New family of finite-range pseudopotential-based energy density functionals

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New developments in nuclear energy density functionals
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Outline

1. Introduction: generators of the nuclear EDF
2. PVC corrections to single-particle energies
3. Pseudopotentials
4. Regularized pseudopotentials
5. First results
6. Simple regularization scheme
7. 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

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

Direct

Exchange

Standard functional 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*

$$V(\vec{r}_1\vec{r}_2;\vec{r}\,'_1\vec{r}\,'_2) = \Big\{t_0(1+x_0P^\sigma) + \tfrac{1}{6}t_3(1+x_3P^\sigma)\rho^\alpha\left(\tfrac{1}{2}(\vec{r}_1+\vec{r}_2)\right)$$

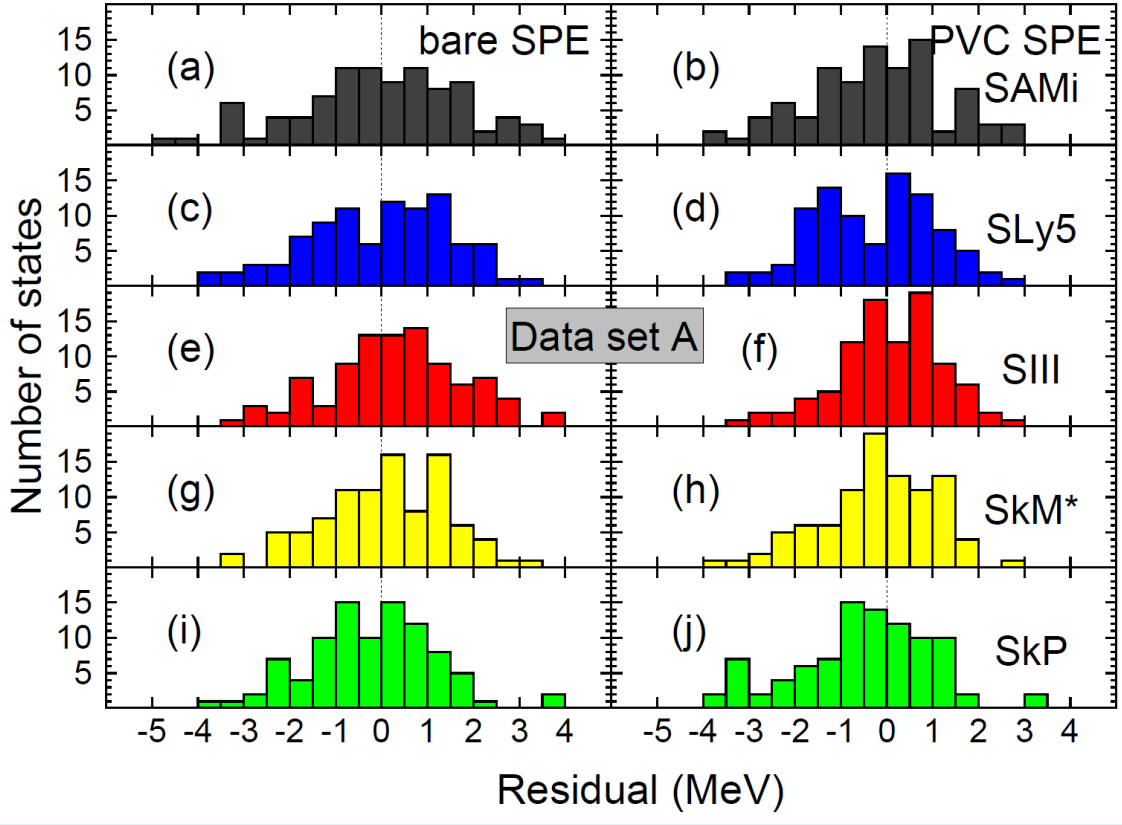
$$+\tfrac{1}{2}t_1(1+x_1P^\sigma)[\vec{k}'^{*2}+\vec{k}^2] + t_2(1+x_2P^\sigma)\vec{k}'^{*}\cdot\vec{k}\Big\}\,\delta(\vec{r}_1-\vec{r}\,'_1)\delta(\vec{r}_2-\vec{r}\,'_2)\delta(\vec{r}_1-\vec{r}_2),$$

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.

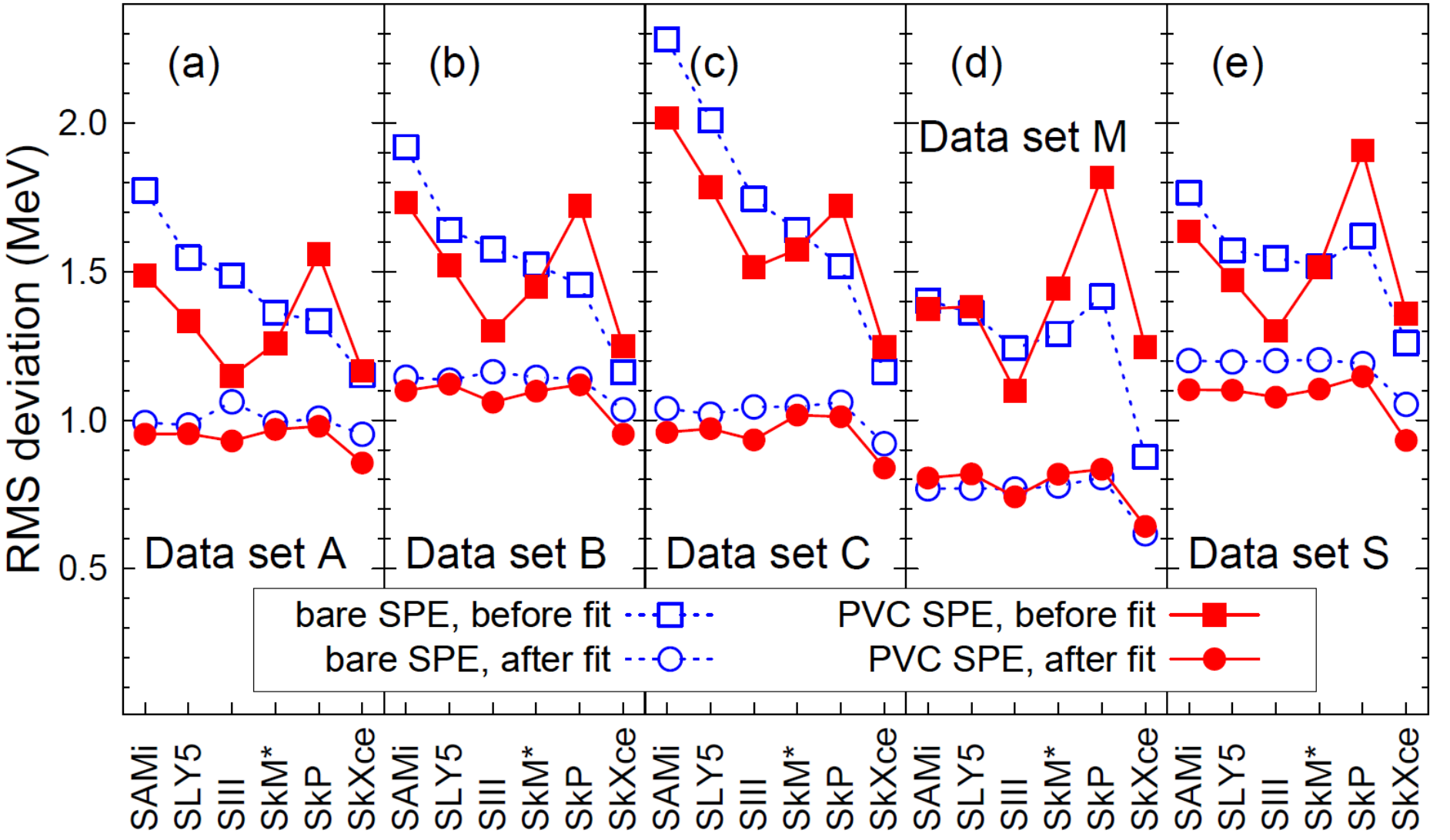
Particle-vibration-coupling (PVC) corrections

$$\delta\epsilon_i = \frac{1}{2j_i+1}\left(\sum_{nJp}\frac{|\langle i||V||p,nJ\rangle|^2}{\epsilon_i-\epsilon_p-\hbar\omega_{nJ}+i\eta} + \sum_{nJh}\frac{|\langle i||V||h,nJ\rangle|^2}{\epsilon_i-\epsilon_h+\hbar\omega_{nJ}-i\eta}\right),$$



