# Novel energy density functionals for low-energy nuclear phenomena

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# Outline

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# 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

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

Direct

Exchange

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3/16

# Standard effective interactions

- ## Gogny*

$$V(\vec{r}_1\vec{r}_2; \vec{r}\,'_1\vec{r}\,'_2) = \delta(\vec{r}_1 - \vec{r}\,'_1)\delta(\vec{r}_2 - \vec{r}\,'_2)V(\vec{r}_1 - \vec{r}_2),$$

where,

$$V(\vec{r}_1 - \vec{r}_2) = \sum_{i=1,2} e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_i^2} \times (W_i + B_iP_\sigma - H_iP_\tau - M_iP_\sigma P_\tau)$$

$$+t_3(1 + P_\sigma)\delta(\vec{r}_1 - \vec{r}_2)\rho^{1/3}\left[\tfrac{1}{2}(\vec{r}_1 + \vec{r}_2)\right].$$

$P_\sigma = \tfrac{1}{2}(1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2)$ and $P_\tau = \tfrac{1}{2}(1 + \vec{\tau}_1 \cdot \vec{\tau}_2)$ 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 $\mu_i = 0.7$ and $1.2\,\text{fm}$, $W_i$, $B_i$, $H_i$, $M_i$, and $t_3$ are parameters.
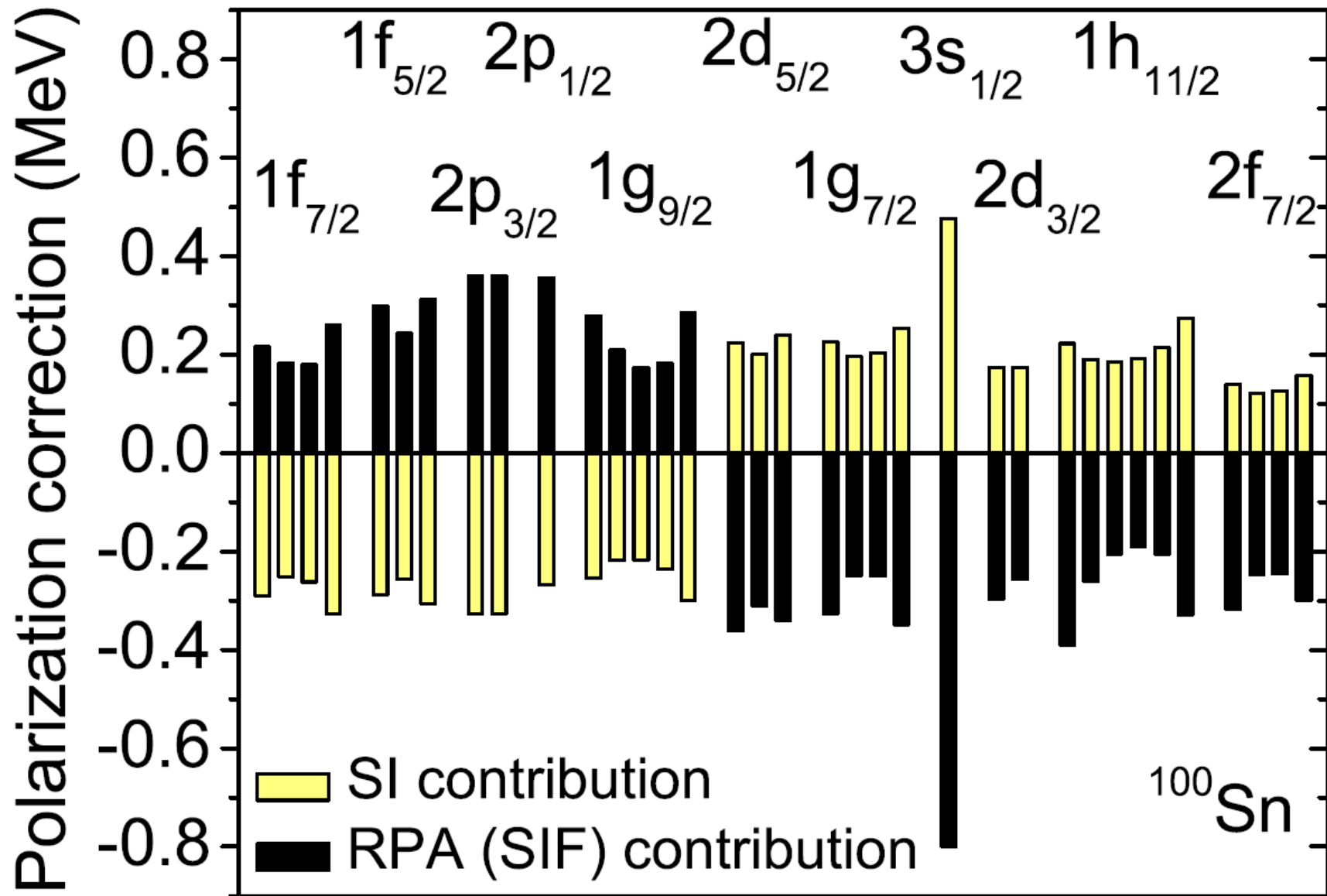
- ## Skyrme*

