MR-DFT - past, present, and future

Jacek Dobaczewski
University of York, University of Jyväskylä, University of Warsaw

Workshop on MR-DFT - past, present, and future
University of Warsaw
25-26 June 2015, Warsaw, Poland

UNIVERSITY of York

UNIVERSITY OF WARSAW

JYVÄSKYLÄN YLIOPISTO
UNIVERSITY OF JYVÄSKYLÄ

Past

1. MR-DFT is mandatory for:
   a) collective excitations
   b) symmetry restoration
2. MR-DFT technology well developed over the years
3. Density dependence is incompatible with MR-DFT
4. Simple regularization scheme is possible
5. A crisis has been born – should we continue "saving the furniture"?

The density dependence causes havoc

Particle-number projection impossible

Strong self interaction present

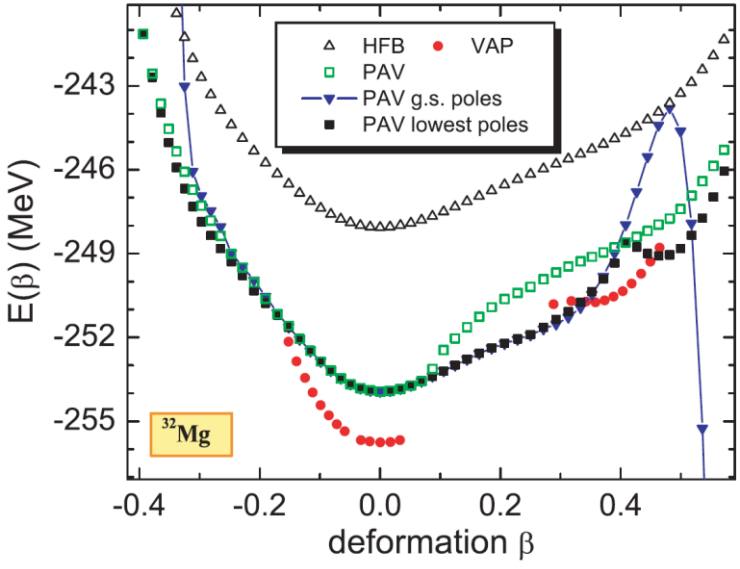


FIG. 11. (Color online) Deformation energy $E(\beta)$ as a functio quadrupole deformation β calculated for ^{32}Mg with the SIII force volume pairing interaction. Results of the PAV HFB+LN calculati (squares and triangles) are compared with the VAP PNP results (d The standard HFB result is shown by open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

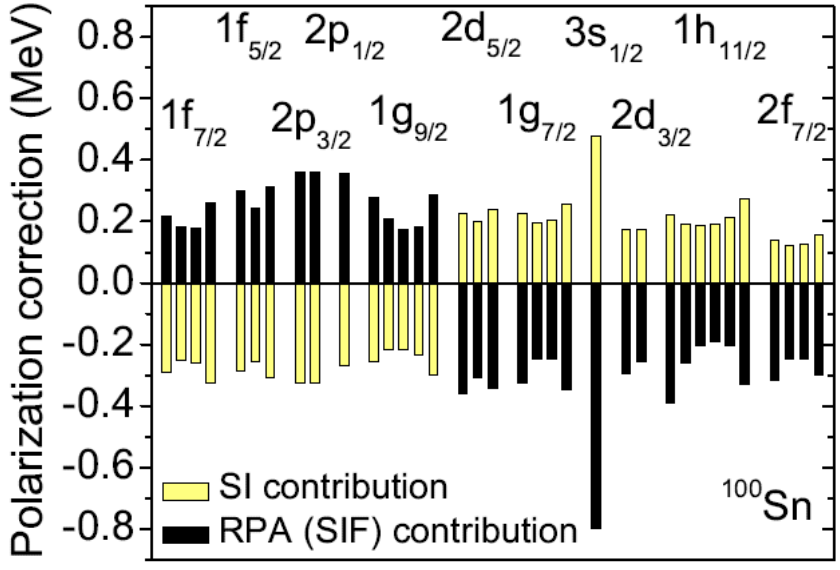
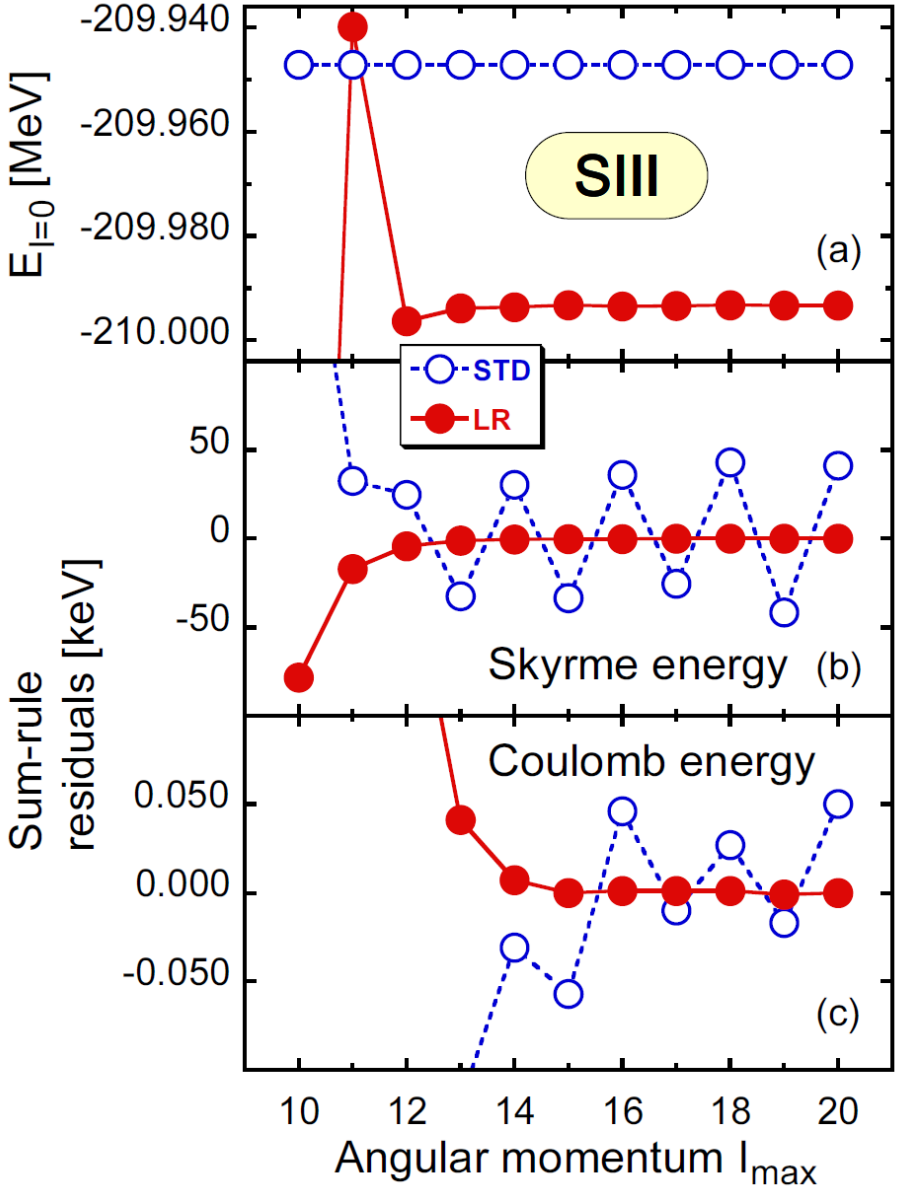