D. Tarpanov *et al.*, arXiv:1405.4823

Particle-vibration-coupling (PVC) corrections



D. Tarpanov *et al.*, arXiv:1405.4823

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)

Regularized finite-range pseudopotentials

Zero range:

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

Finite range:

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

Numbers of terms of the finite-range pseudopotential at different orders up to N^{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

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

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)

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

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

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

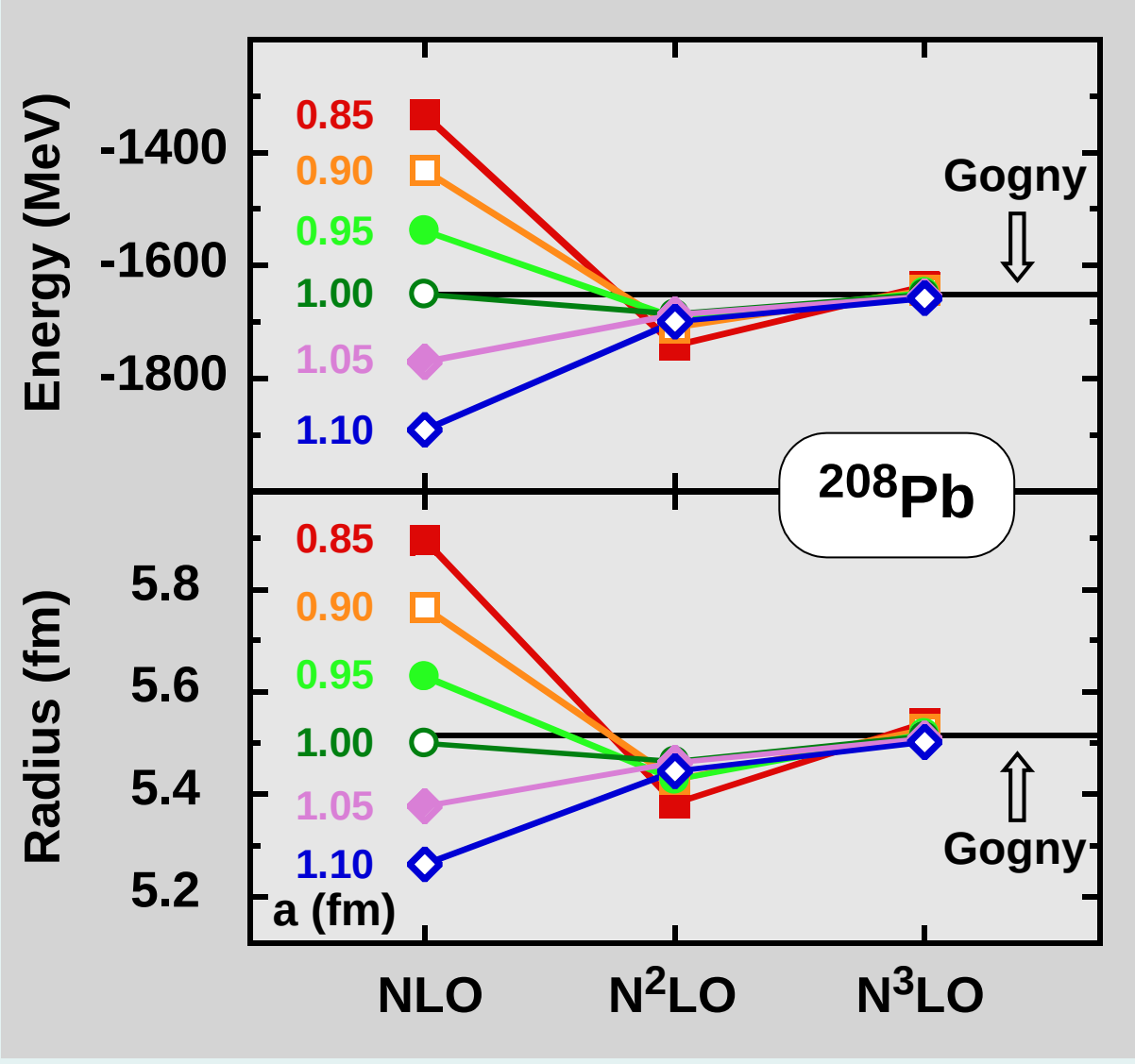
$$M_{2m}^{(i)} \equiv \int r^{2m} G_i(r) \mathrm{d}^3 r = \int r^{2m} V_i(r) \mathrm{d}^3 r,$$

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.

Local regularized pseudopotentials vs. Gogny



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)

Naming conventions

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

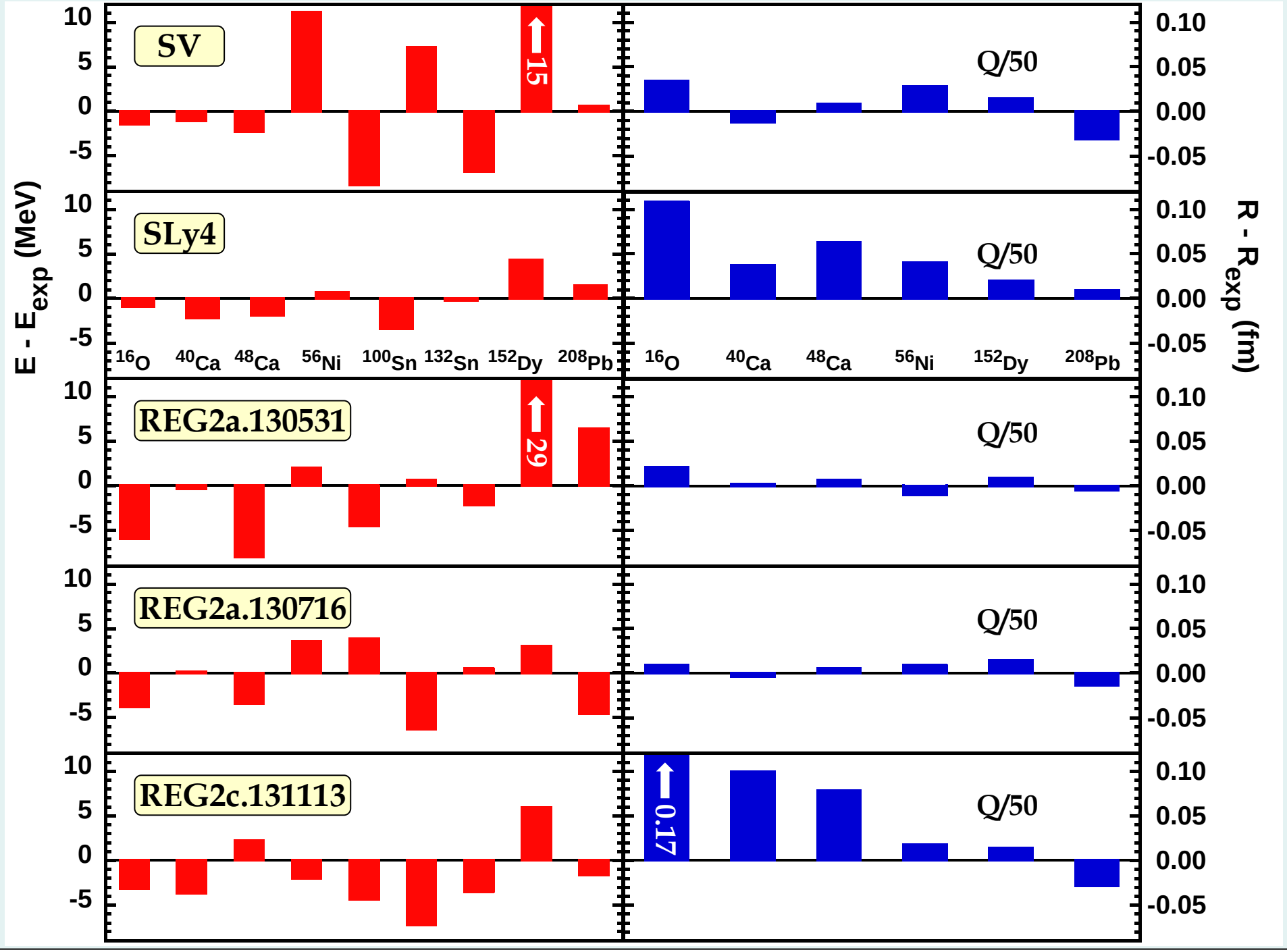
$$\hat{O}_i(\vec{k}\,',\vec{k}) \;=\; \sum\nolimits_{nj} T_j^{(ni)} \hat{O}_j^{(n)}(\vec{k}\,',\vec{k})$$

