The 5th international conference on

"COLLECTIVE MOTION IN NUCLEI UNDER EXTREME CONDITIONS"

COMEX5

Coupling of single-particle motion to nuclear vibrations

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with: D. Tarpanov, J. Toivanen, and B.G. Carlsson

Kraków, Poland

September 14-18, 2015

The 5th international conference on
"COLLECTIVE MOTION IN NUCLEI UNDER EXTREME CONDITIONS"

COMEX5

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Krakó... ...and
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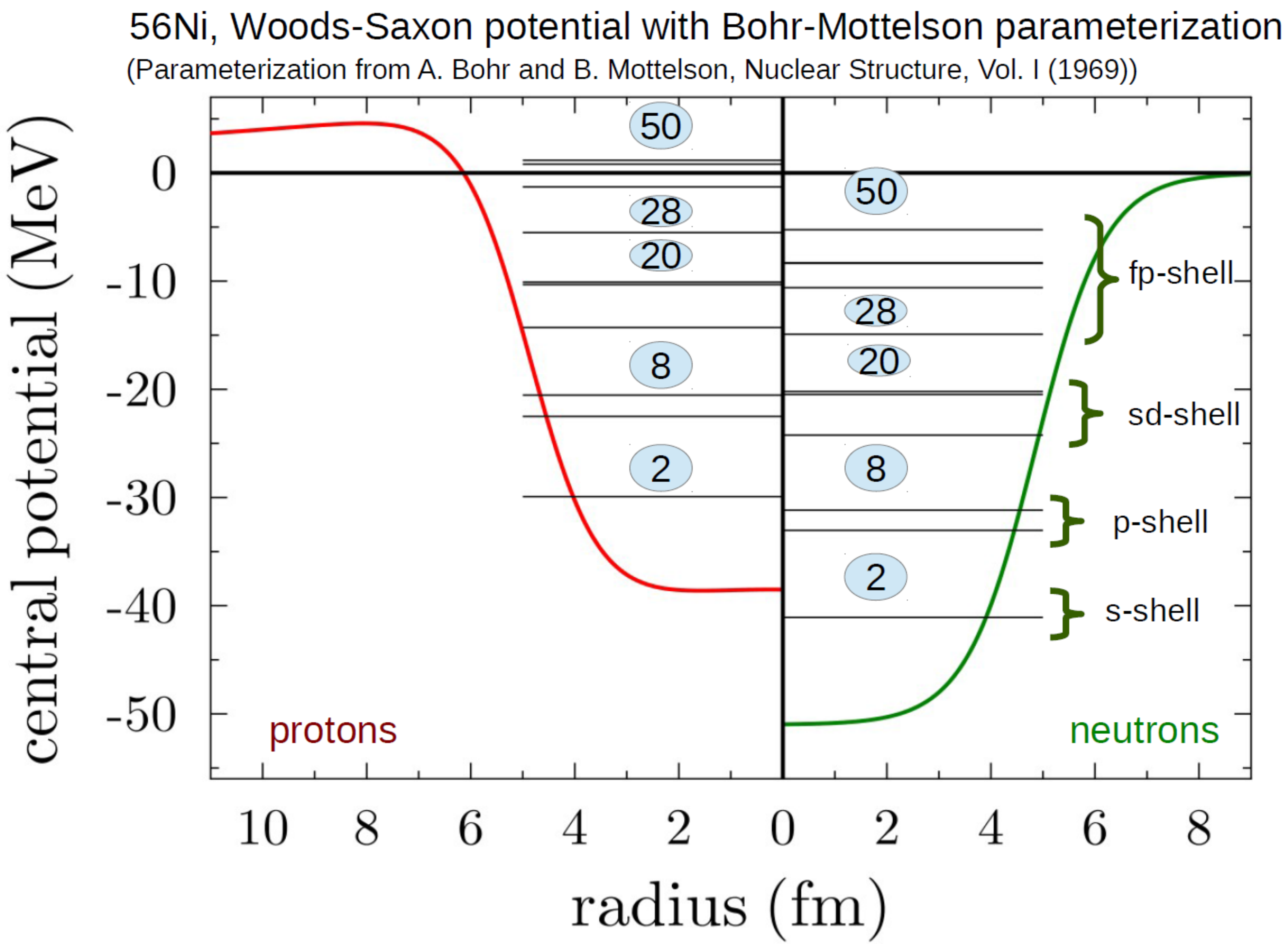
Outline

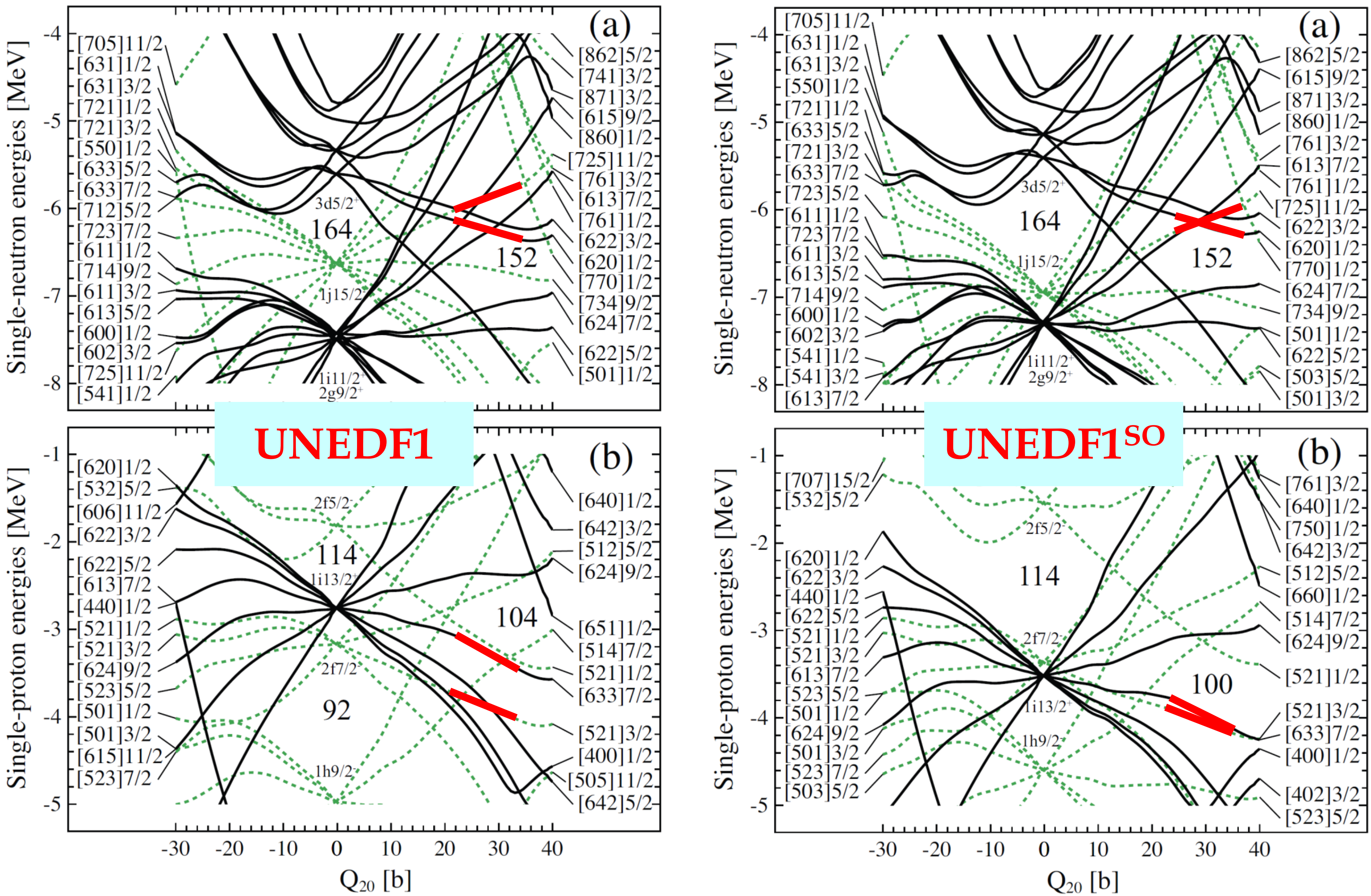
1. Introduction: nuclear single-particle energies (SPEs)
2. Polarization corrections to SPEs
3. Particle-vibration coupling (PVC) corrections to SPEs
4. Conclusions