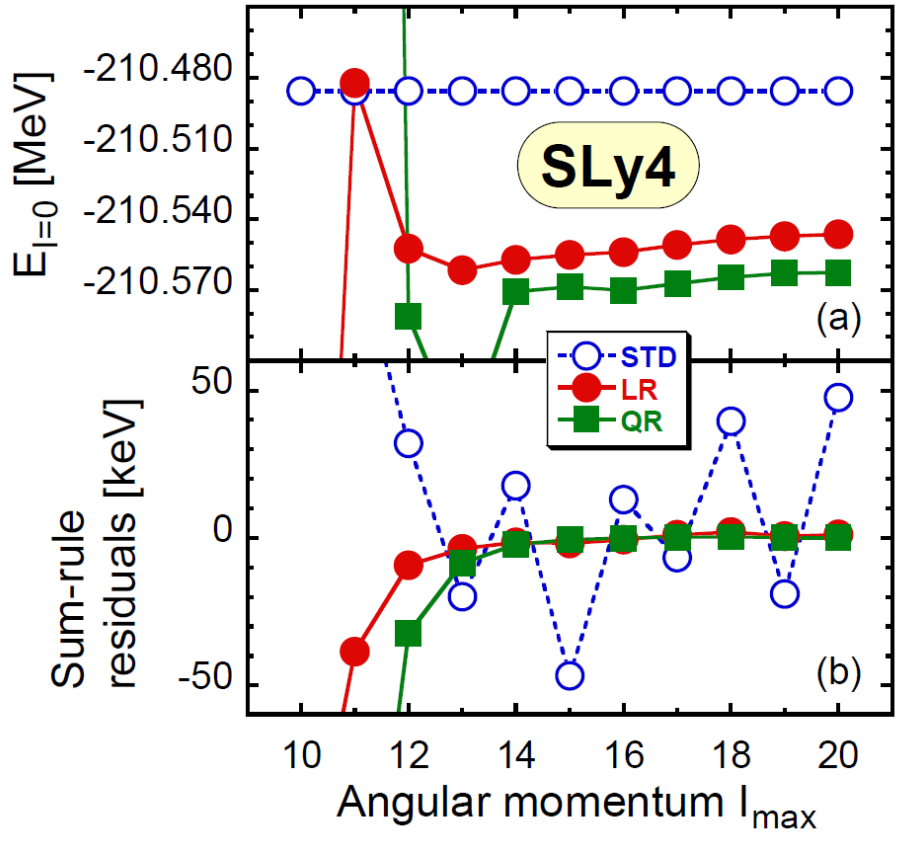
FIG. 6: (Color online) The SIF and SI contributions to the polarization corrections of Eq. (46), calculated in ^{100}Sn for the Skyrme EDF SLy5.

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

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

Simple regularization scheme for multireference density functional theories





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

Present

1. SR-DEFT and MR-DFT based on the EDF generators
2. Pseudopotentials as suitable EDF generators
3. Zero-range, regularized zero-range, finite range (pseudo)potentials
4. Gaussian, Yukawa, ... , formfactors/regulators
5. Expansion in derivatives
6. Three-body, four-body, ... ,

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)

Future

1. More work on the present-day ideas
2. *Ab initio* derivations of the MR-DFT kernels
3. *Ab initio* derivations of model EDFs