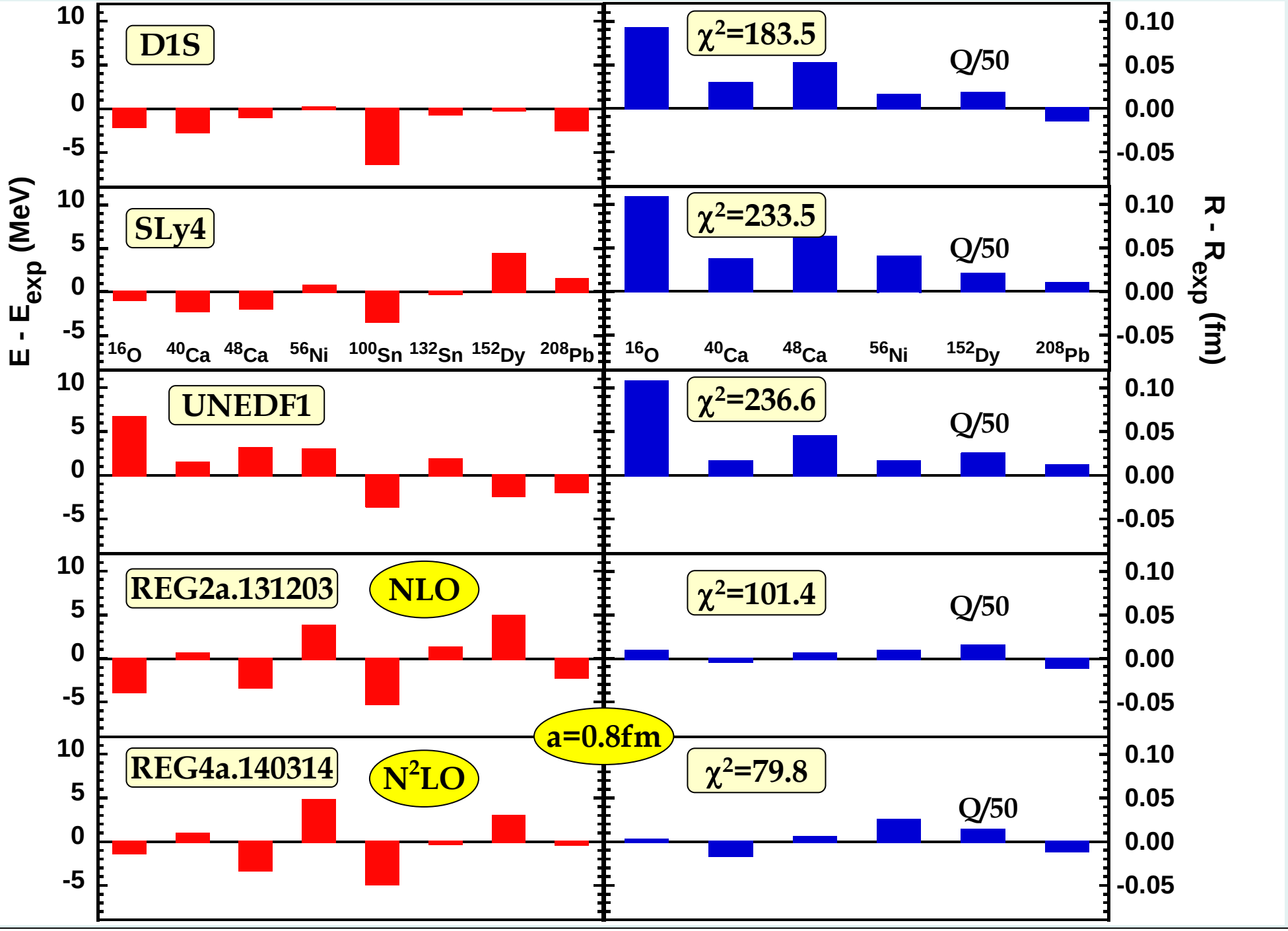
REG2a.date $\Longrightarrow$ 2nd order (NLO), $T_2^{(2i)} = -T_1^{(2i)}$

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

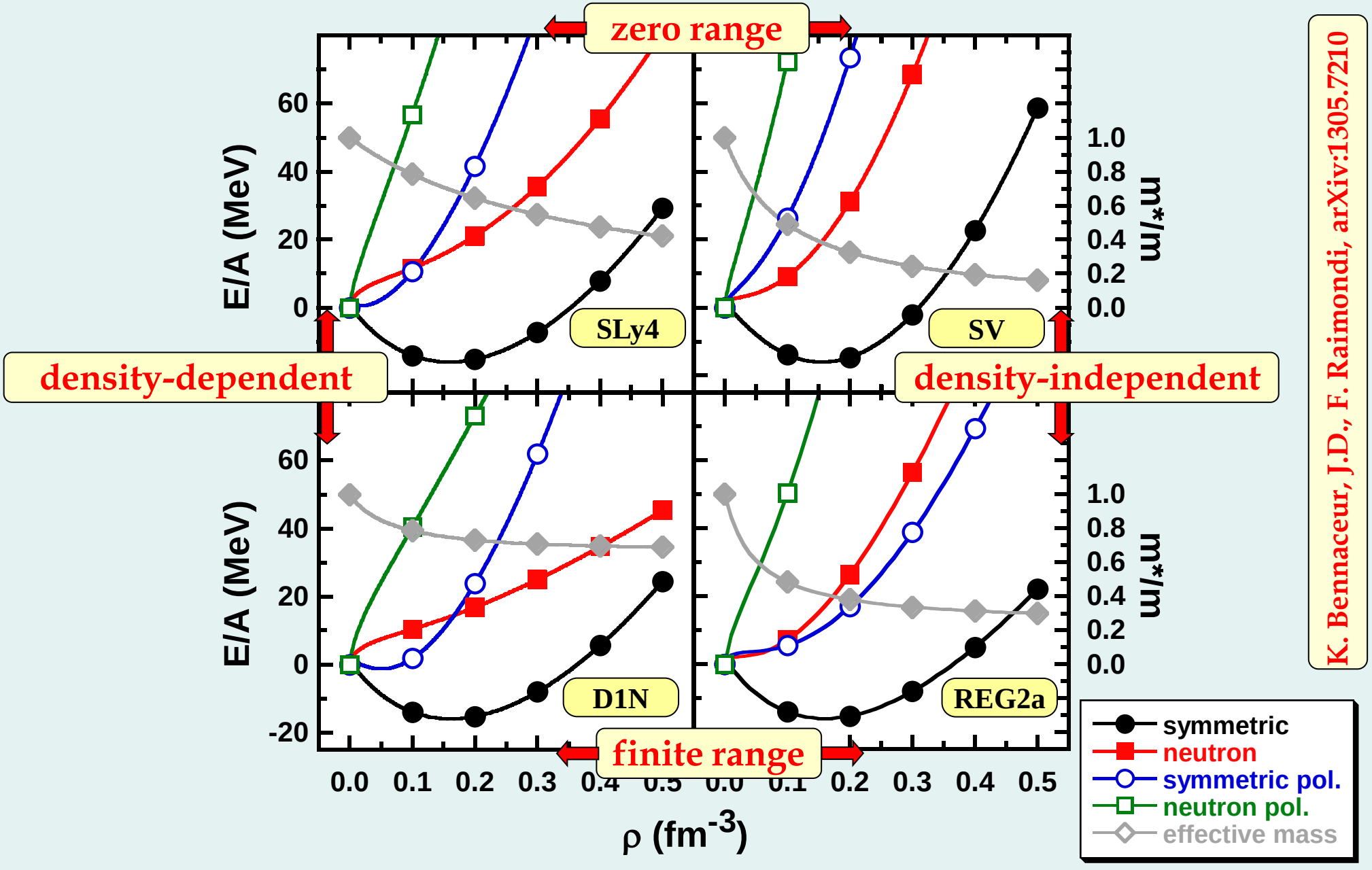
REG2c.date $\Longrightarrow$ 2nd order (NLO), $T_2^{(i)} = -T_1^{(i)}$, 3-body zero-range