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

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

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

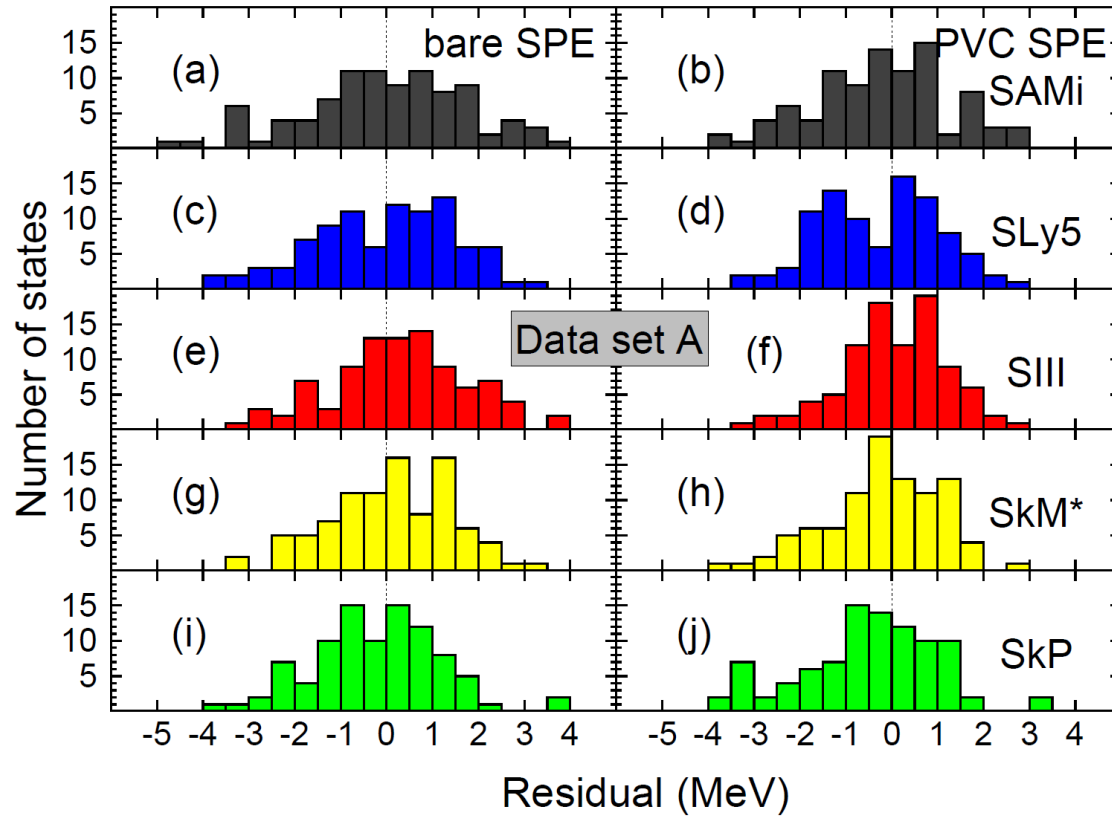*We omit the spin-orbit and tensor terms for simplicity.