Ab initio derivations 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,

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

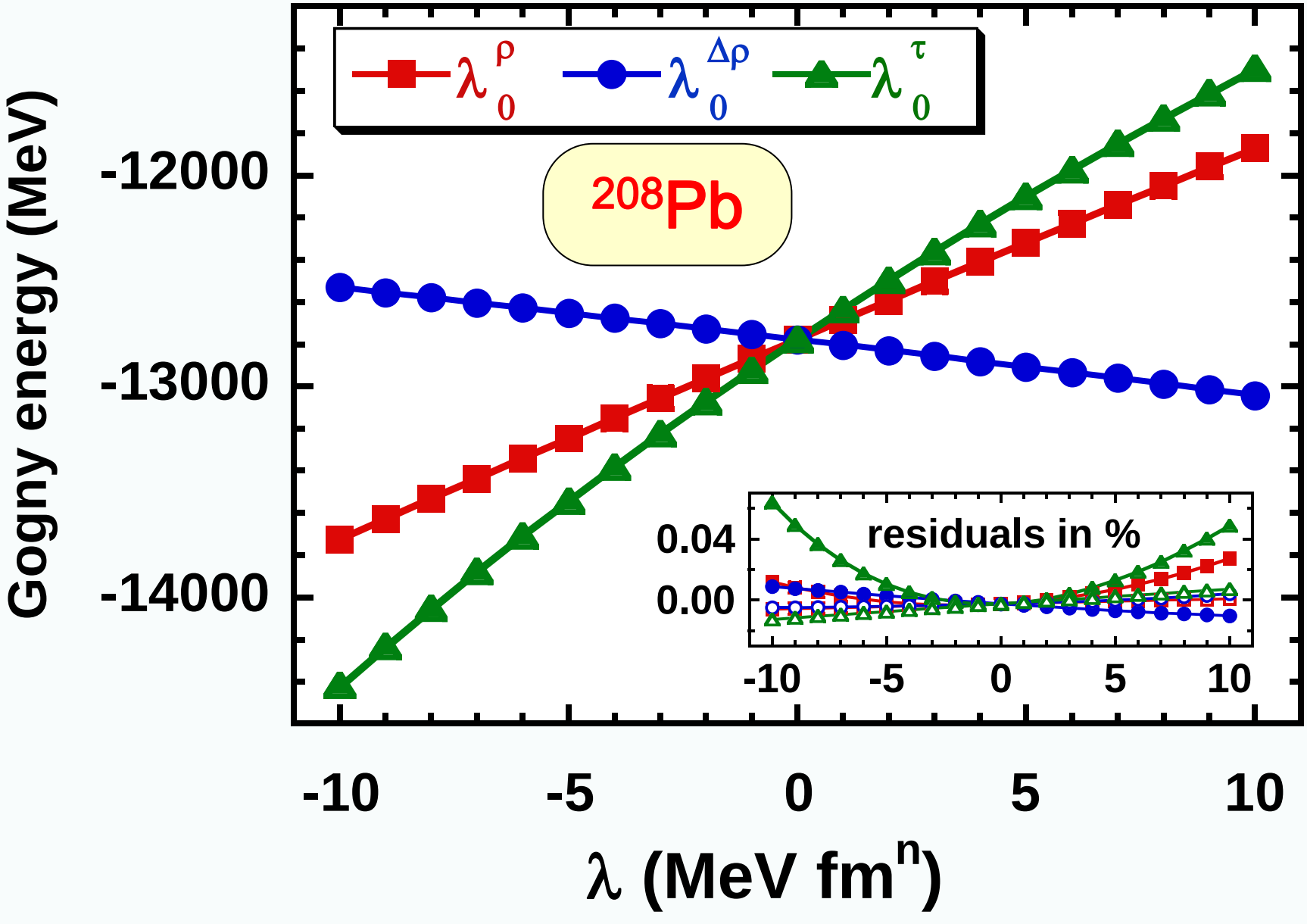
for a suitable set of values of a finite number of Lagrange multipliers λ^i, which is perfectly manageable a task.

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., to be published

Ab initio derivations of model EDFs



J.D., to be published

Ab initio derivations of model EDFs

S1Sd

		$t=0$	$t=1$
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 S1Sd.

	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., to be published

Thank you

Skyrme's three-body interaction

1.C:
1.D.1

Nuclear Physics **9** (1959) 615—634; © *North-Holland Publishing Co., Amsterdam*
Not to be reproduced by photoprint or microfilm without written permission from the publisher

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

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

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:

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

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*

Not to be reproduced by photoprint or microfilm without written permission from the publisher

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.