Phenomenological nuclear mean field



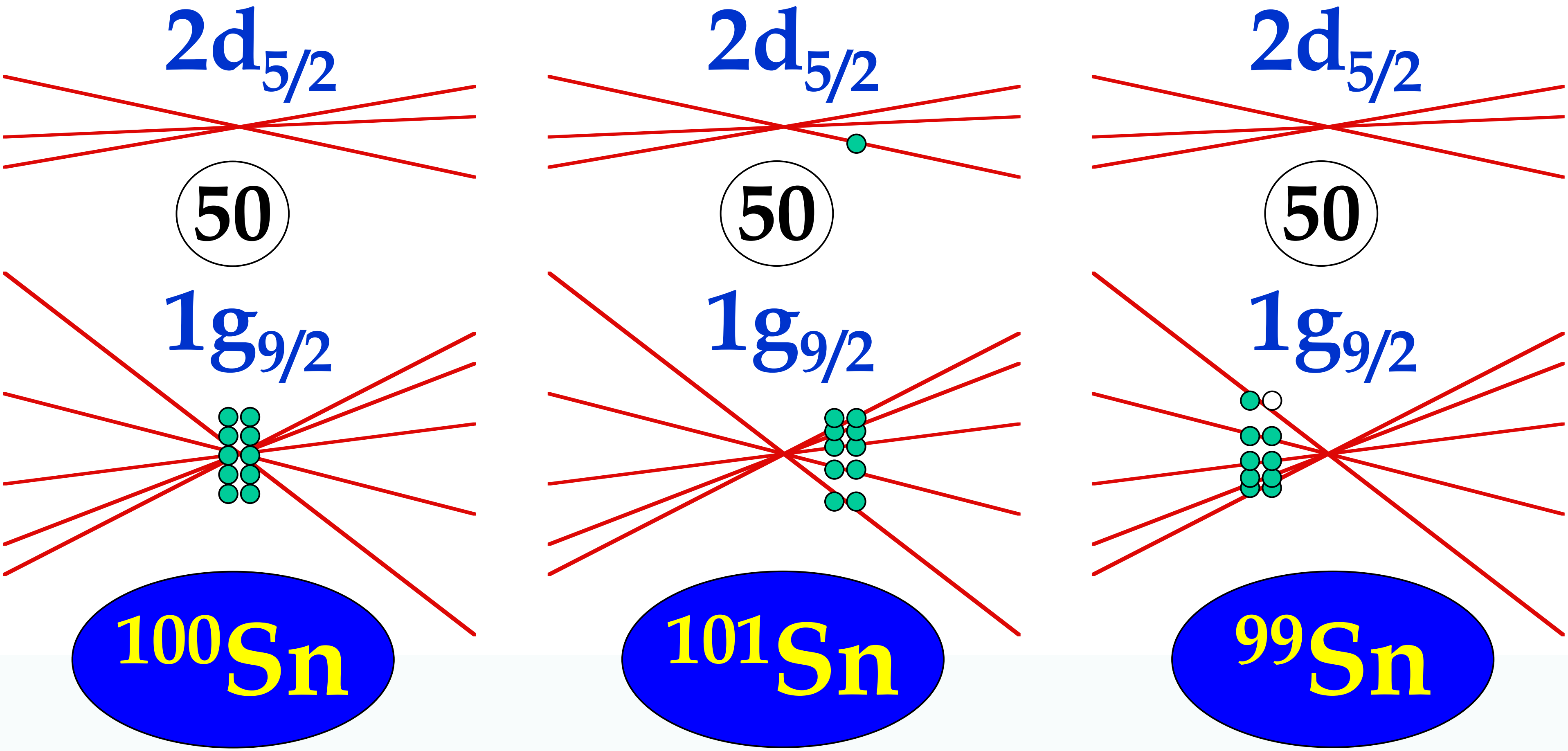
Slide by Markus Kortelainen

Nilsson diagrams in ^{254}No



Yue Shi, *et al.*, Phys. Rev. C89, 034309 (2014)

Polarization effects by odd particles or holes



Blaizot and Ripka
Problem 10.14

$$E_\lambda^{A\pm1} = E_0^A \pm e_\lambda + \tfrac{1}{2}\begin{pmatrix} \delta\rho^*, & \delta\rho \end{pmatrix}\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} \delta\rho \\ \delta\rho^* \end{pmatrix} \pm \begin{pmatrix} \delta\rho^*, & \delta\rho \end{pmatrix}\begin{pmatrix} f \\ f^* \end{pmatrix}$$

$$\begin{aligned} A_{p'h',ph} &= (e_p - e_h)\delta_{pp'}\delta_{hh'} \pm h(\rho^\lambda)_{p'p}\delta_{h'h} \mp h(\rho^\lambda)_{hh'}\delta_{pp'} + \bar{v}_{hp'ph'}, \\ B_{p'h',ph} &= \bar{v}_{pp'hh'}. \end{aligned}$$

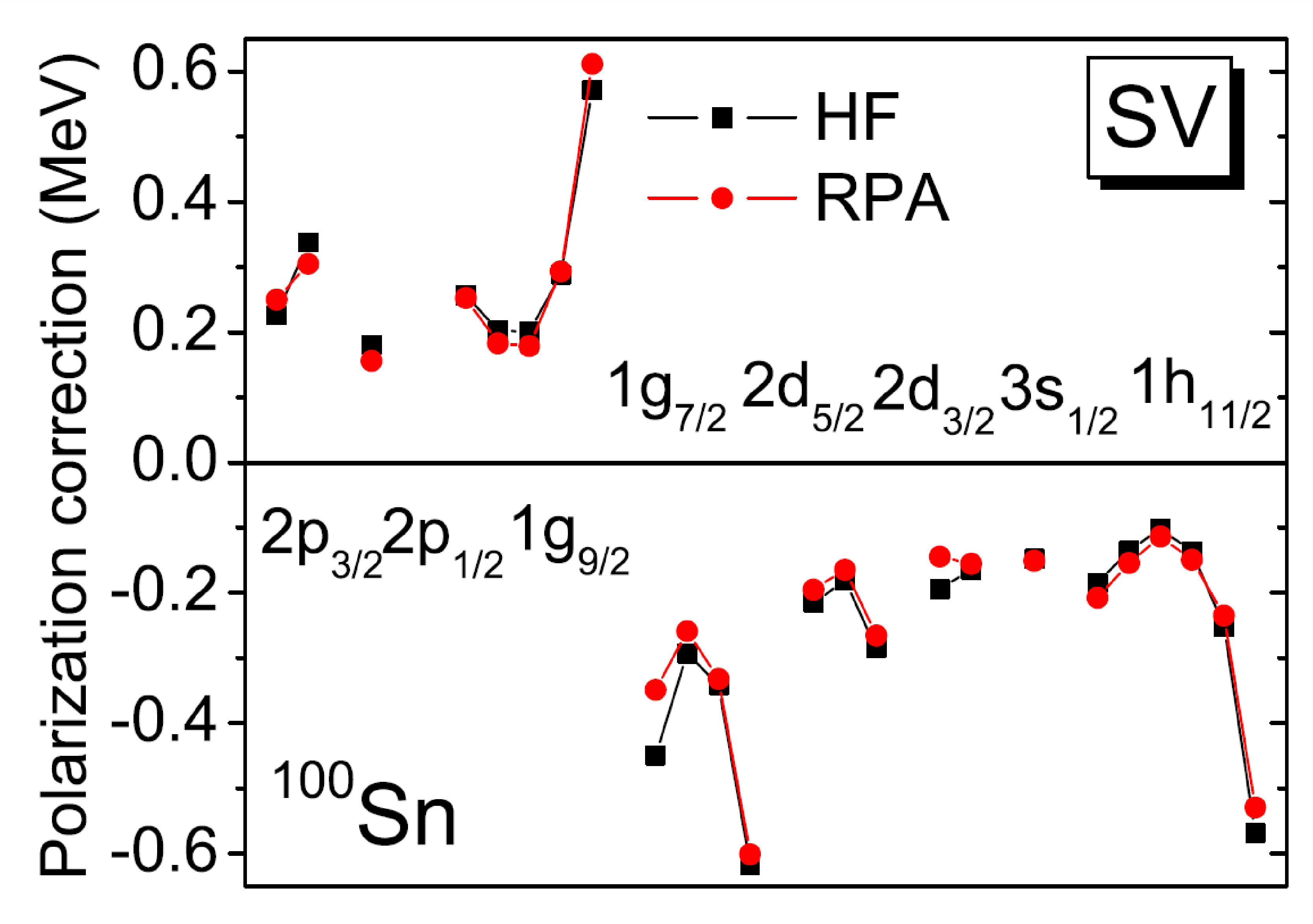
$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} \delta\rho \\ \delta\rho^* \end{pmatrix} = \mp\begin{pmatrix} f \\ f^* \end{pmatrix}$$

$$\begin{aligned} f_{ph} &= h(\rho^\lambda)_{ph} = \bar{v}_{p\lambda h\lambda}, \\ f_{hp} &= h(\rho^\lambda)_{hp} = \bar{v}_{h\lambda p\lambda}, \end{aligned}$$

$$E_\lambda^{A\pm1} = E_0^A \pm e_\lambda - \tfrac{1}{2}\begin{pmatrix} \delta\rho^*, & \delta\rho \end{pmatrix}\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} \delta\rho \\ \delta\rho^* \end{pmatrix}$$

G.E. Brown, in Facets of Physics (Academic Press, 1970)