# Self Interaction

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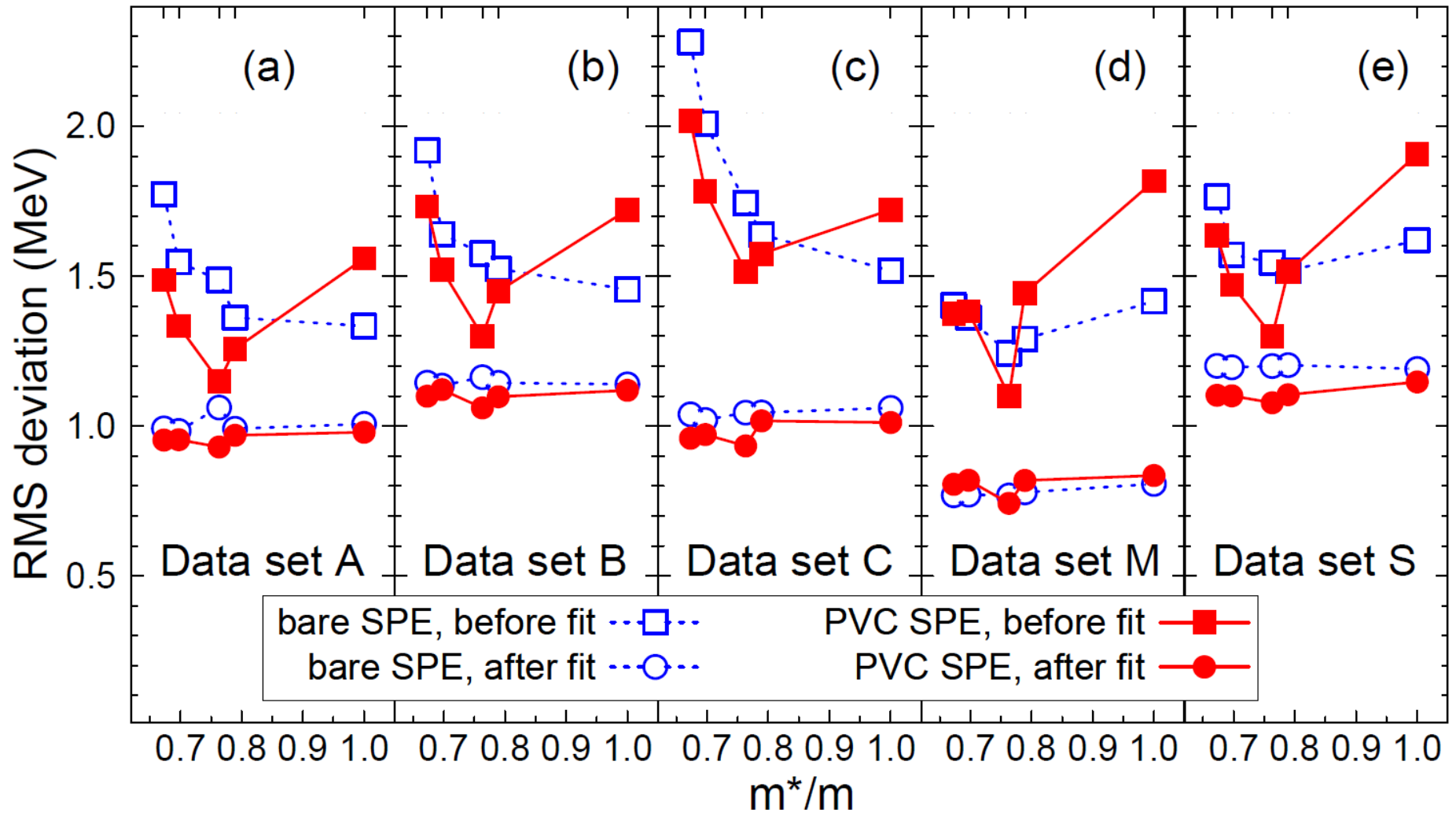
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# Particle-vibration-coupling (PVC) corrections