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

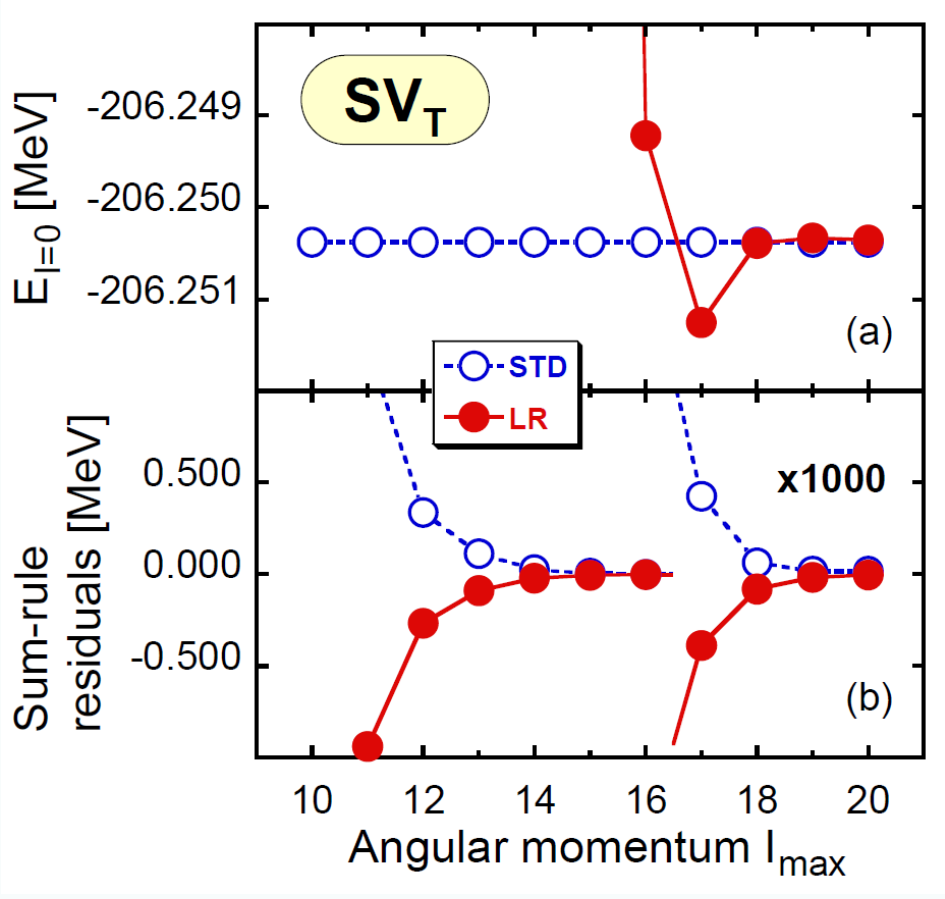
$$A^{IMK}_{I'M'K'} = \sum_{I''M''K''} c^{\mathcal{N}}_{I''M''K''}\mathrm{C}^{IM}_{I''M''I'M'}\mathrm{C}^{IK}_{I''K''I'K'}.$$

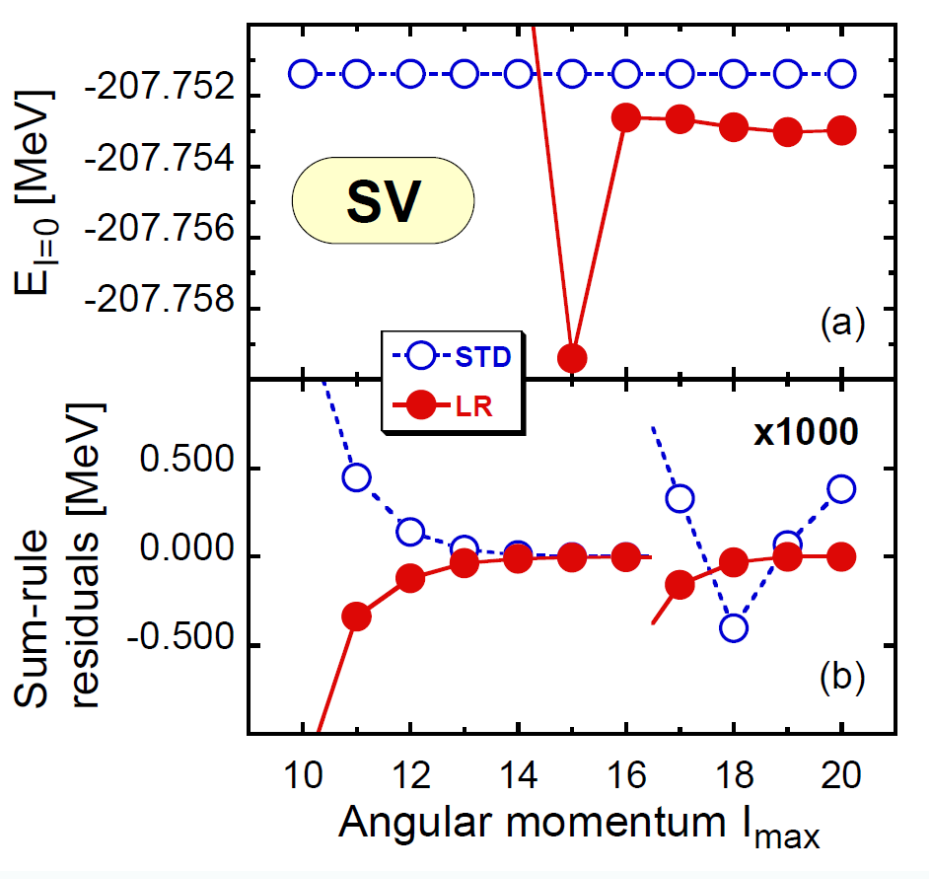
The problem of finding the regularized matrix elements is thus reduced to calculating auxiliary quantities and then solving a set of linear equations.

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)

