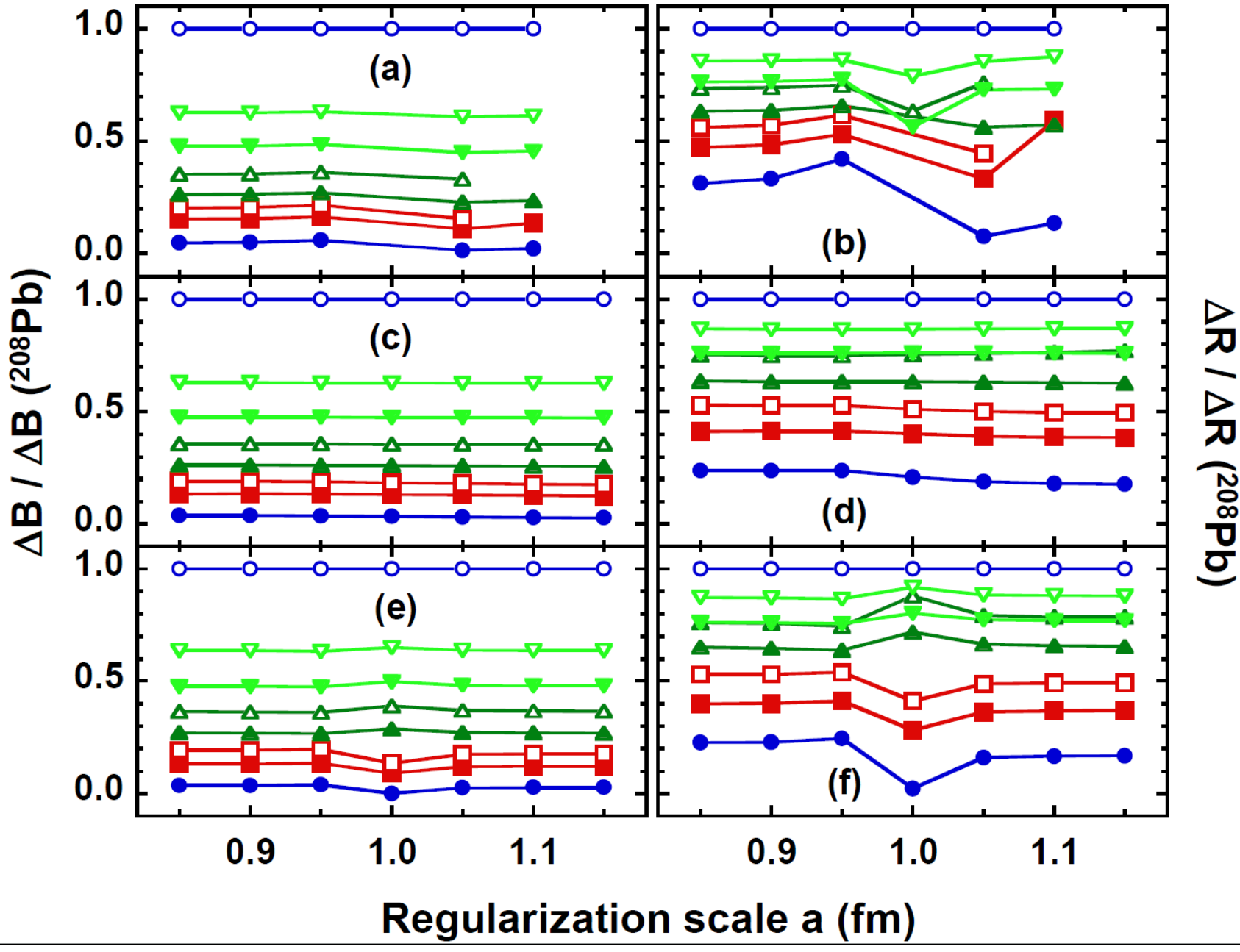


K. Bennaceur, J.D., F. Raimondi, arXiv:1305.7210

Two-body a=1.4, Three-body zero range



Regularized pseudopotentials vs. Gogny



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

Naming conventions

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

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

REG2a.date $\Longrightarrow$ **2nd order (NLO),** $T_2^{(2i)} = -T_1^{(2i)}$

REG2b.date $\Longrightarrow$ **2nd order (NLO),** $T_2^{(2i)} \neq -T_1^{(2i)}$

REG2c.date $\Longrightarrow$ **2nd order (NLO),** $T_2^{(i)} = -T_1^{(i)}$**, 3-body zero-range**

REG4a.date $\Longrightarrow$ **4th order (N2LO),** $T_2^{(4i)} = -T_1^{(4i)}$, $T_3^{(4i)} = 0$, $T_4^{(4i)} = 0$

Density-independent finite-range interactions

Saturation properties with SV:

$\rho_{\rm sat}$	E/A	K_∞	m^*/m	J	L	$K_{\rm sym}$
0.1551 fm^{-3}	−16.05 MeV	305.7 MeV	0.38	32.82 MeV	96.09 MeV	24.17 MeV

Saturation properties with REG2a.130531
($a = 0.8$ fm, $T_2^{(i)} = -T_1^{(i)}$), manual fit:

$\rho_{\rm sat}$	E/A	K_∞	m^*/m	J	L	$K_{\rm sym}$
0.160 fm^{-3}	−16.00 MeV	230.0 MeV	0.41	32.00 MeV	100.2 MeV	83.26 MeV

Saturation properties with REG2b.130531
($a = 0.8$ fm, $T_2^{(i)} \neq -T_1^{(i)}$), manual fit:

$\rho_{\rm sat}$	E/A	K_∞	m^*/m	J	L	$K_{\rm sym}$
0.160 fm^{-3}	−16.00 MeV	230.0 MeV	0.41	32.00 MeV	58 MeV	−175 MeV

Saturation properties with REG2a.130716
($a = 0.8$ fm, $T_2^{(i)} = -T_1^{(i)}$), pounders fit:

$\rho_{\rm sat}$	E/A	K_∞	m^*/m	J	L	$K_{\rm sym}$
0.157 fm^{-3}	−16.58 MeV	276.4 MeV	0.39	40.92 MeV	167 MeV	253 MeV

Saturation properties with REG2c.131113
($a = 1.4$ fm, $T_2^{(i)} = -T_1^{(i)}$), 3-body zero-range, manual fit:

$\rho_{\rm sat}$	E/A	K_∞	m^*/m	J	L	$K_{\rm sym}$
0.160 fm^{-3}	−15.90 MeV	231.0 MeV	0.77	30.50 MeV	48 MeV	−288 MeV

K. Bennaceur, J.D., F. Raimondi, arXiv:1305.7210 and to be publised