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

$$\left.+\sum_{nJh}\frac{|\langle i||V||h,nJ\rangle|^2}{\epsilon_i-\epsilon_h+\hbar\omega_{nJ}-i\eta}\right),$$



D. Tarpanov et al., arXiv:1405.4823

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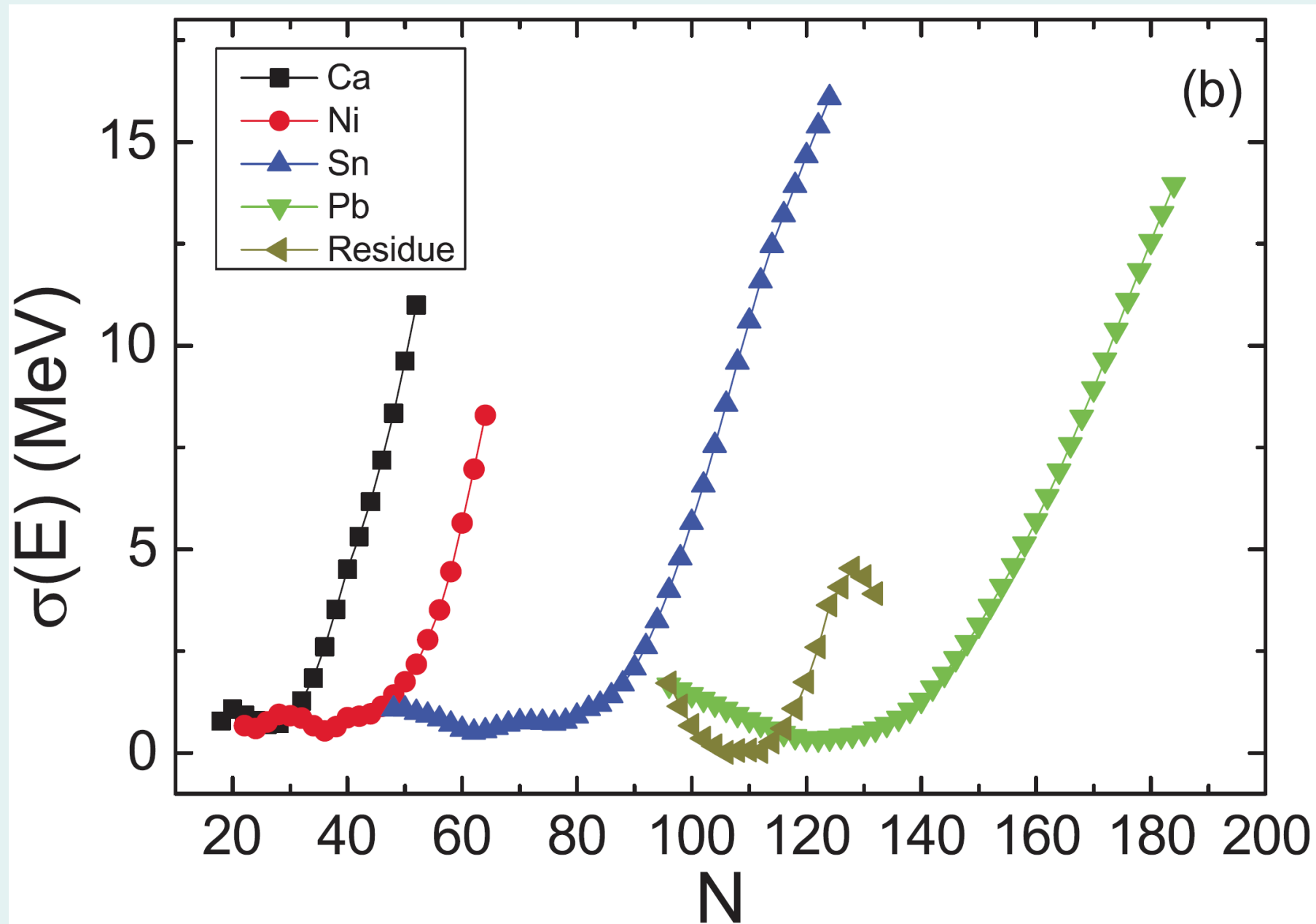UNIVERSITY OF JYVÄSKYLÄ