Polarization corrections & self-interaction

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

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

antisymmetric, the SI term (44b),

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

Self-interaction

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

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

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

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

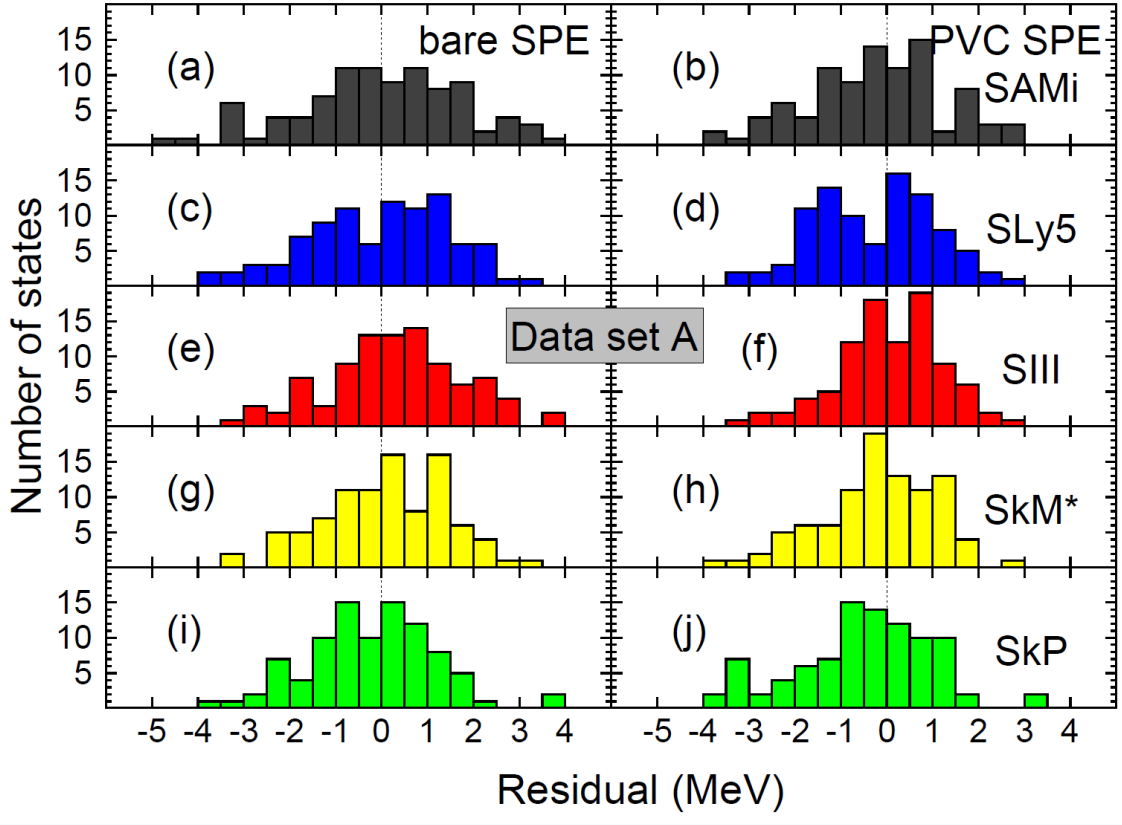
RPA: Self-interaction free

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

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

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*, Phys. Rev. Lett. 113, 252501 (2014)

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,

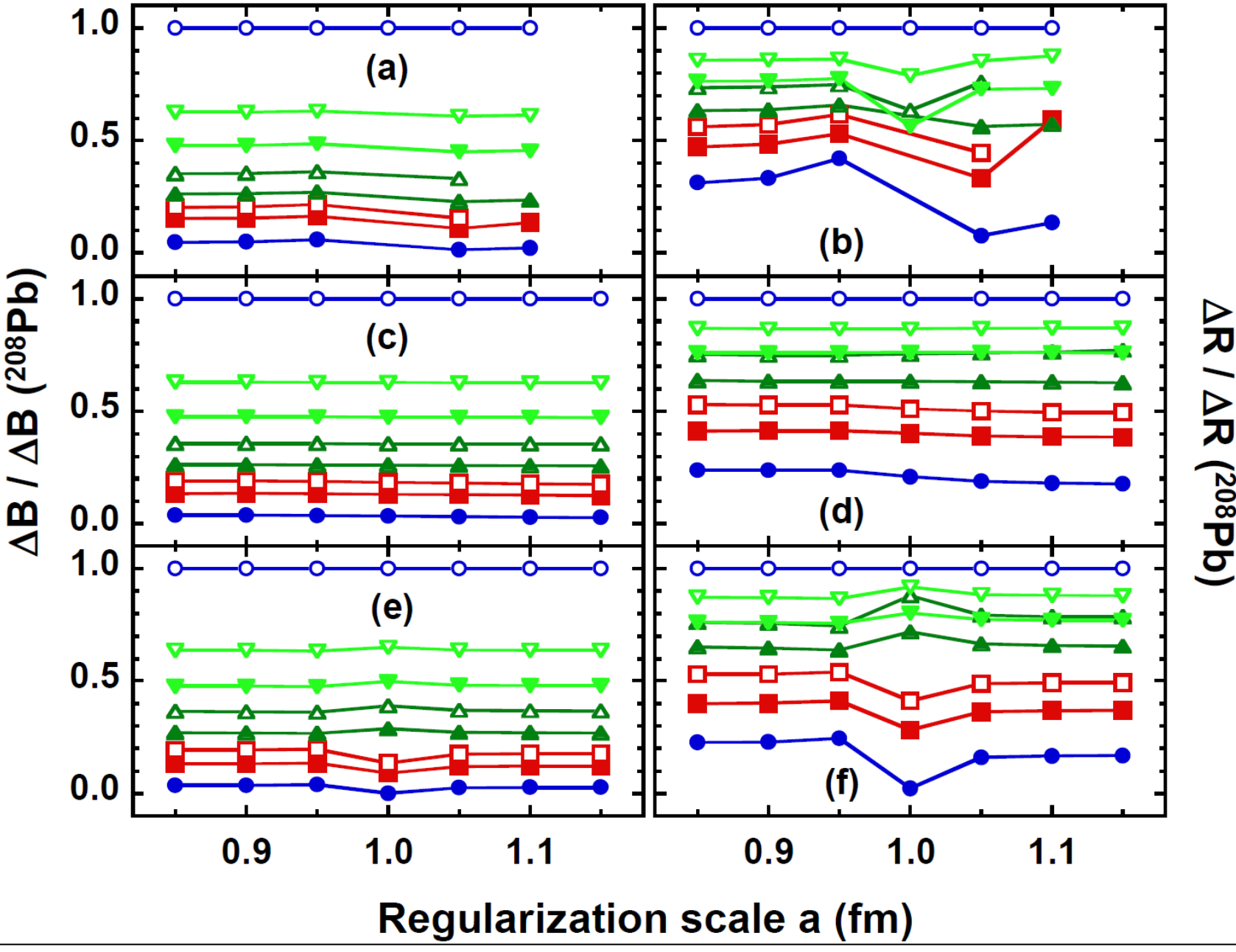
$$M_{2m}^{(i)} \equiv \int r^{2m} G_i(r) \mathrm{d}^3 r = \int r^{2m} V_i(r) \mathrm{d}^3 r,$$

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.