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


SV
SLy4
REG2a.130531
REG2a.130716
REG2c.131113
Q/50
15
29
0.17
E - E_exp (MeV)
R - R_exp (fm)
16O 40Ca 48Ca 56Ni 100Sn 132Sn 152Dy 208Pb

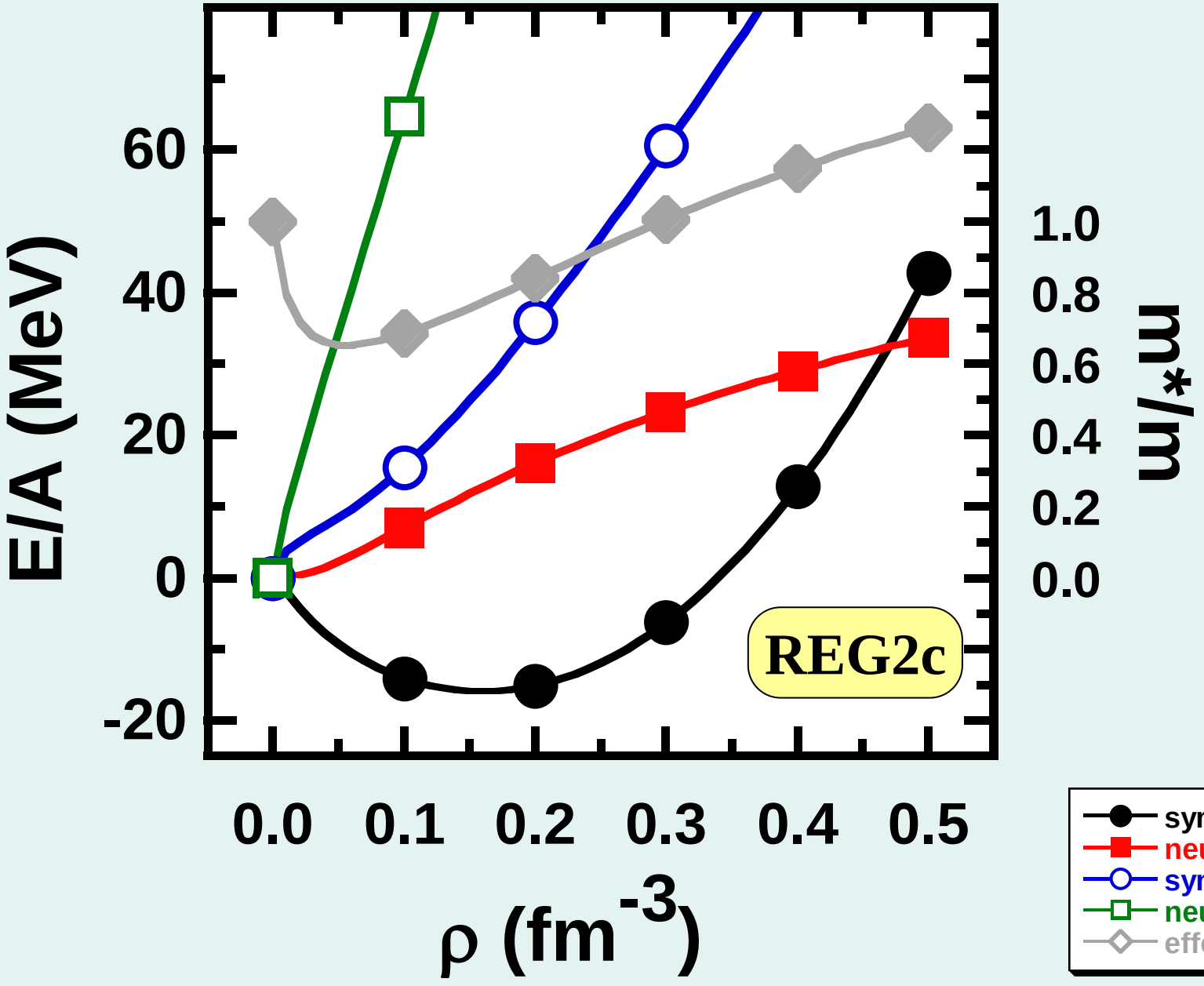

D1S
SLy4
UNEDF1
REG2a.131203
NLO
REG4a.140314
N²LO
a=0.8fm
χ²=183.5
χ²=233.5
χ²=236.6
χ²=101.4
χ²=79.8
Q/50
E - E_exp (MeV)
R - R_exp (fm)
10
5
0
-5
0.10
0.05
0.00
-0.05
16O
40Ca
48Ca
56Ni
100Sn
132Sn
152Dy
208Pb

Equations of state



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

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



Simple regularization scheme for multireference density functional theories

The matrix element between the unprojected and AMP state reads:

$$V^{2\mathrm{B}}_{IMK} \equiv \langle\Psi|\hat{V}_{2\mathrm{B}}\hat{P}^{I}_{MK}|\Psi\rangle = = \frac{2I+1}{8\pi^2}\int d\Omega\, D^{I\star}_{MK}(\Omega)\langle\Psi|\hat{V}_{2\mathrm{B}}|\tilde{\Psi}\rangle.$$

The proposed regularization scheme amounts to replacing the calculation of matrix elements $V^{2\mathrm{B}}_{IMK}$ by the calculation of an auxiliary quantity defined as:

$$V^{2\mathrm{B,n}}_{IMK} = \frac{2I+1}{8\pi^2}\int d\Omega\, D^{I\star}_{MK}(\Omega)\langle\Psi|\hat{V}_{2\mathrm{B}}|\tilde{\Psi}\rangle\langle\Psi|\tilde{\Psi}\rangle^{n}.$$

Requesting that the ralation between the auxiliary quantity and matrix element is the same as for regular interactions gives rise to a set of linear equations for regularized matrix elements $\tilde{V}^{2\mathrm{B}}_{I'M'K'}$:

$$V^{2\mathrm{B,1}}_{IMK} = \sum_{I'M'K'} A^{IMK}_{I'M'K'}\tilde{V}^{2\mathrm{B}}_{I'M'K'},$$