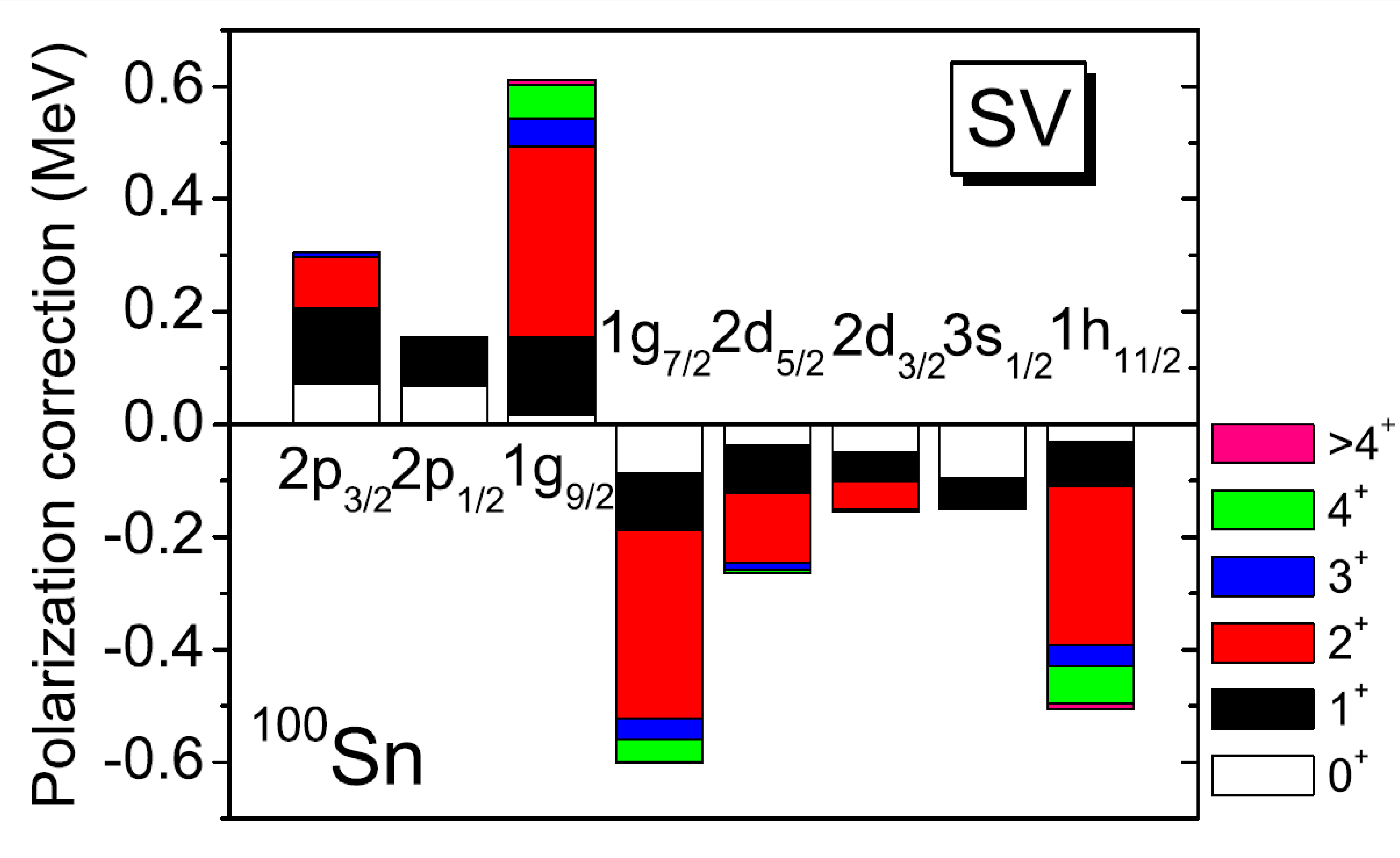
- no density dependence
- no c-o-m correction
- full tensor



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

- no density dependence
- no c-o-m correction
- full tensor

- orbital with highest |K|



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

Phenomenological 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,

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

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

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,

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

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

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

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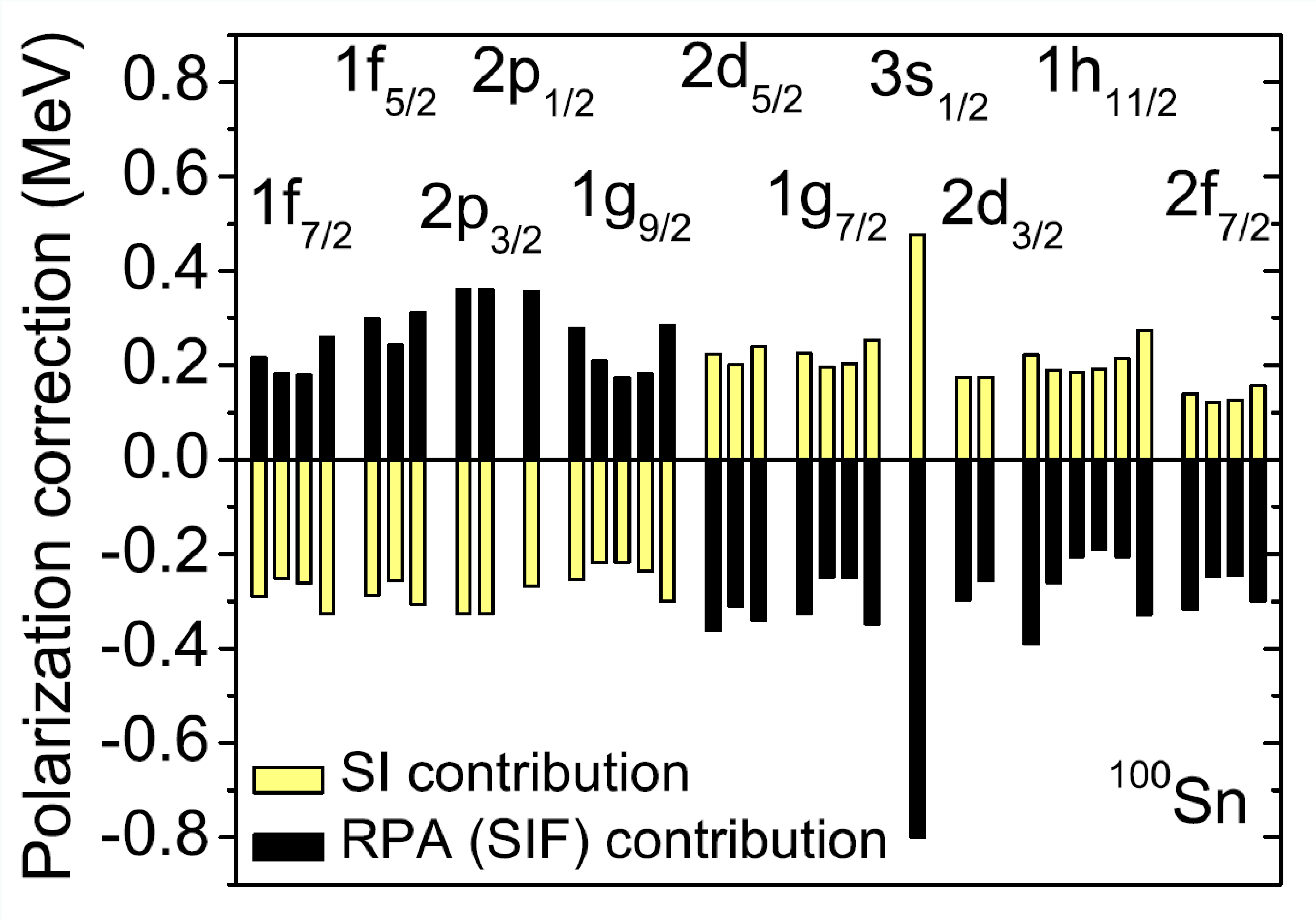
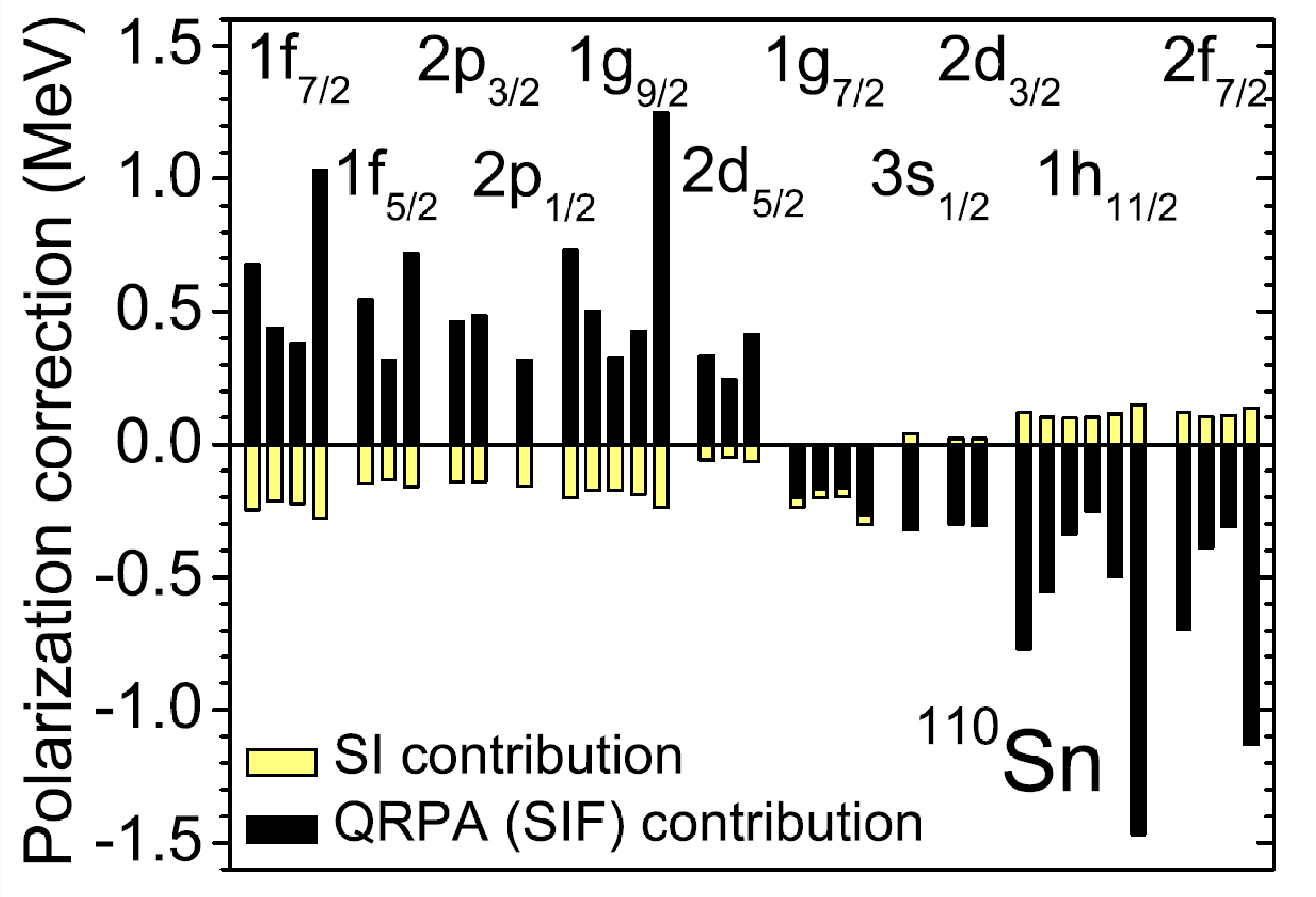
Self Interaction