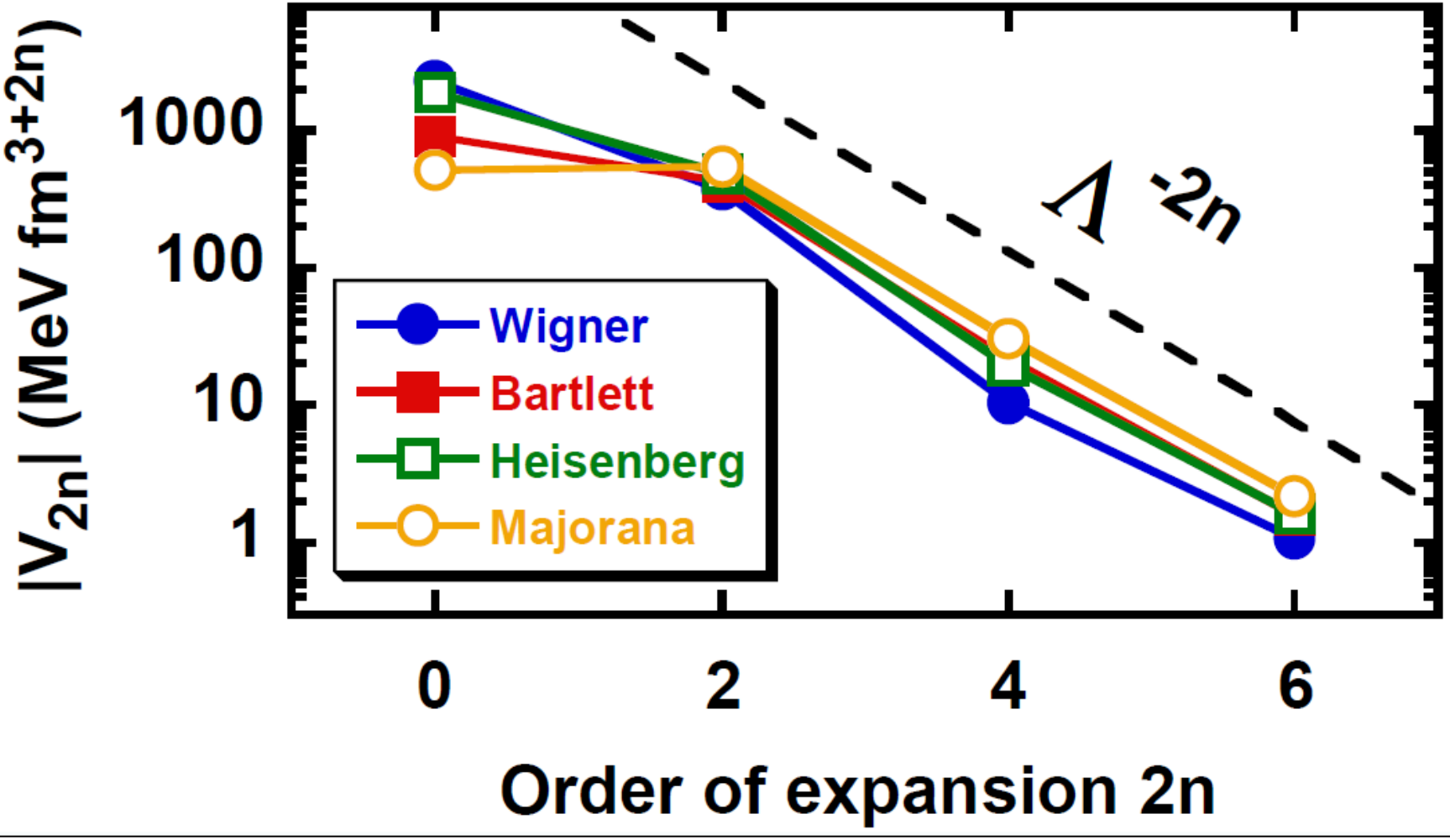
Regularized pseudopotentials vs. Gogny



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

Coupling constants of the regularized pseudopotentials

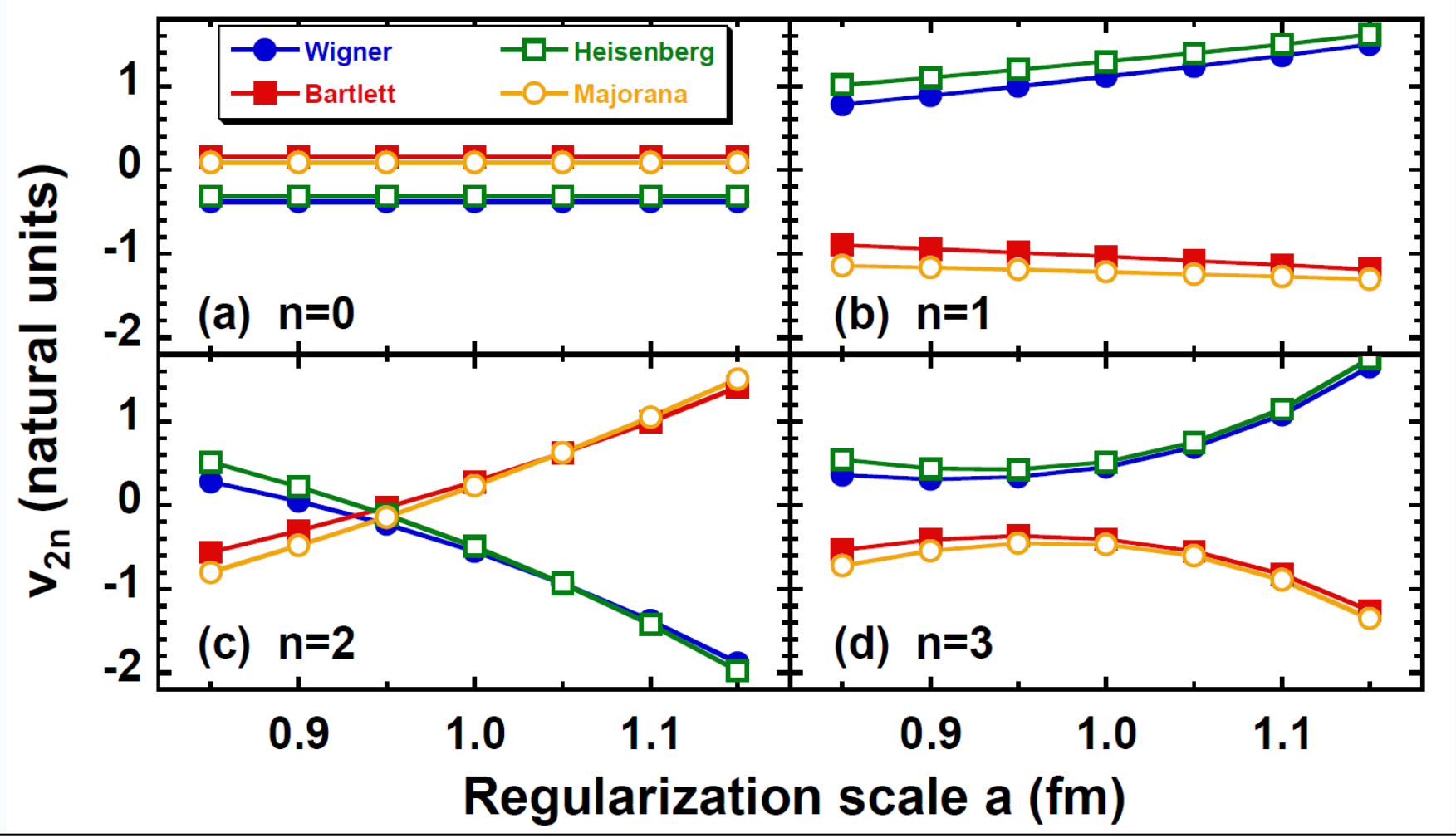
$\Lambda \approx 700$ MeV/$\hbar c \approx 3.8$ fm^{-1}



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)