where

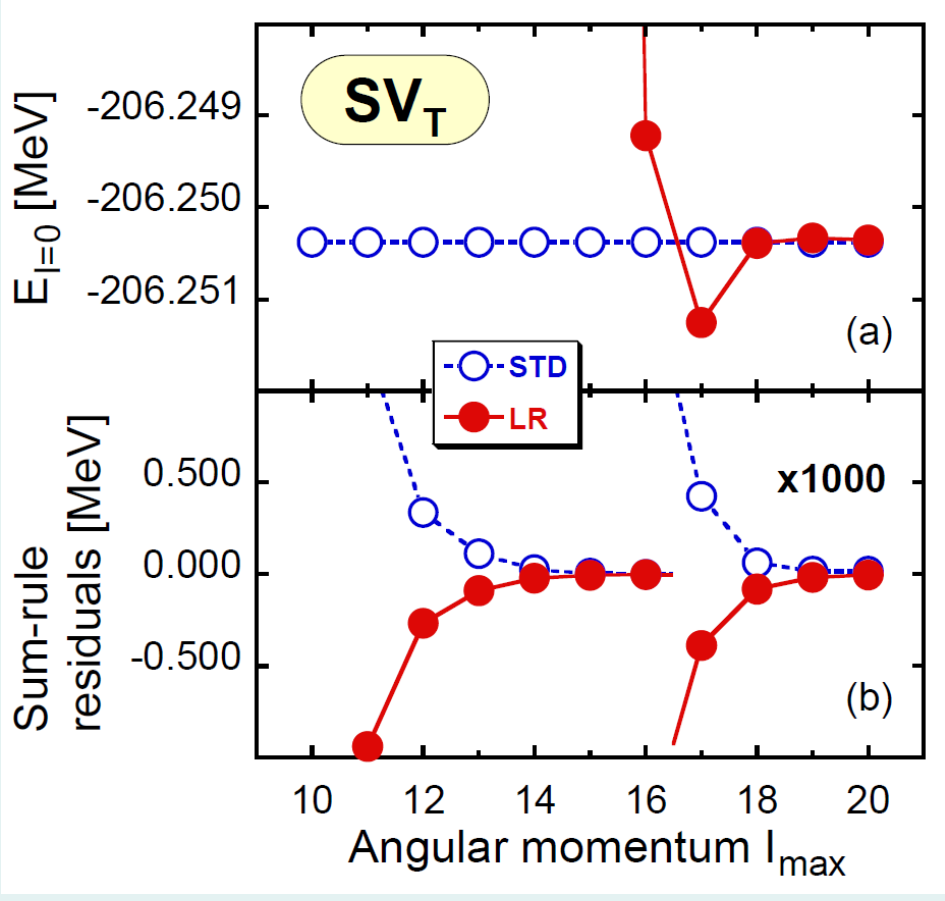
$$A^{IMK}_{I'M'K'} = \sum_{I''M''K''} c^{\mathcal{N}}_{I''M''K''}\mathrm{C}^{IM}_{I''M''I'M'}\mathrm{C}^{IK}_{I''K''I'K'}.$$

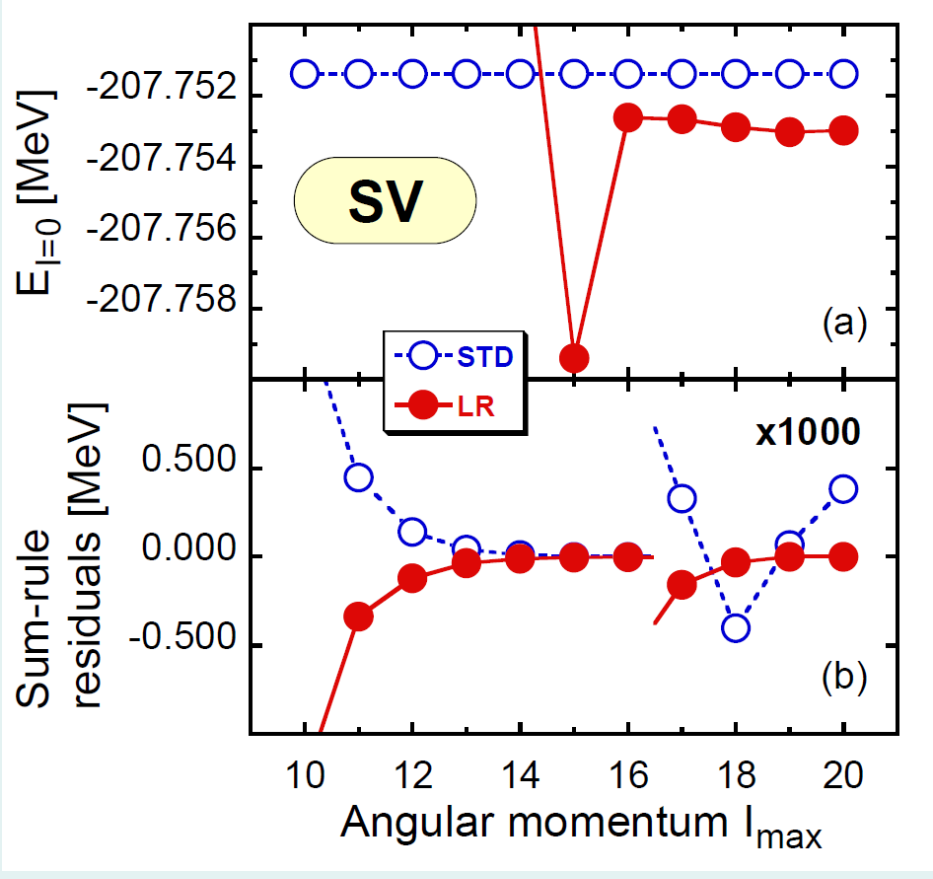
The problem of finding the regularized matrix elements is thus reduced to calculating auxiliary quantities and then solving a set of linear equations.

W. Satuła and J.D, Phys. Rev. C90, 054303 (2014)

Simple regularization scheme for multireference density functional theories

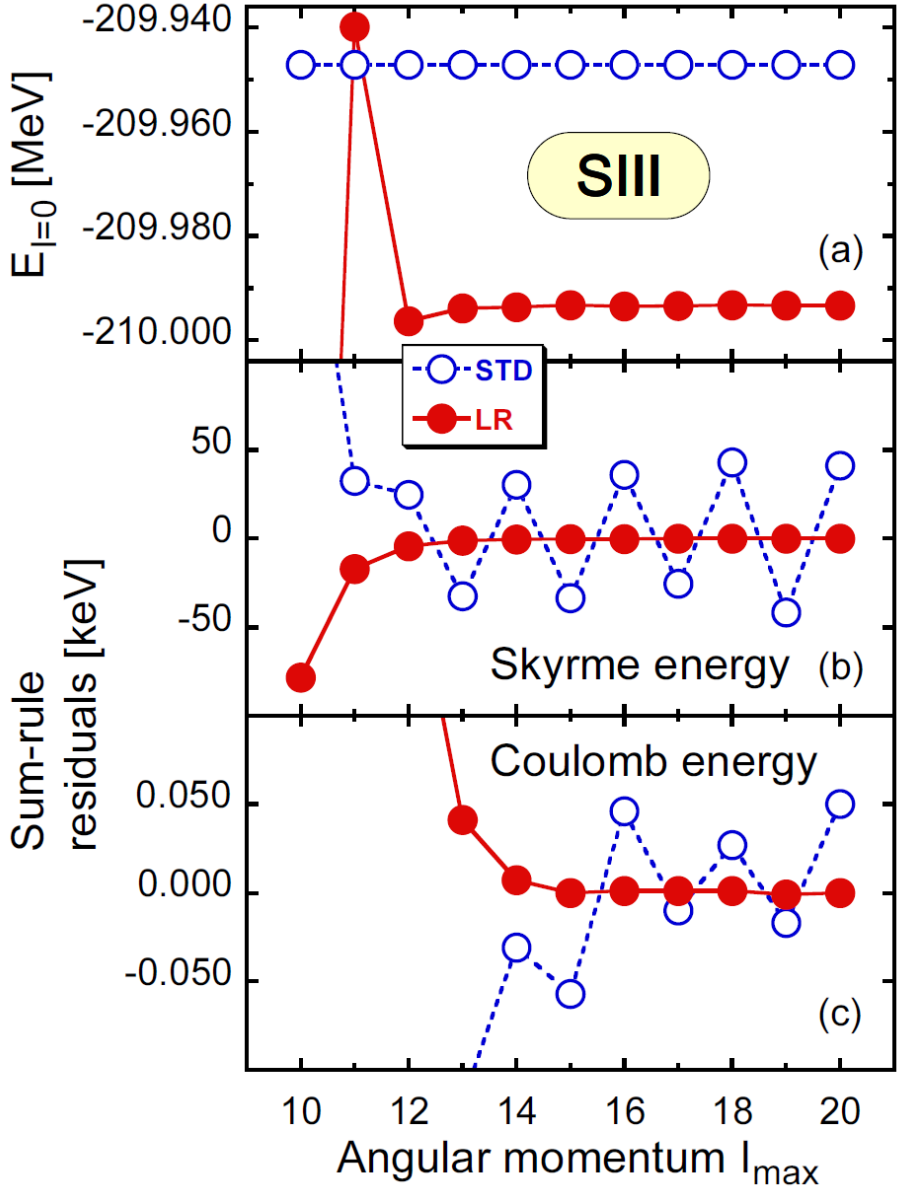
Test for the antialigned configuration in ^{26}Al