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

Self Interaction



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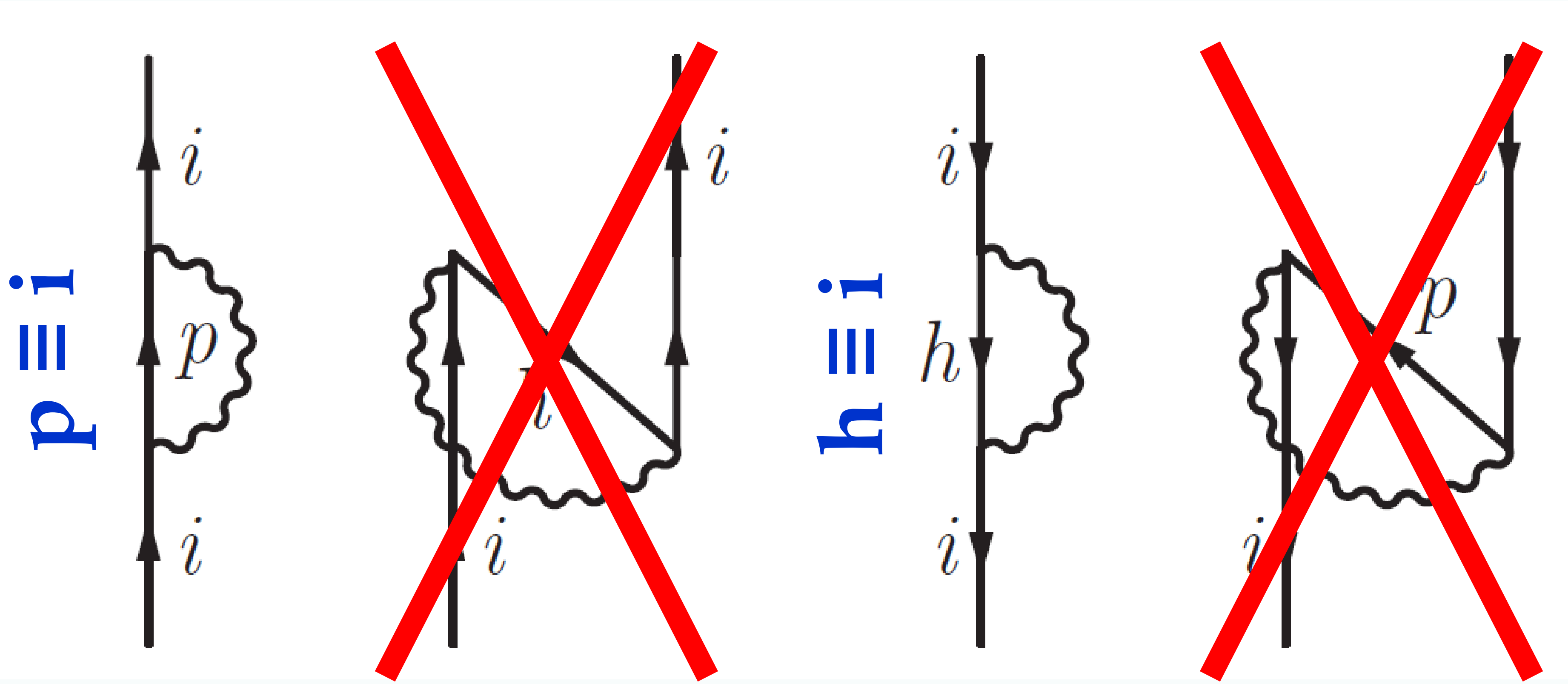
Lessons learnt

- **For density-independent effective interactions, mean field polarization effects are exactly equivalent to diagonal RPA corrections.**
- **For density-dependent effective interactions, mean-field energies of odd nuclei are polluted by the self-interaction energies.**

Polarization corrections

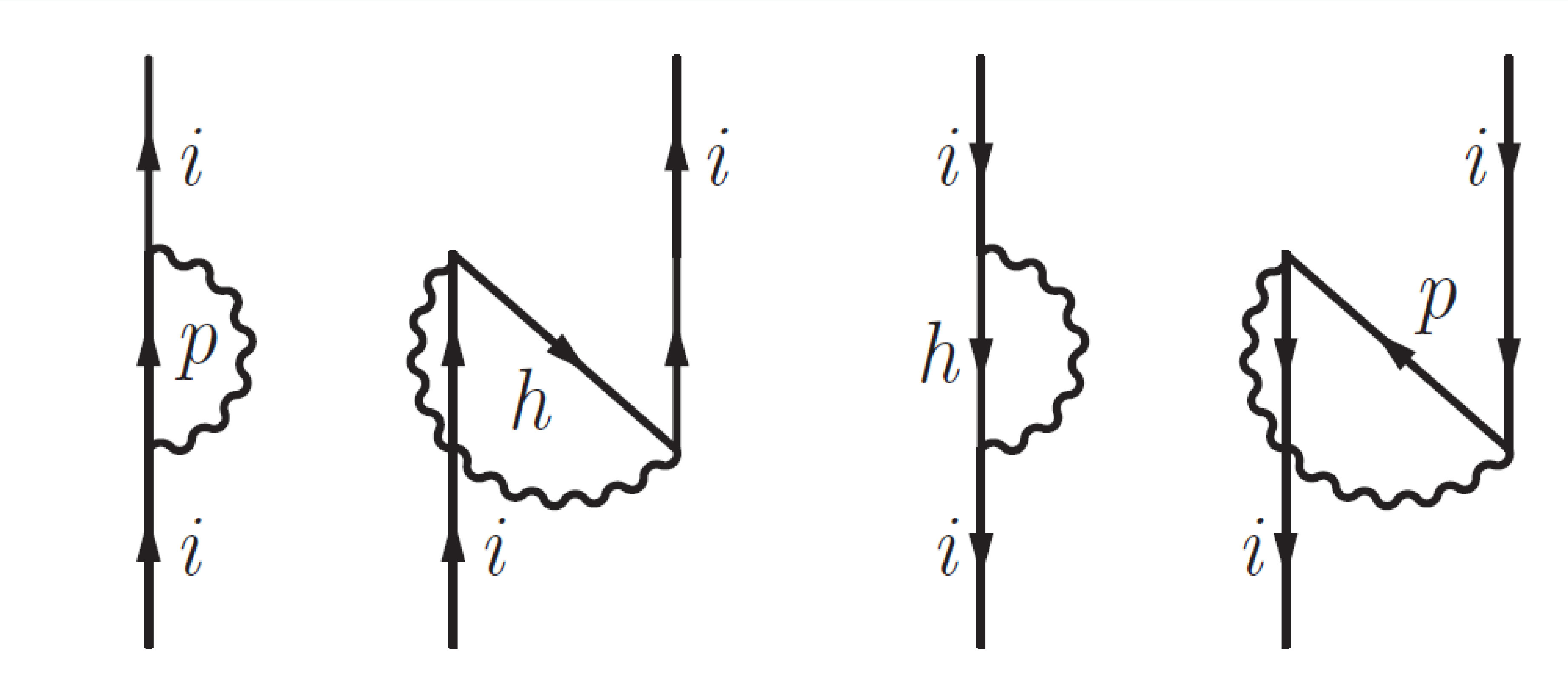


$$\delta E^{\lambda}_{\mathrm{SIF}} = -\sum_{\omega>0} \frac{\left|\sum_{\mathrm{ph}} \tilde{\tilde{h}}^{\lambda *}_{\mathrm{ph}} X^{\omega}_{\mathrm{ph}} + \tilde{\tilde{h}}^{\lambda}_{\mathrm{ph}} Y^{\omega}_{\mathrm{ph}}\right|^2}{\hbar\omega}.$$