# Particle-vibration-coupling (PVC) corrections



D. Tarpanov et al., arXiv:1405.4823

# Propagation of uncertainties



(b)

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

# non-relativistic EDF @ ARIS2014

| Class/ Author | range | | locality | | | derivatives | | | | pseudopotential-based | density dependence | many-body | | | parameters exist? | Token acronym |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | zero-range | finite-range | local pseudopotential | quasilocal EDF | nonlocal EDF | zero order | 2nd order | 4th order | 6th order | | | two-body | three-body | four-body | | |
| Skyrme | X | | | X | | | X | | | | X | X | | | X | UNEDF2 |
| Skyrme | X | | | X | | | X | | | X | | X | | | X | SV |
| Gogny | | X | X | | X | X | | | | | X | X | | | X | D1S |
| Nakada | | X | X | | X | X | | | | | X | X | | | X | M3Y |
| Carlsson | X | | | X | | | | | X | | X | X | | | | |
| Sadoudi | X | | | X | | | X | | | X | | X | X | X | X | SLyMR0 |
| Sadoudi | X | | | X | | | X | | | X | | X | X | | | |
| Bennaceur | | X | X | | X | X | | | | X | | X | | | X | REG2a |
| Bennaceur | | X | | | X | | X | | | X | | X | | | X | REG2b |
| Bennaceur | | X | | | X | | X | | | | X | X | | | X | REG2c |
| Raimondi | | X | | | X | | | | X | X | | X | | | | |

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9/16

# 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,

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

$K_{\tilde{n}\tilde{L}}$ 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,

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

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.

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# Quasilocal EDF up to N³LO

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 $n$th-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 $m$th-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.