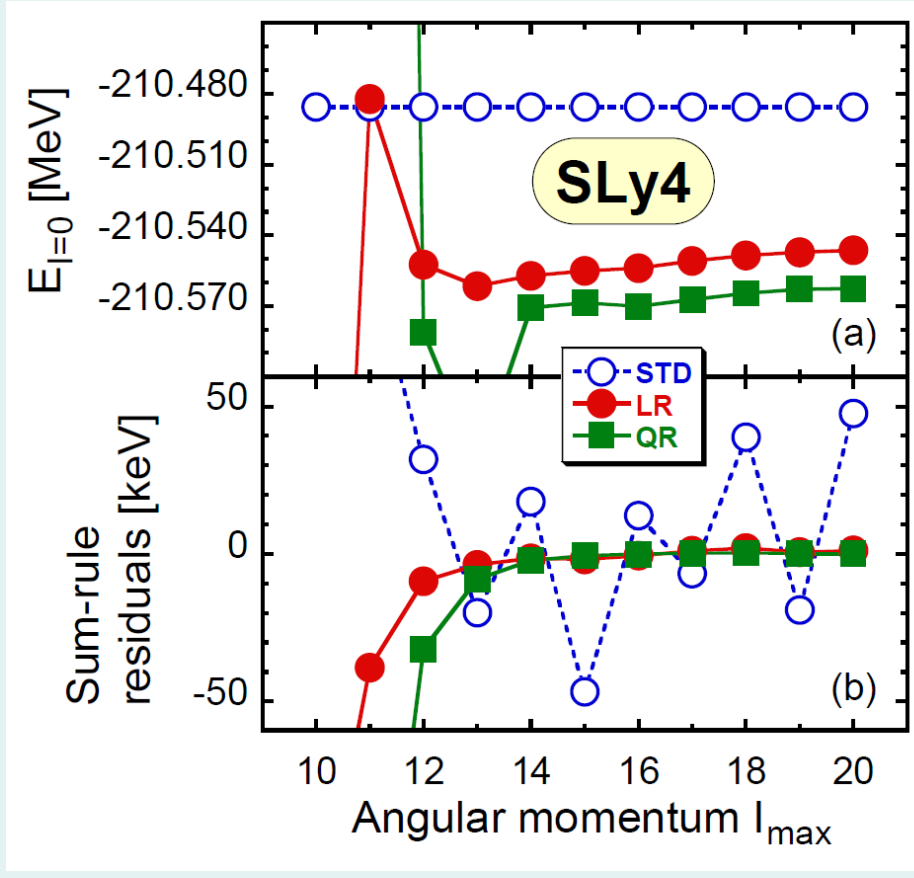




W. Satuła and J.D, Phys. Rev. C90, 054303 (2014)

Simple regularization scheme for multireference density functional theories





W. Satuła and J.D, Phys. Rev. C90, 054303 (2014)

Conclusions

1. We introduced a new class of energy density functionals that are based on **regularized pseudopotentials**. They allow for constructing **density-independent** finite-range interactions.
2. Future prospects for using the proposed regularized pseudopotentials are high.
3. The regularized pseudopotentials give us a possibility of building an **order-by-order correctible theory**.
4. We proposed a **method to regularize** the two-body off-diagonal MR DFT kernels and we presented the first application thereof to a representative case of the angular-momentum projection. }
5. Refinements of energy density functionals towards reaching **spectroscopic-quality description** of low-energy data are mandatory.

Thank you

Skyrme's three-body interaction

1.C:
1.D.1

Nuclear Physics **9** (1959) 615—634; © *North-Holland Publishing Co., Amsterdam*

THE EFFECTIVE NUCLEAR POTENTIAL

T. H. R. SKYRME
Atomic Energy Research Establishment, Harwell, Didcot, Berks.

Received 18 October 1958

The effective interaction potential will *not* be the same as that defined in the self-consistent many-body theory (to which the variational principle is not applicable). The potential used in our analysis must contain three-body, and generally many-body, terms which describe the way in which interaction between two particles is influenced by the presence of others; the two-body terms alone should be related closely to the scattering between free nucleons.

These considerations have led to the following ansatz for the form of the effective potential:

$$T = \sum_{i<j}\sum t_{ij} + \sum_{i<j<k}\sum\sum t_{ijk} \qquad (2)$$

in which the many-body effects have been simulated by three-body terms alone, for the sake of simplicity of calculation.

The density dependence is born

PHYSICAL REVIEW C VOLUME 5, NUMBER 3 MARCH 1972

Hartree-Fock Calculations with Skyrme's Interaction. I. Spherical Nuclei*

D. Vautherin and D. M. Brink

For the three-body force Skyrme also assumed a zero-range force

$$v_{123}^{(3)} = t_3 \delta(\vec{r}_1 - \vec{r}_2)\delta(\vec{r}_2 - \vec{r}_3). \quad (7)$$

In the following we will show that for Hartree-Fock calculations of even-even nuclei, this force is equivalent to a two-body density-dependent interaction:

$$v_{12} = \tfrac{1}{6} t_3 (1 + P_\sigma)\delta(\vec{r}_1 - \vec{r}_2)\rho\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right). \quad (8)$$

Such a term provides a simple phenomenological representation of many-body effects, and describes the way in which the interaction between two nucleons is influenced by the presence of others.

Volume 56B, number 3 PHYSICS LETTERS 28 April 1975

SPIN SATURATION AND THE SKYRME INTERACTION ☆

B.D. CHANG*

Received 18 March 1975

Of existing variants of the Skyrme interaction, those with strong three-body terms – in particular the variant SIII that is in best accord with experiment – overbind odd-mass and odd-odd nuclei and produce unstable spin-saturated Hartree-Fock ground states in nuclear matter and in even-even light nuclei. This difficulty can be removed either by imposition of an additional stability condition or by abandoning the three-body term in favor of the two-body density-dependent interaction equivalent to it in spin-saturated HF states.

The density dependence is exploited

1.E.2

Nuclear Physics **A238** (1975) 29—69; © *North-Holland Publishing Co., Amsterdam*

NUCLEAR GROUND-STATE PROPERTIES AND SELF-CONSISTENT CALCULATIONS WITH THE SKYRME INTERACTION

(I). Spherical description

M. BEINER, H. FLOCARD and NGUYEN VAN GIAI

TABLE 5

Binding energy per particle E/A, Fermi momentum k_F, incompressibility coefficient K, effective mass ratio m^*/m and symmetry coefficients ε_1 and ε_2 [see eq. (17)] in nuclear matter calculated with the interactions SII to SVI

	t_3 (MeV fm^6)	E/A (MeV)	k_F (fm^{-1})	K (MeV)	m^*/m	ε_1 (MeV)	ε_2 (MeV)
SVI	17000	−15.77	1.29	364	0.95	26.89	0.67
SIII	14000	−15.87	1.29	356	0.76	28.16	0.83
SII	9331	−16.00	1.30	342	0.58	34.2	1.10
SIV	5000	−15.98	1.31	325	0.47	31.22	1.37
SV	0	−16.06	1.32	306	0.38	32.72	1.70

The interactions have been ordered according to the decreasing values of the parameter t_3.

The density dependence causes havoc

Particle-number projection impossible

Strong self interaction present

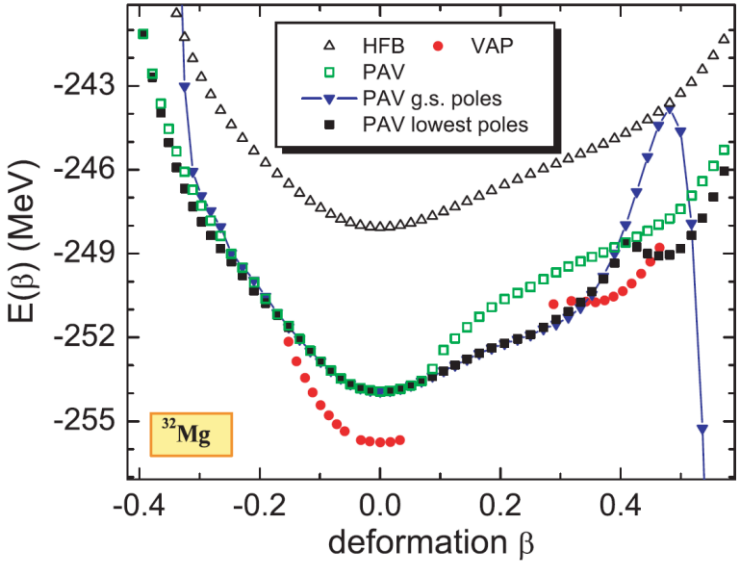


FIG. 11. (Color online) Deformation energy $E(\beta)$ as a functio quadrupole deformation β calculated for ^{32}Mg with the SIII force volume pairing interaction. Results of the PAV HFB+LN calculati (squares and triangles) are compared with the VAP PNP results (d The standard HFB result is shown by open triangles.