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

G. Colò *et al.*, Phys. Rev. C82, 064307 (2010)

Particle-vibration-coupling (PVC) corrections



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

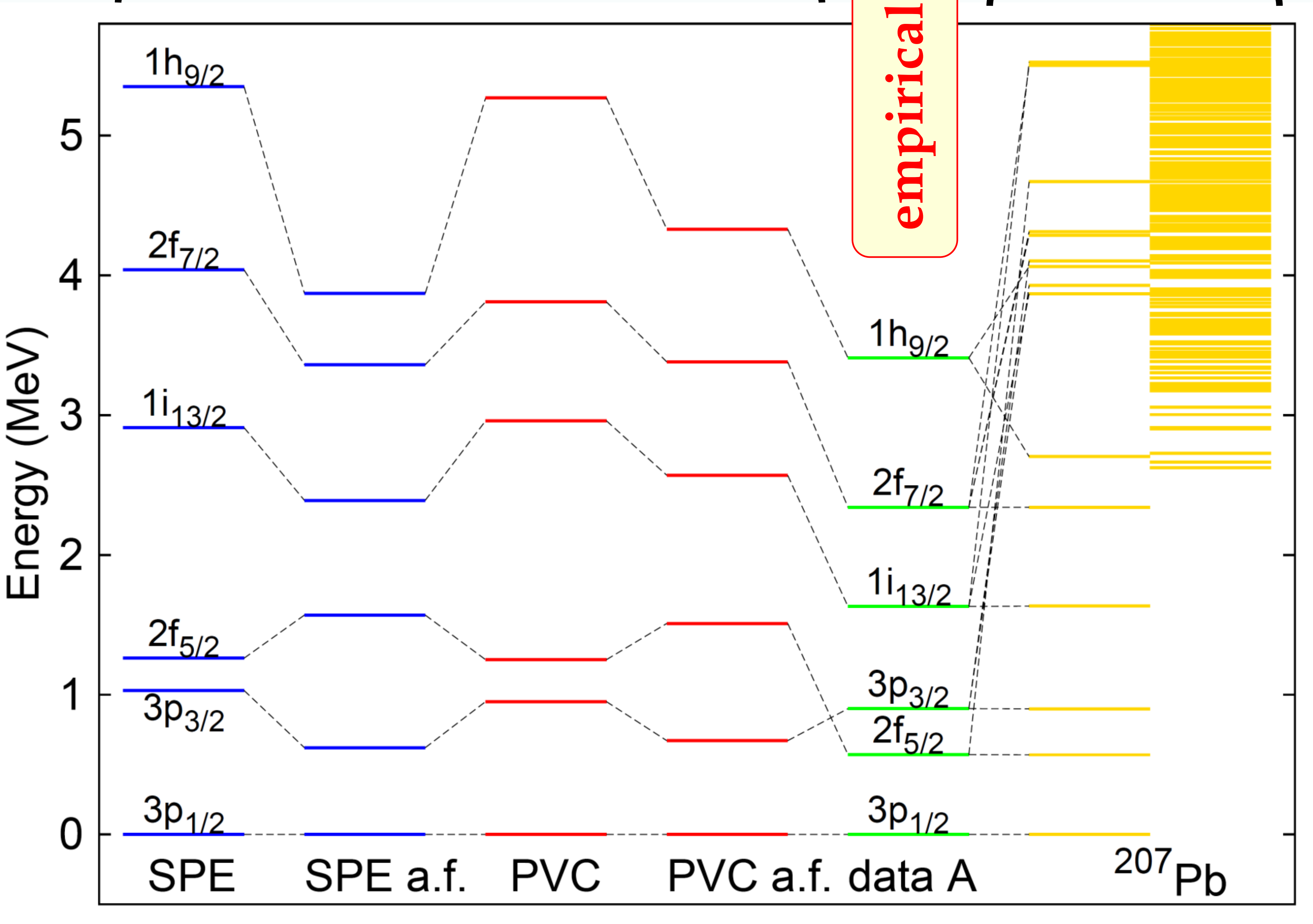
G. Colò *et al.*, Phys. Rev. C82, 064307 (2010)

^{207}Pb

Skyrme SIII

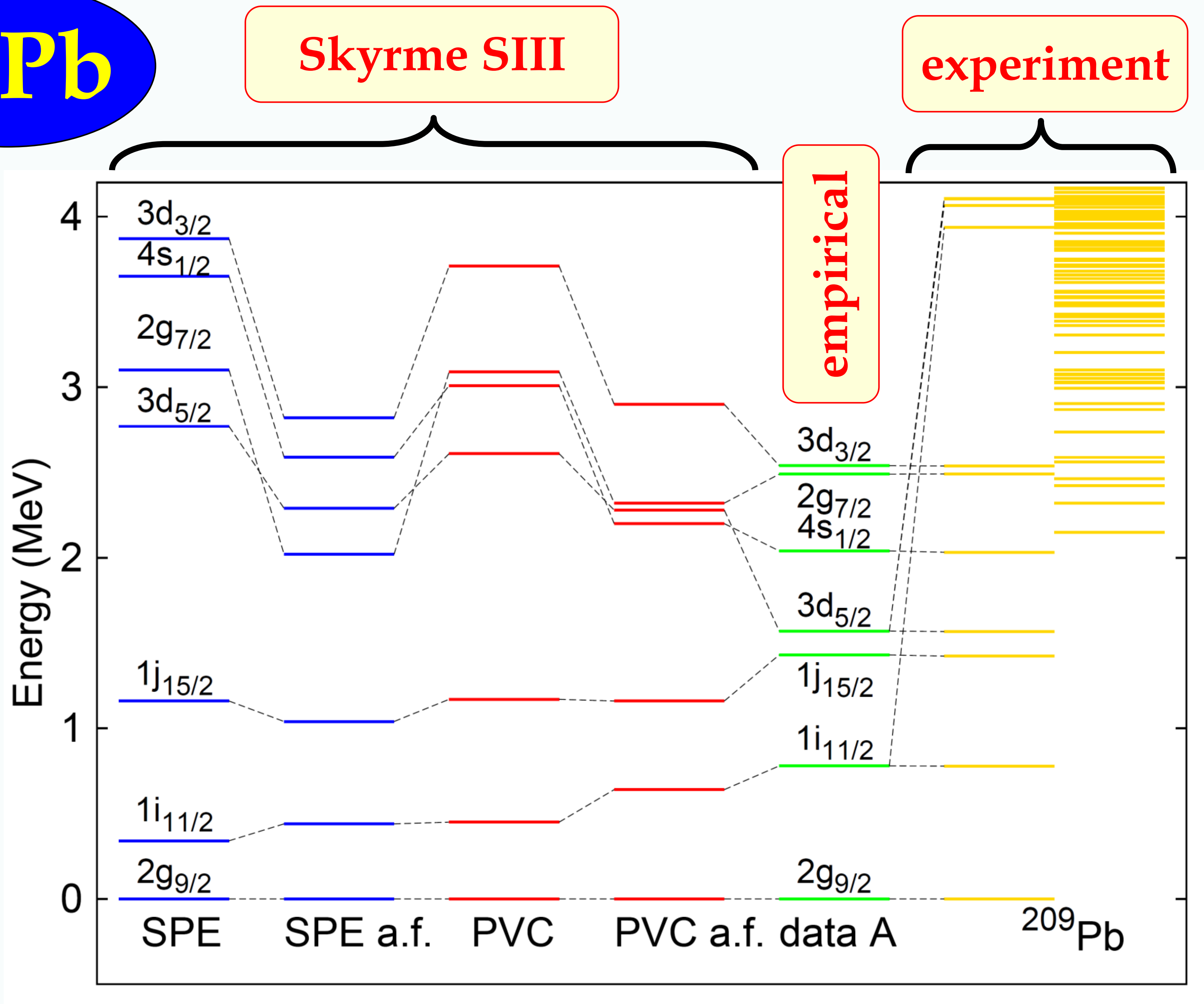
experiment

empirical



D. Tarpanov *et al*, Phys. Rev. Lett. 113, 252501 (2014)

^{209}Pb



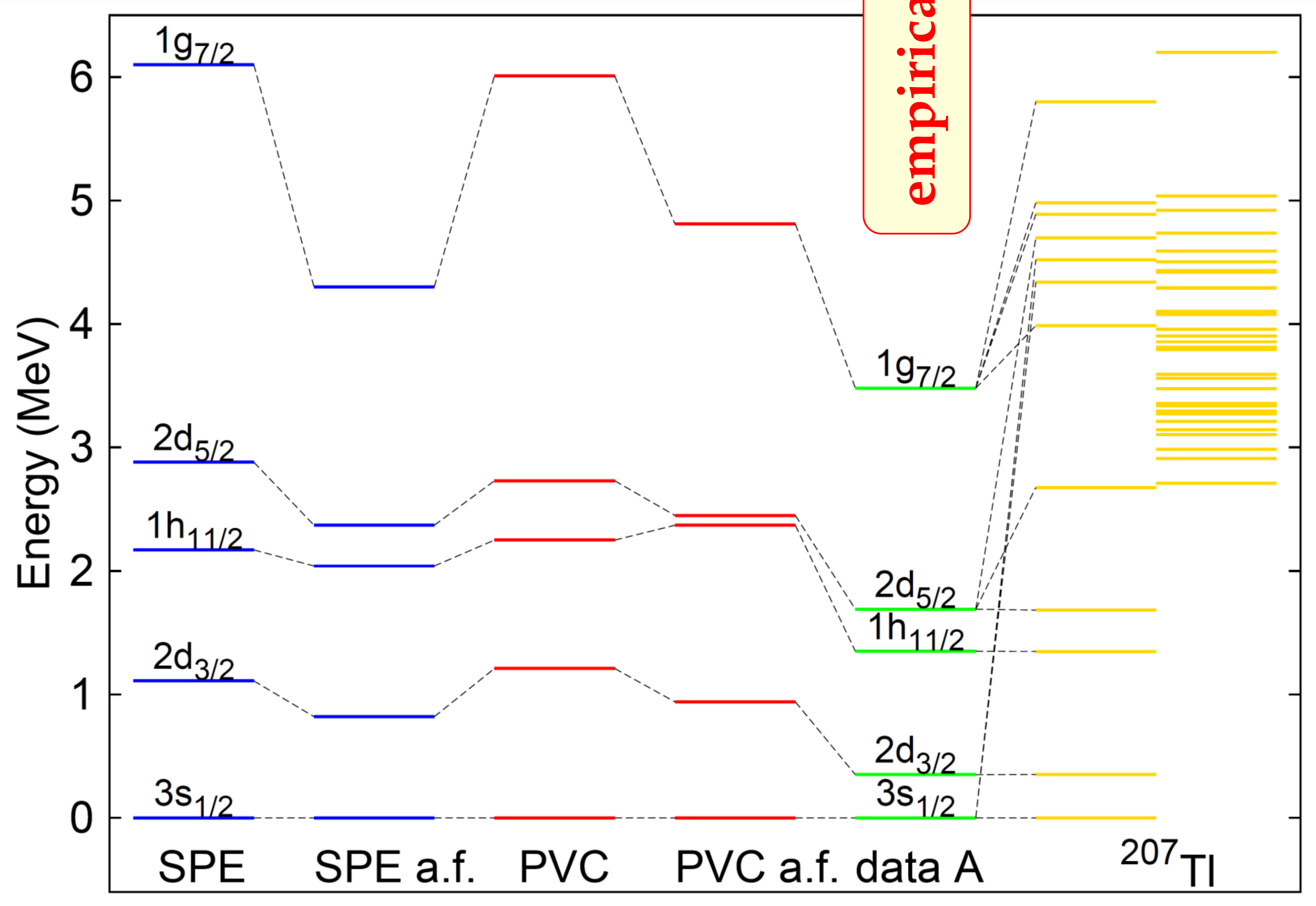
D. Tarpanov *et al*, Phys. Rev. Lett. 113, 252501 (2014)