# Regularized 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,

$$V(\vec{r}_1 \vec{r}_2; \vec{r}\,'_1 \vec{r}\,'_2) = \sum_{i=1}^{4} \hat{P}_i \hat{O}_i(\vec{k}, \vec{k}\,') \delta(\vec{r}_1 - \vec{r}\,'_1) \delta(\vec{r}_2 - \vec{r}\,'_2) g_a(\vec{r}_1 - \vec{r}_2),$$
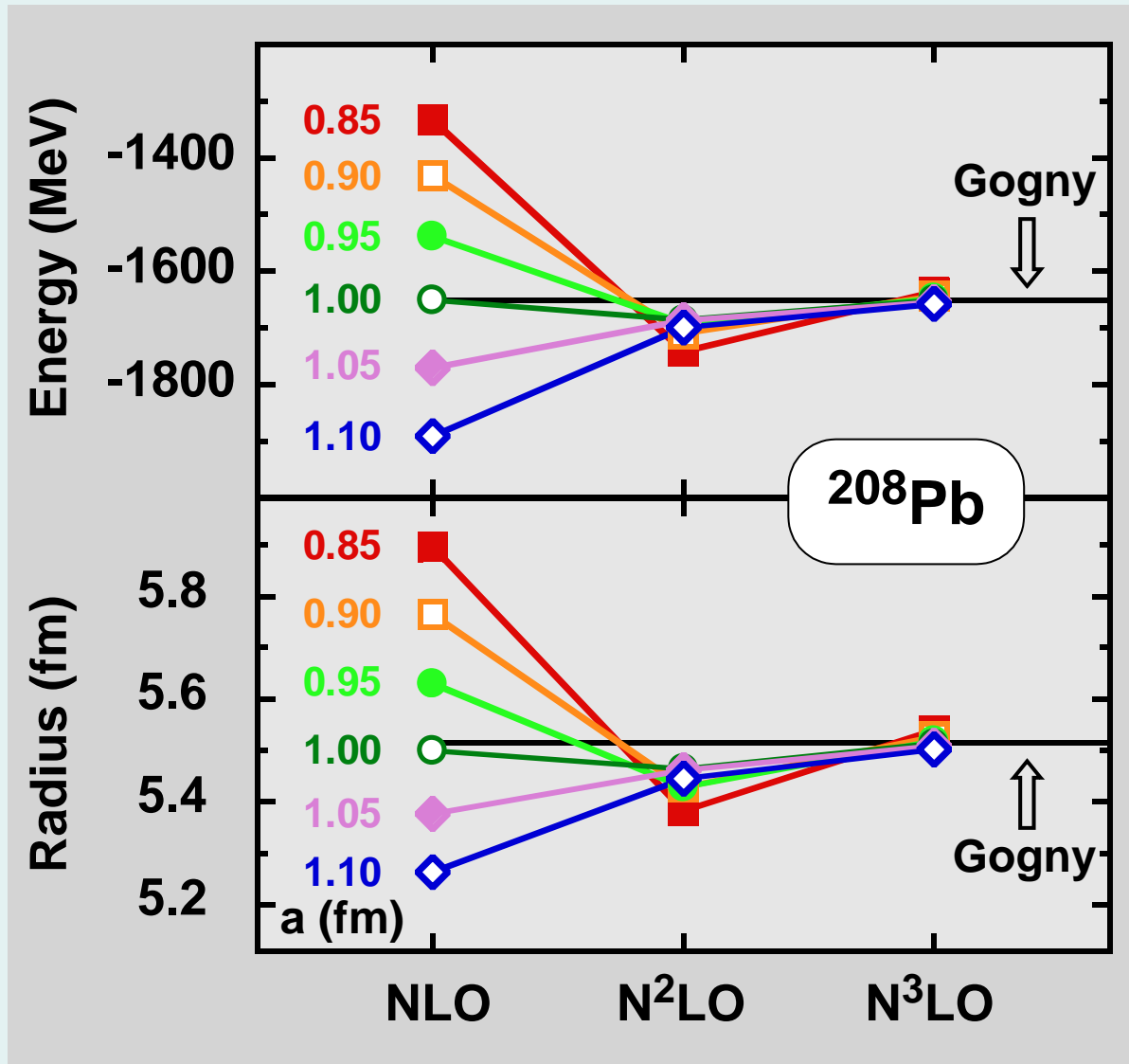
where $\vec{k} = \frac{1}{2i}(\vec{\nabla}_1 - \vec{\nabla}_2)$ and $\vec{k}' = \frac{1}{2i}(\vec{\nabla}\,'_1 - \vec{\nabla}\,'_2)$ are the standard relative-momentum operators, and the Wigner, Bartlett, Heisenberg, and Majorana terms are given by the standard spin and isospin exchange operators, $\hat{P}_1 \equiv 1$, $\hat{P}_2 \equiv \hat{P}_\sigma$, $\hat{P}_3 \equiv -\hat{P}_\tau$, $\hat{P}_4 \equiv -\hat{P}_\sigma \hat{P}_\tau$.