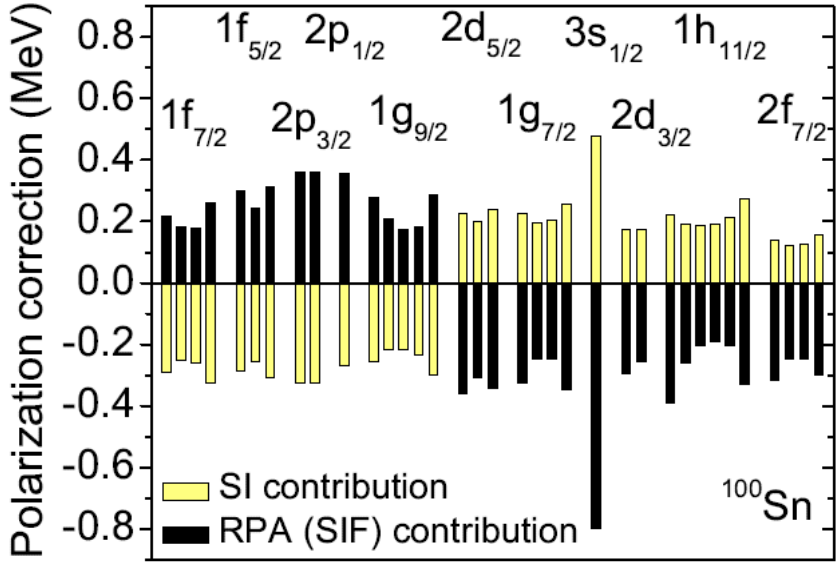
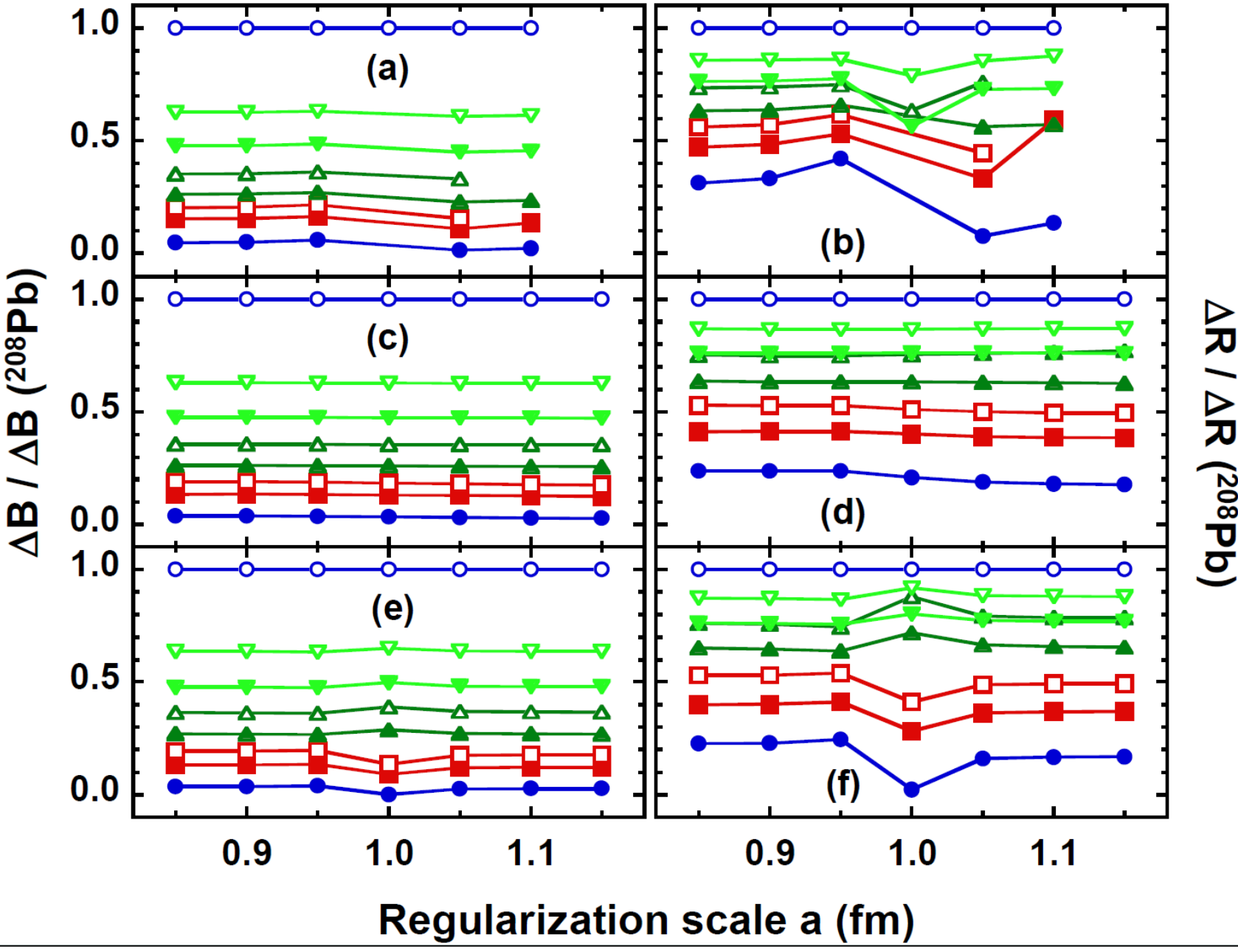


FIG. 6: (Color online) The SIF and SI contributions to the polarization corrections of Eq. (46), calculated in ^{100}Sn for the Skyrme EDF SLy5.

J.D. *et al.*, Phys. Rev. C 76, 054315 (2007)