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:

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

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

Naming conventions

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

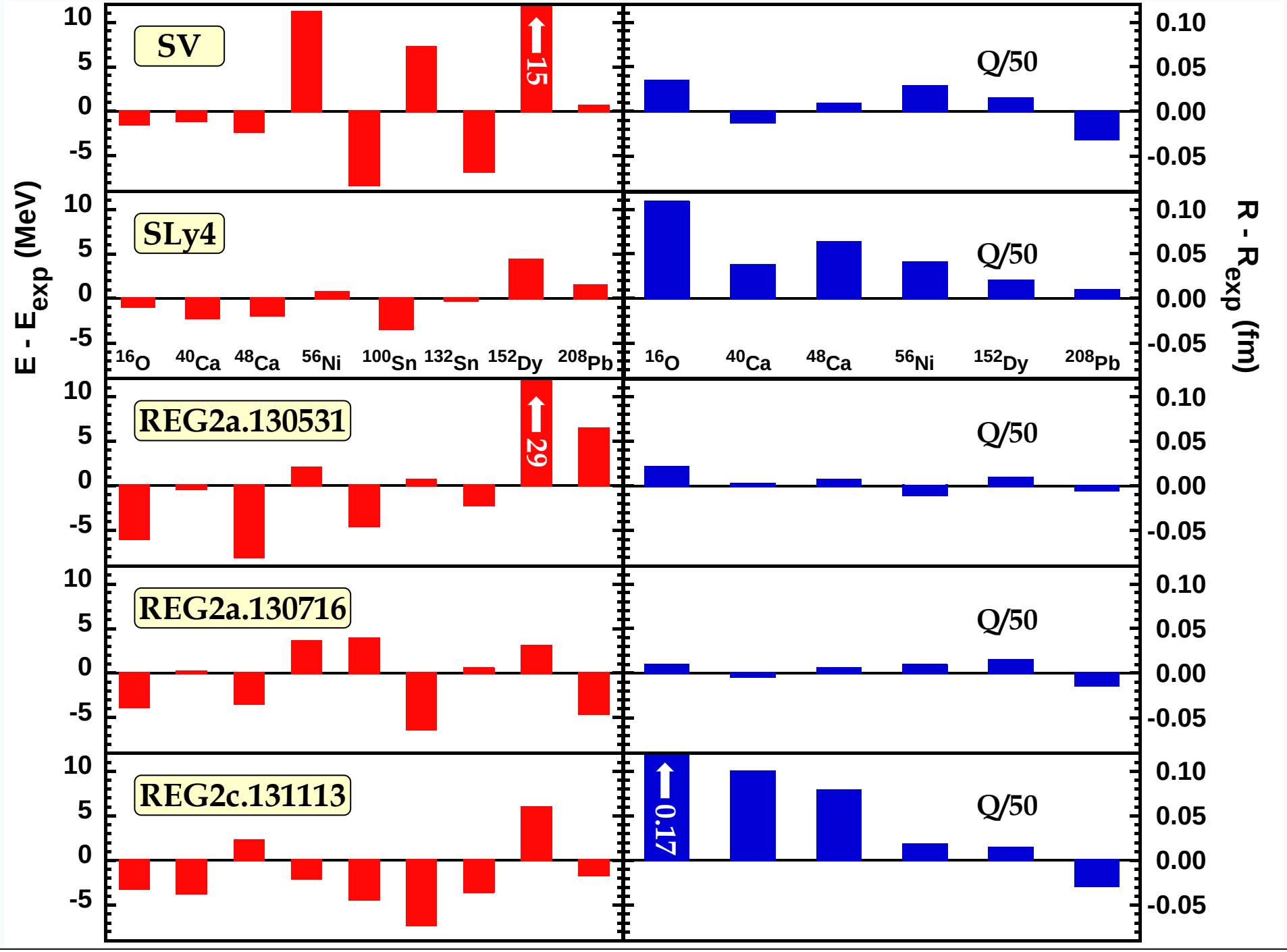
$$\hat{O}_i(\vec{k}\,',\vec{k}) \;=\; \sum\nolimits_{nj} T_j^{(ni)} \hat{O}_j^{(n)}(\vec{k}\,',\vec{k})$$