^{207}Tl

Skyrme SIII

experiment

empirical



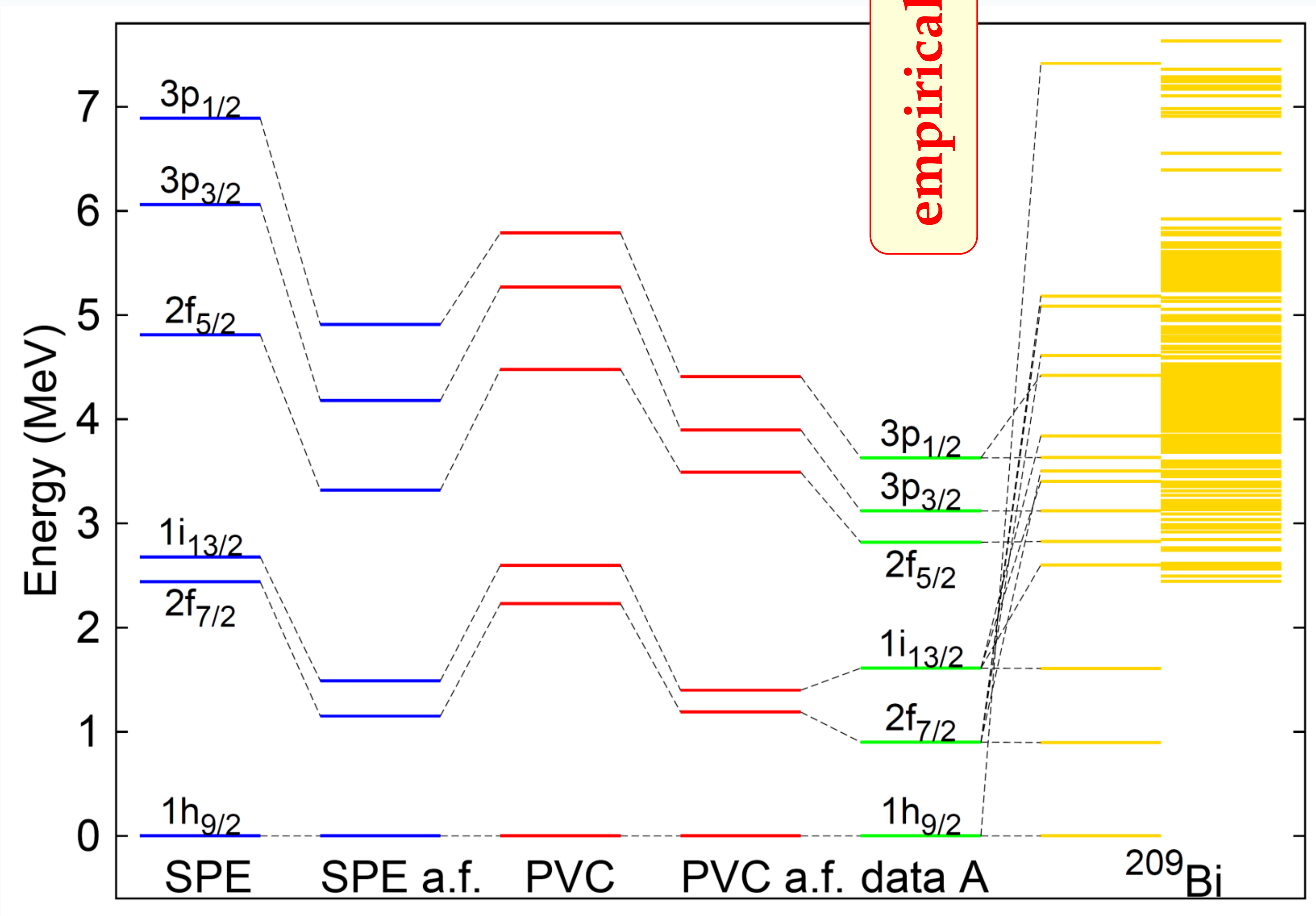
D. Tarpanov *et al*, Phys. Rev. Lett. 113, 252501 (2014)

^{209}Bi

Skyrme SIII

experiment

empirical



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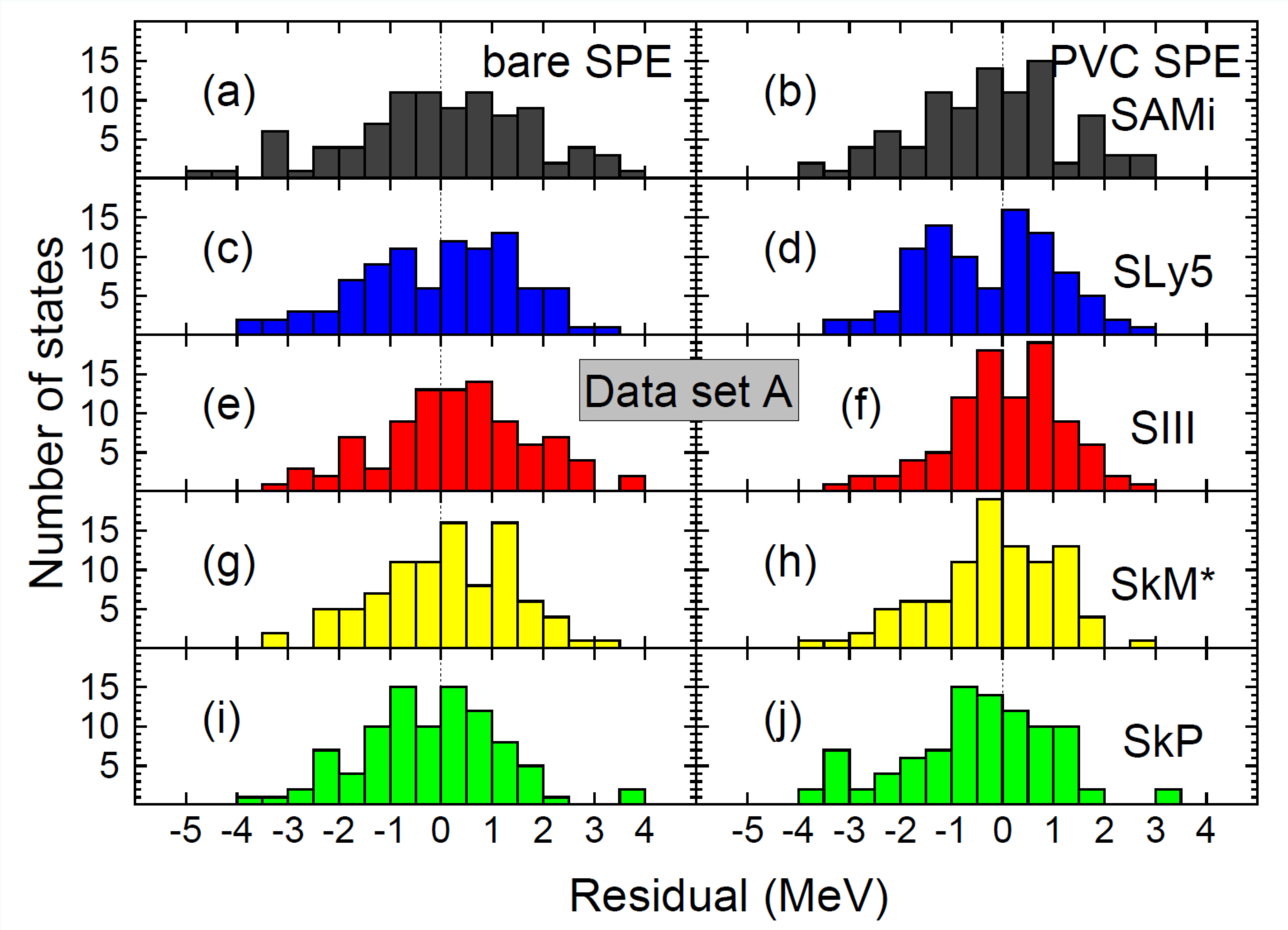
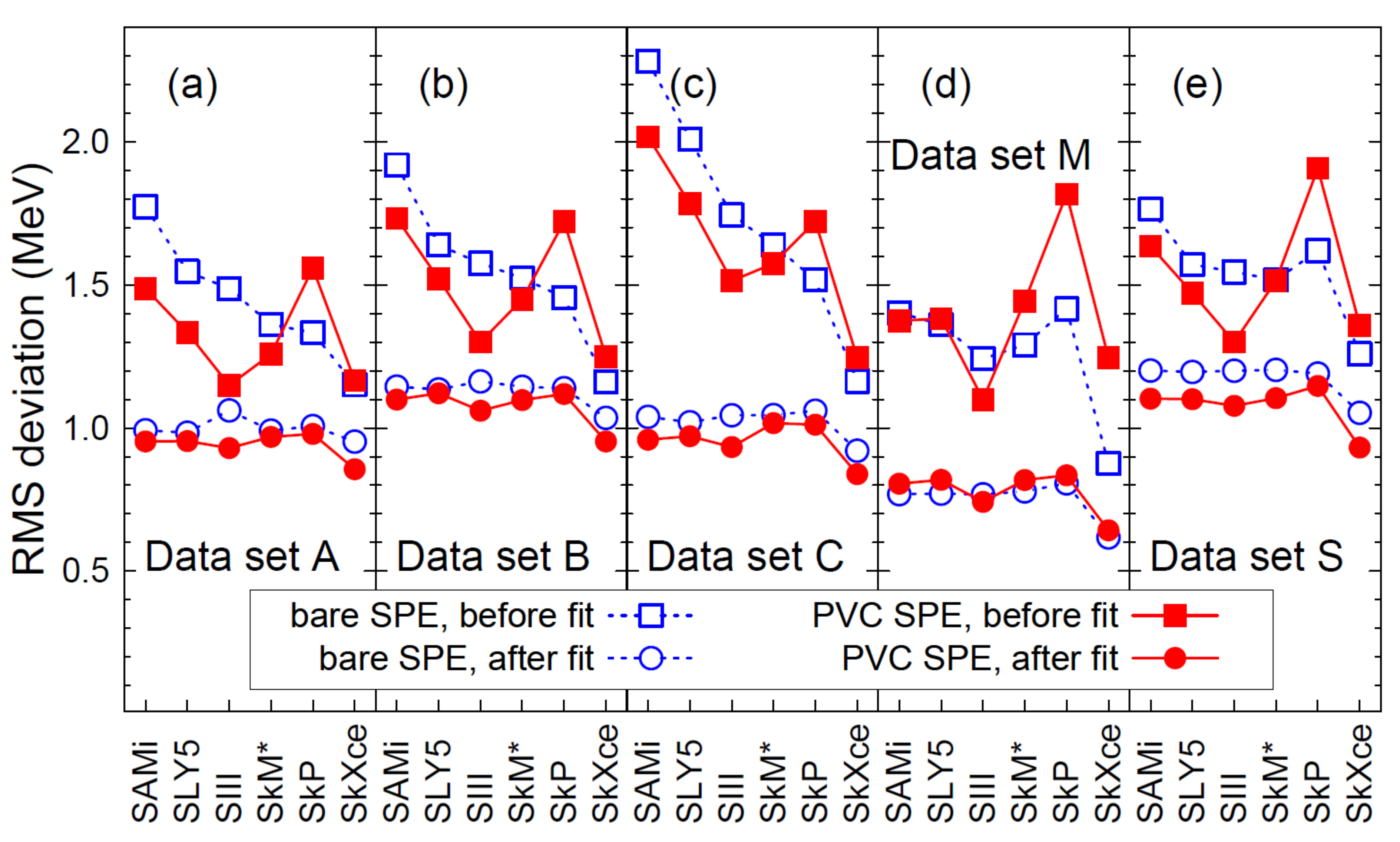
Particle-vibration-coupling (PVC) corrections