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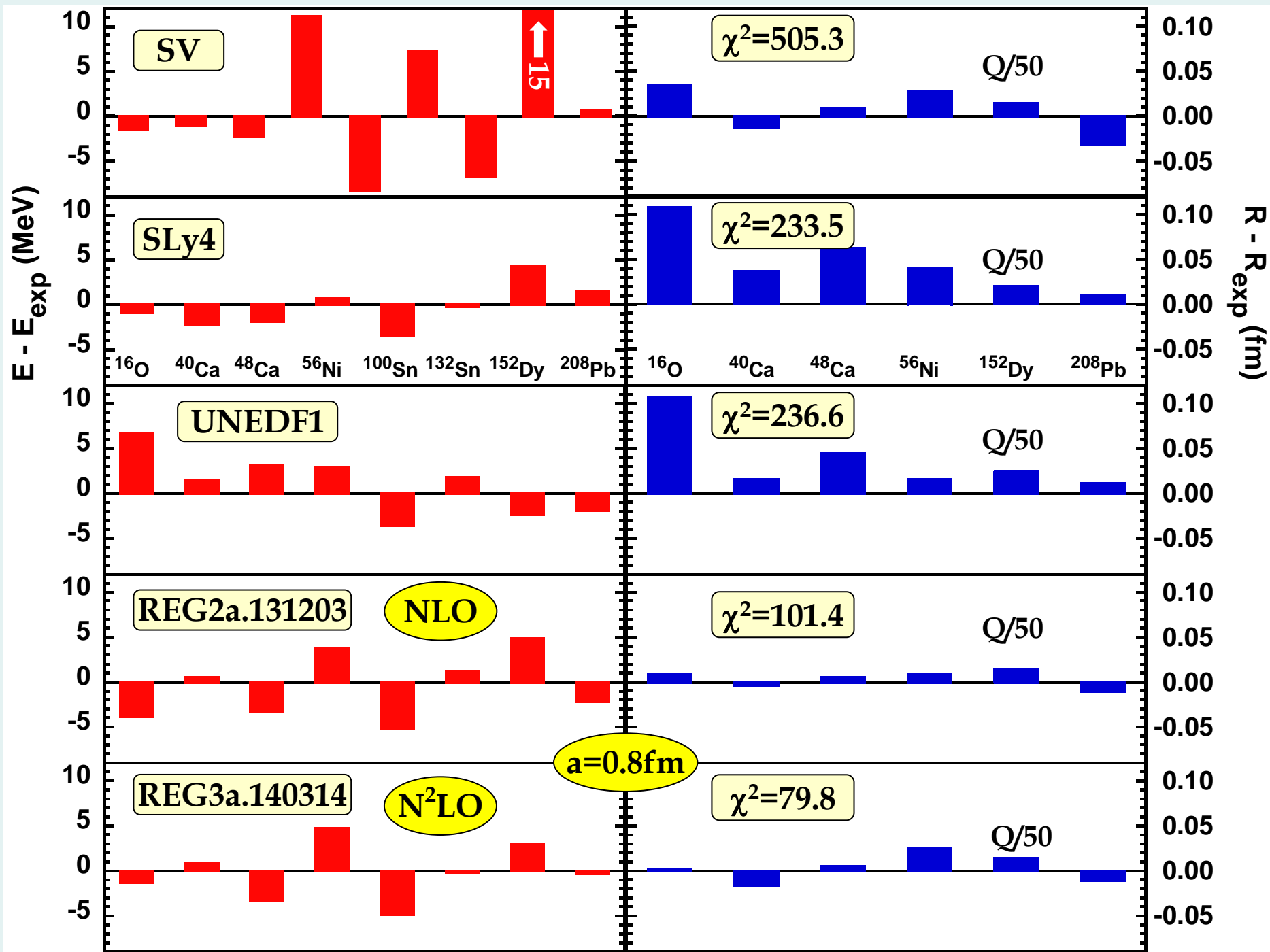
$$\hat{O}_i(\vec{k}, \vec{k}') = T_0^{(i)} + \frac{1}{2} T_1^{(i)} \left(\vec{k}'^{*2} + \vec{k}^2\right) + T_2^{(i)} \vec{k}'^* \cdot \vec{k},$$

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

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# Regularized pseudopotentials vs. Gogny