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

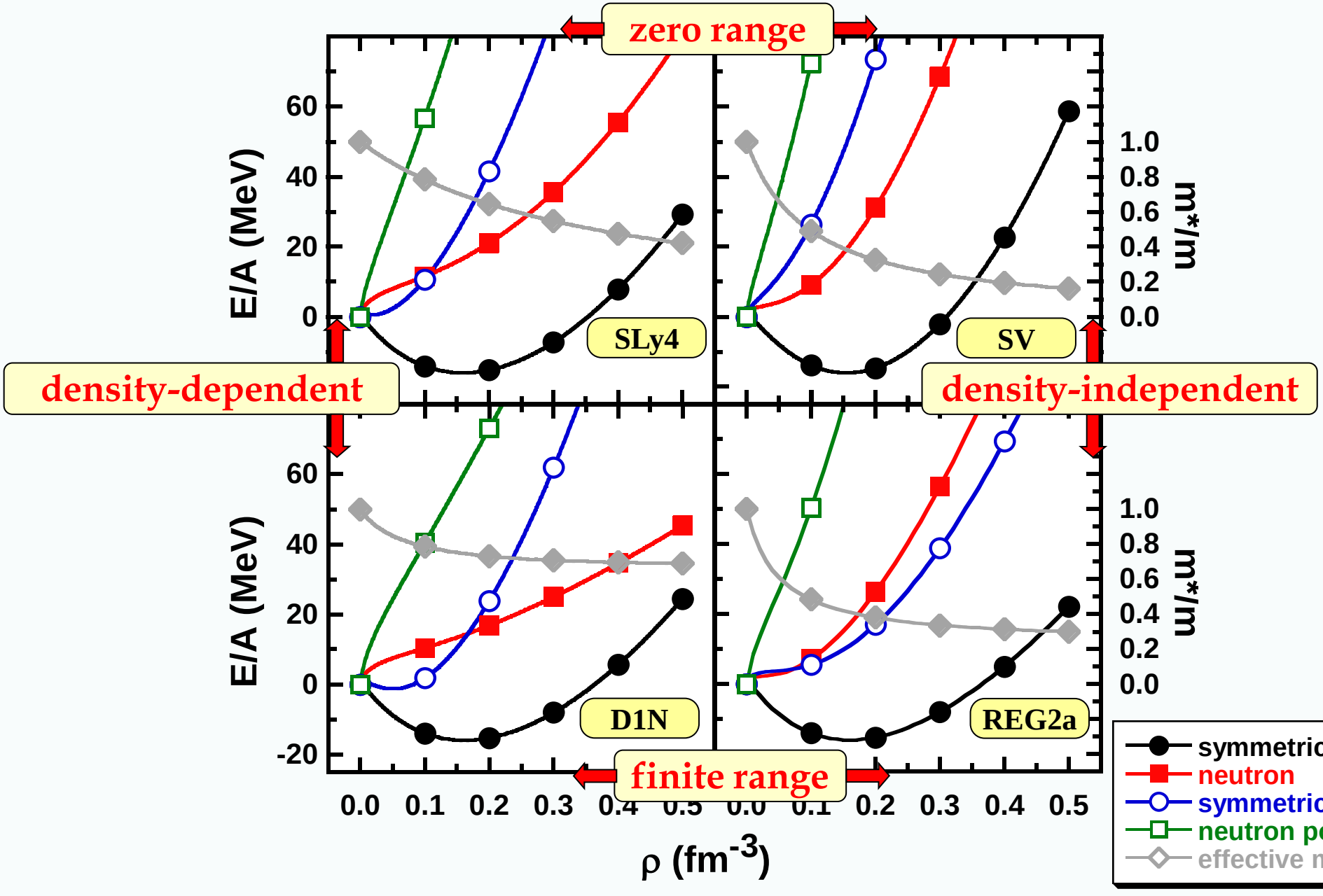
REG2b.date $\Longrightarrow$ 2nd order (NLO), $T_2^{(2i)} \neq -T_1^{(2i)}$

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
17
E - E_exp (MeV)
R - R_exp (fm)
16O 40Ca 48Ca 56Ni 100Sn 132Sn 152Dy 208Pb

Equations of state



K. Bennaceur, J.D., F. Raimondi, EPJ WoC 66, 02031 (2014)

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