D. Tarpanov *et al*, Phys. Rev. Lett. 113, 252501 (2014)

Particle-vibration-coupling (PVC) corrections



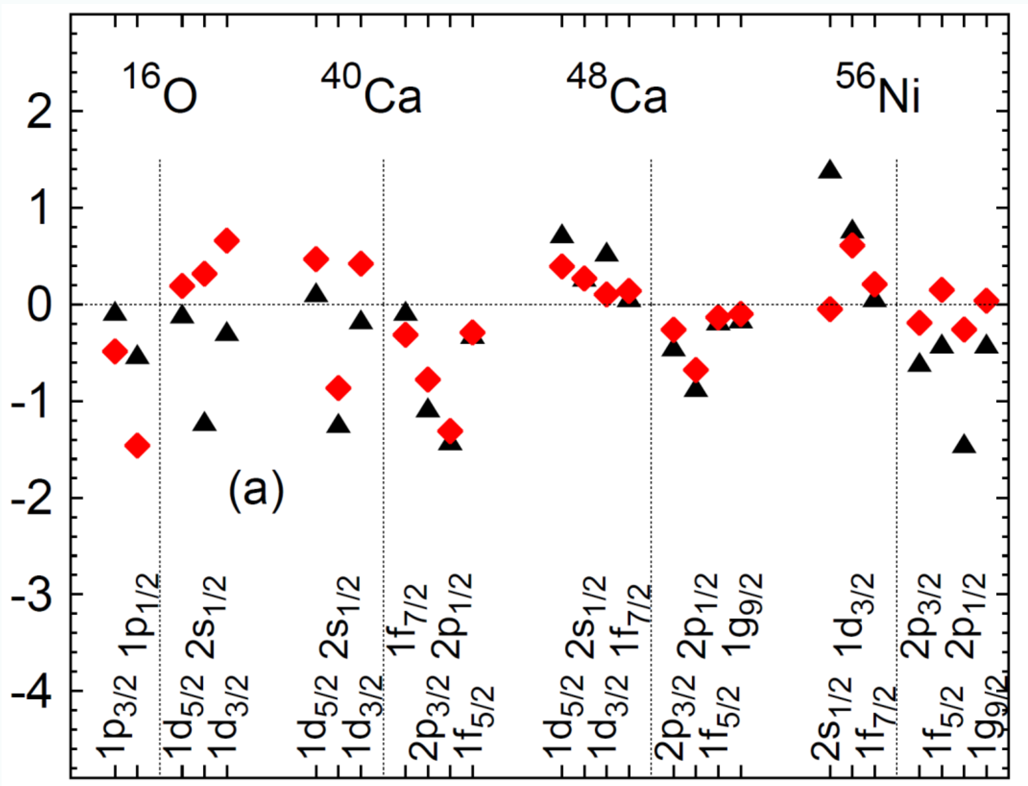
D. Tarpanov *et al*, Phys. Rev. Lett. 113, 252501 (2014)