D. Tarpanov. *et al.*, Phys. Rev. C 89, 014307 (2014)

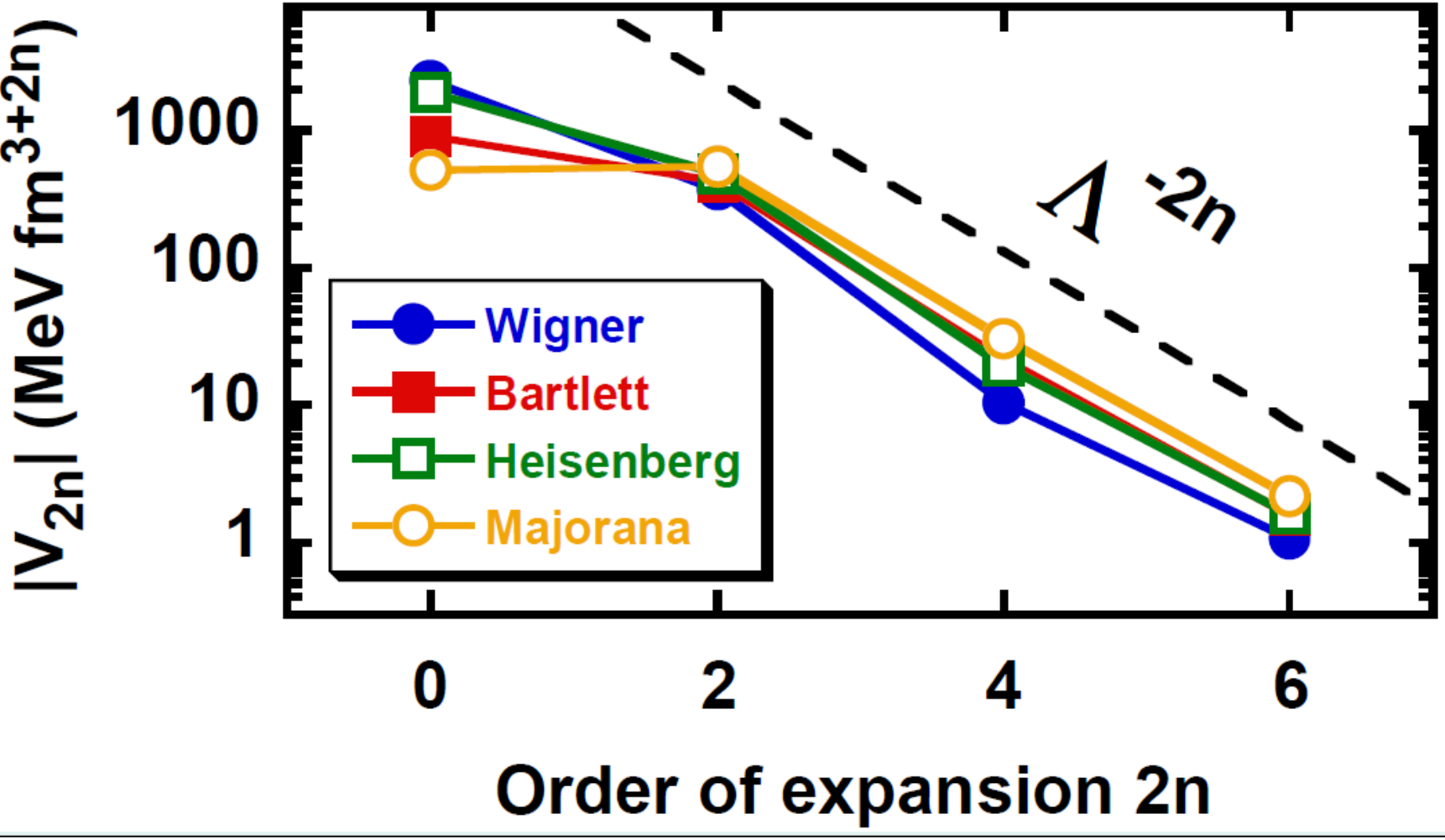
Regularized pseudopotentials vs. Gogny



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

Coupling constants of the regularized pseudopotentials

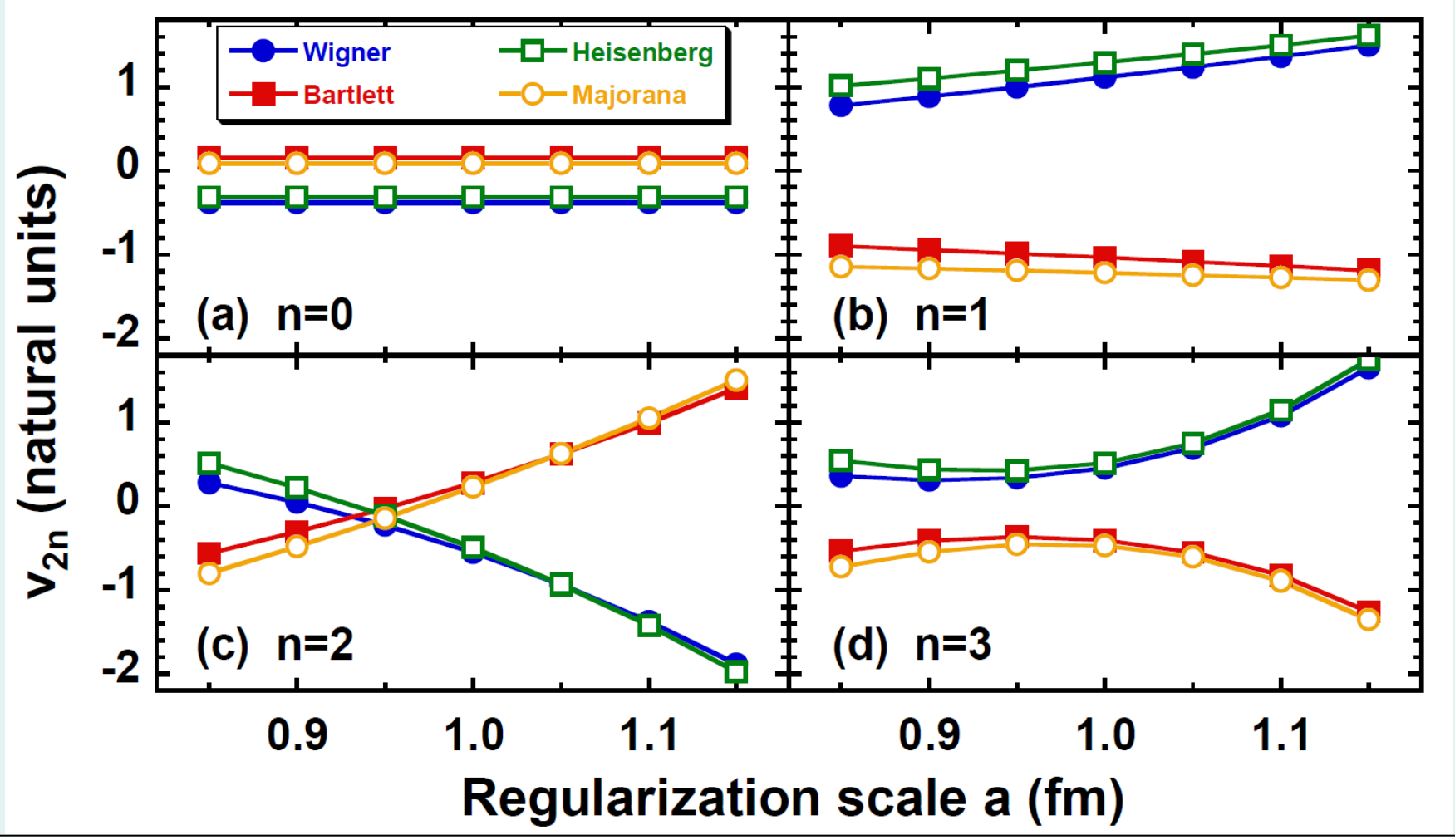
$\Lambda \approx 700$ MeV/$\hbar c \approx 3.8$ fm^{-1}



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)

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

Polarization corrections & self-interaction

$$E^A = \mathrm{Tr}(t\rho^A) + \tfrac{1}{2}\mathrm{Tr}_1\mathrm{Tr}_2(\rho^A \bar{v}[\rho^A]\rho^A), \tag{38a}$$

$$E^{A\pm1} = \mathrm{Tr}(t\rho^{A\pm1}) + \tfrac{1}{2}\mathrm{Tr}_1\mathrm{Tr}_2(\rho^{A\pm1} \bar{v}[\rho^{A\pm1}]\rho^{A\pm1}). \tag{38b}$$

antisymmetric, the SI term (44b),

$$E^\lambda_{\mathrm{SI}} = \tfrac{1}{2}\tilde{\tilde{h}}^\lambda_{\lambda\lambda}, \tag{45}$$

Self-interaction

is nonzero, and explicitly appears in Eq. (43). This leads to corrections to s.p. energies now having the form,

$$\delta e_\lambda = \pm\delta E = \pm\left(\delta E^\lambda_{\mathrm{SIF}} + E^\lambda_{\mathrm{SI}}\right), \tag{46}$$

where, based on the analogy with Eq. (37), the first term can be called self-interaction-free (SIF) polarization correction,

$$\delta E^\lambda_{\mathrm{SIF}} = -\sum_{\omega>0} \frac{\left|\sum_{\mathrm{ph}} \tilde{\tilde{h}}^{\lambda *}_{\mathrm{ph}} X^\omega_{\mathrm{ph}} + \tilde{\tilde{h}}^\lambda_{\mathrm{ph}} Y^\omega_{\mathrm{ph}}\right|^2}{\hbar\omega}. \tag{47}$$

RPA: Self-interaction free

$$\tilde{\tilde{h}}^\lambda_{i'i} = \sum_{k'k} \left.\frac{\partial \tilde{h}_{i'i}}{\partial \rho_{k'k}}\right|_{\rho=\rho^A} \rho^\lambda_{k'k},$$

D. Tarpanov *et al.*, Phys. Rev. C89, 014307 (2014)