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



REG2c

Legend:
- symmetric
- neutron
- symmetric pol.
- neutron pol.
- effective mass
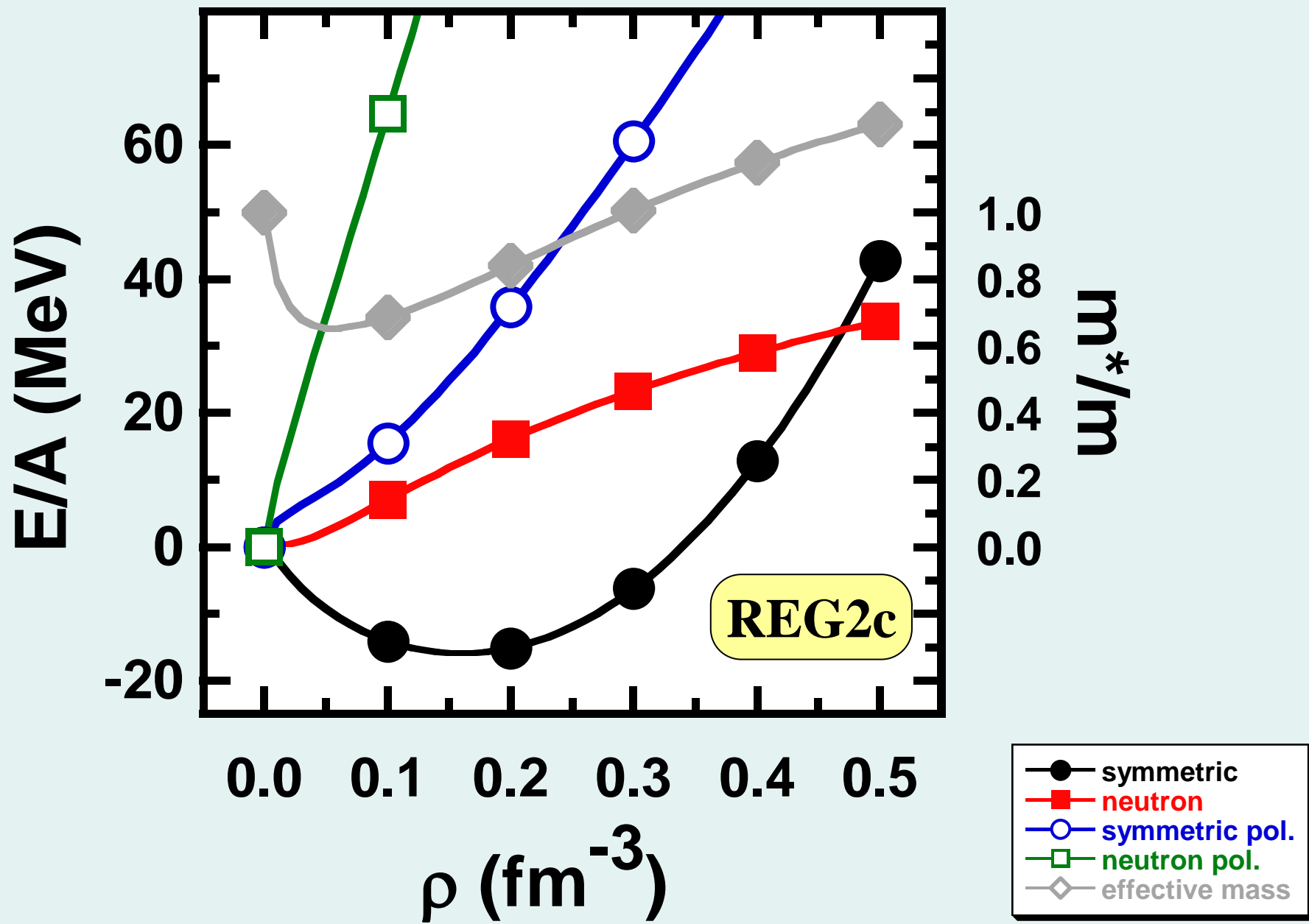
# Conclusions

1. Nuclear DFT provides us with one of the most spectacularly successful approaches in nuclear physics.
2. Based on a dozen odd parameters, nuclear DFT fairly well describes thousands of experimental data
3. In 2014, nuclear DFT lacks three things: precision, precision, and precision
4. New functionals are rooted in
   a) effective theories
   b) *ab initio* derivations
   c) systematic expansions
   d) correctible theory
   e) …

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# **Thank you**

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# 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:

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

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

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

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

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

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:

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

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# Regularized pseudopotentials vs. Gogny

Below we determine coupling constants $V_{2n}^{(i)}$ in Eq. (??) 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,

$$V_{2n}^{(i)} = \sum_{m=0}^{n} \left(-\frac{a^2}{4}\right)^{n-m} \frac{M_{2m}^{(i)}}{(n-m)!(2m+1)!}$$

$$= \frac{1}{4^n n!} \sum_{k=1,2} G_k^{(i)} \left(a_k^2 - a^2\right)^n,$$

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

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# Regularized pseudopotentials

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,

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

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 $\Delta$ 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 $2n$.

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