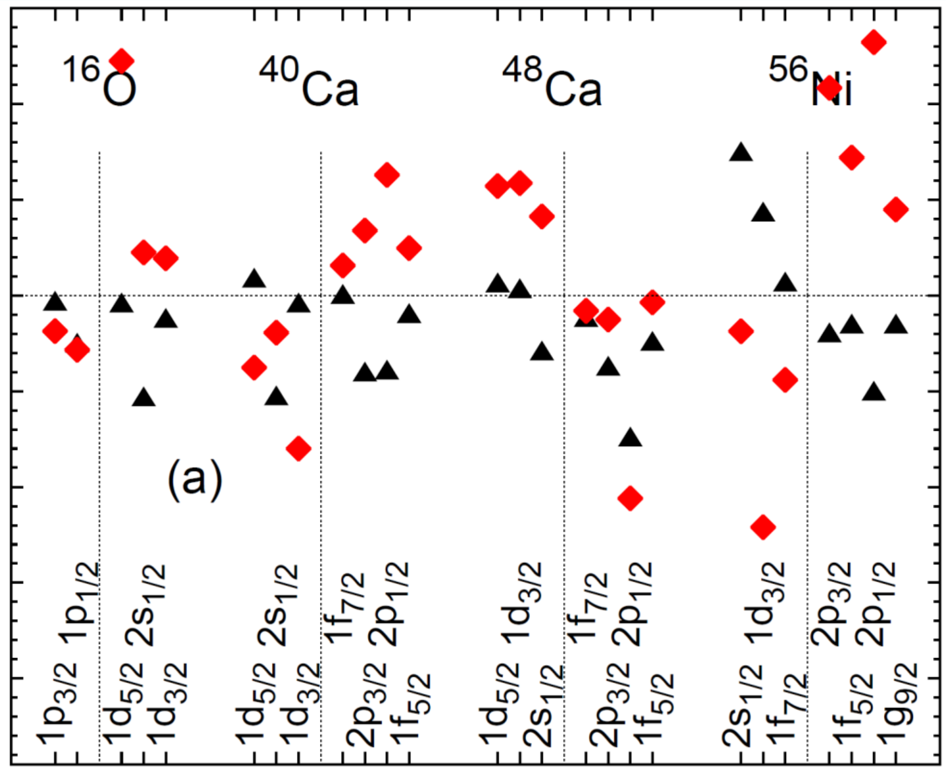
Like-particle vs. unlike-particle PVC

Neutron states

PVC ▲
pnPVC ◆

Proton states





PRELIMINARY

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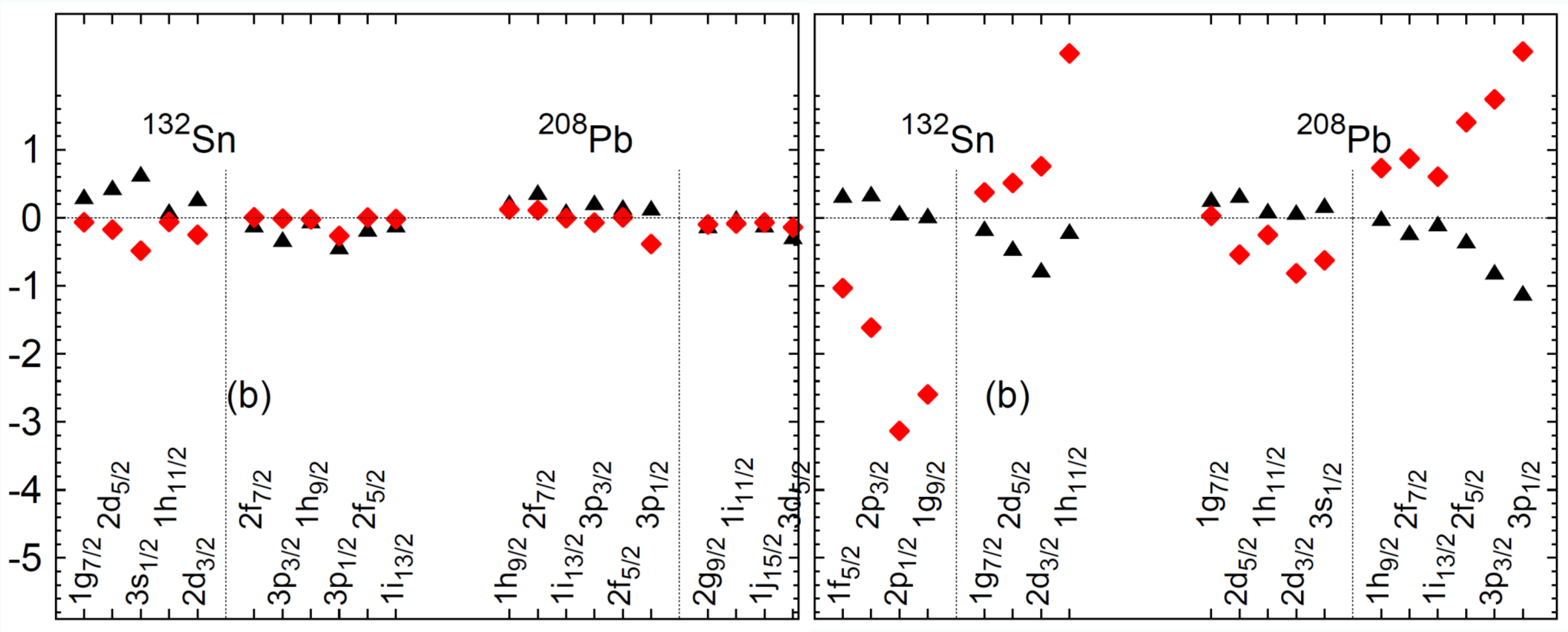
Like-particle vs. unlike-particle PVC

Neutron states

Proton states



PRELIMINARY

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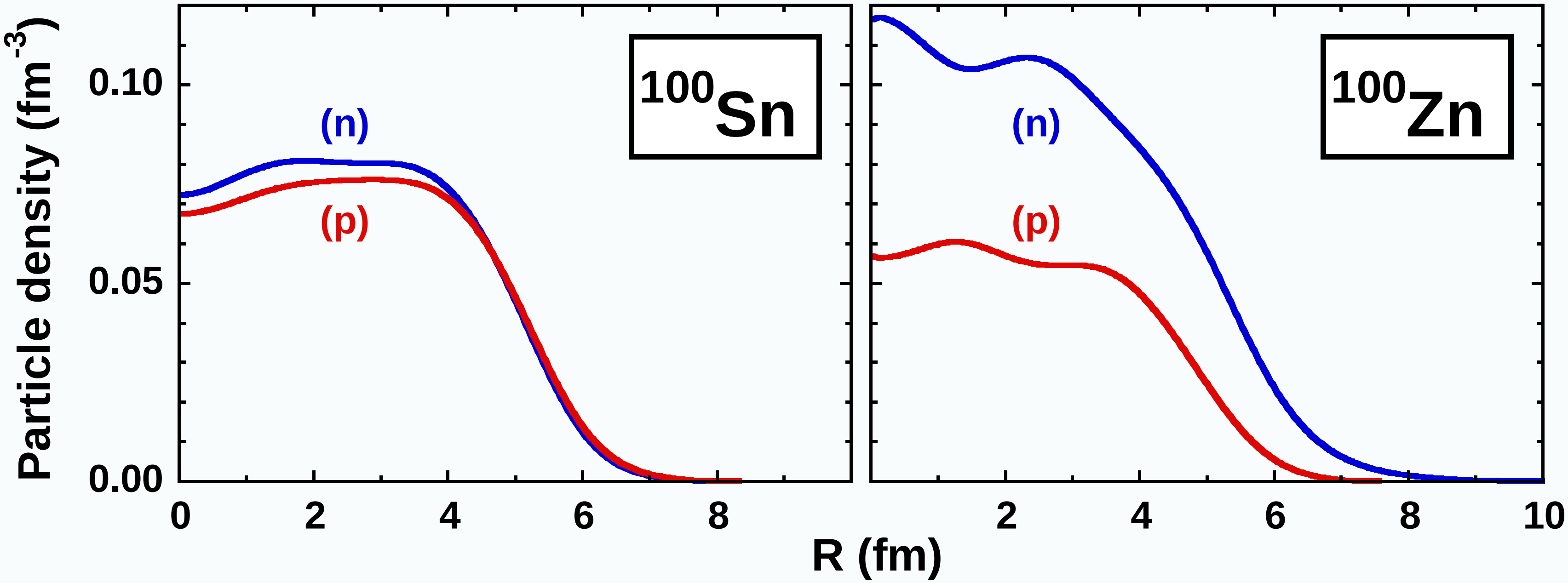
Conclusions

- For density-dependent effective interactions, mean-field energies of odd nuclei are polluted by the self-interaction energies.
- The single-particle energies (SPEs) with particle-vibration-coupling (PVC) corrections included and then adjusted to empirical data do not give satisfactory description of experiment.
- The main source of disagreement with data is still in the underlying mean fields, and not in including or neglecting the PVC corrections.
- The search for better energy density functionals (EDFs), which is currently pursued in various directions, remains an important priority for the field.

Thank you

Nuclear densities as composite fields



Modern Mean-Field Theory ≡ Energy Density Functional

ρ, τ, $\overleftrightarrow{J}$, $\vec{j}$, $\vec{T}$, $\vec{s}$, $\vec{F}$,

- Hohenberg-Kohn
- Kohn-Sham
- Negele-Vautherin
- Landau-Migdal
- Nilsson-Strutinsky

mean field ⇒ one-body densities

zero range ⇒ local densities

finite range ⇒ non-local densities

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

Introduction

The energy required to remove a particle with quantum numbers i, outside of the nucleus with A+1 particles

$$E^{i}_{separation} = E^{A}_{0} - E^{A+1}_{i}$$

in mean-field formalism the energies of the systems with A and A+1 particles are given by the expectation value of the Hartree-Fock Hamiltonian in a proper state:

$$E^{A}_{0} = \langle \phi_0 | \, H \, | \phi_0 \rangle = E[\rho^{A}]$$

- Separation energies.
- Single-particle levels.
- Polarization corrections.

$$E^{A+1}_{\lambda} - E^{A}_{0} = e_{\lambda} - \sum_{N>0} \frac{|\langle \lambda \, | H_{pv} | \, N\lambda \rangle|^2}{\omega_N}$$

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UNIVERSITY OF JYVÄSKYLÄ

Blaizot and Ripka
Problem 10.14

$$\rho^{A\pm1} = \rho_0^A \pm |\lambda\rangle\langle\lambda| + \delta\rho$$

Density in the odd-even system

$$\begin{aligned}
E_\lambda^{A\pm1} &= \mathrm{Tr}(t\rho^{A\pm1}) + \tfrac{1}{2}\mathrm{Tr}_1\mathrm{Tr}_1(\rho^{A\pm1}v\rho^{A\pm1}) \\
&= \sum_{ii'} t_{i'i}\rho_{ii'}^{A\pm1} + \frac{1}{2}\sum_{ii'kk'} \rho_{i'i}^{A\pm1}\bar{v}_{ik'i'k}\rho_{kk'}^{A\pm1} \\
&= E_0^A \pm t_{\lambda\lambda} + \sum_{ii'} t_{i'i}\delta\rho_{ii'} + \tfrac{1}{2}\bar{v}_{\lambda\lambda\lambda\lambda} + \frac{1}{2}\sum_{ii'kk'} \delta\rho_{i'i}\bar{v}_{ik'i'k}\delta\rho_{kk'} \\
&\pm \frac{1}{2}\sum_{ii'} \rho_{i'i}^A\bar{v}_{i\lambda i'\lambda} \pm \frac{1}{2}\sum_{kk'} \bar{v}_{\lambda k'\lambda k}\rho_{kk'}^A \\
&\pm \frac{1}{2}\sum_{ii'} \delta\rho_{i'i}\bar{v}_{i\lambda i'\lambda} \pm \frac{1}{2}\sum_{kk'} \bar{v}_{\lambda k'\lambda k}\delta\rho_{kk'} \\
&+ \frac{1}{2}\sum_{ii'kk'} \rho_{i'i}^A\bar{v}_{ik'i'k}\delta\rho_{kk'} + \frac{1}{2}\sum_{ii'kk'} \delta\rho_{i'i}\bar{v}_{ik'i'k}\rho_{kk'}^A .
\end{aligned}$$

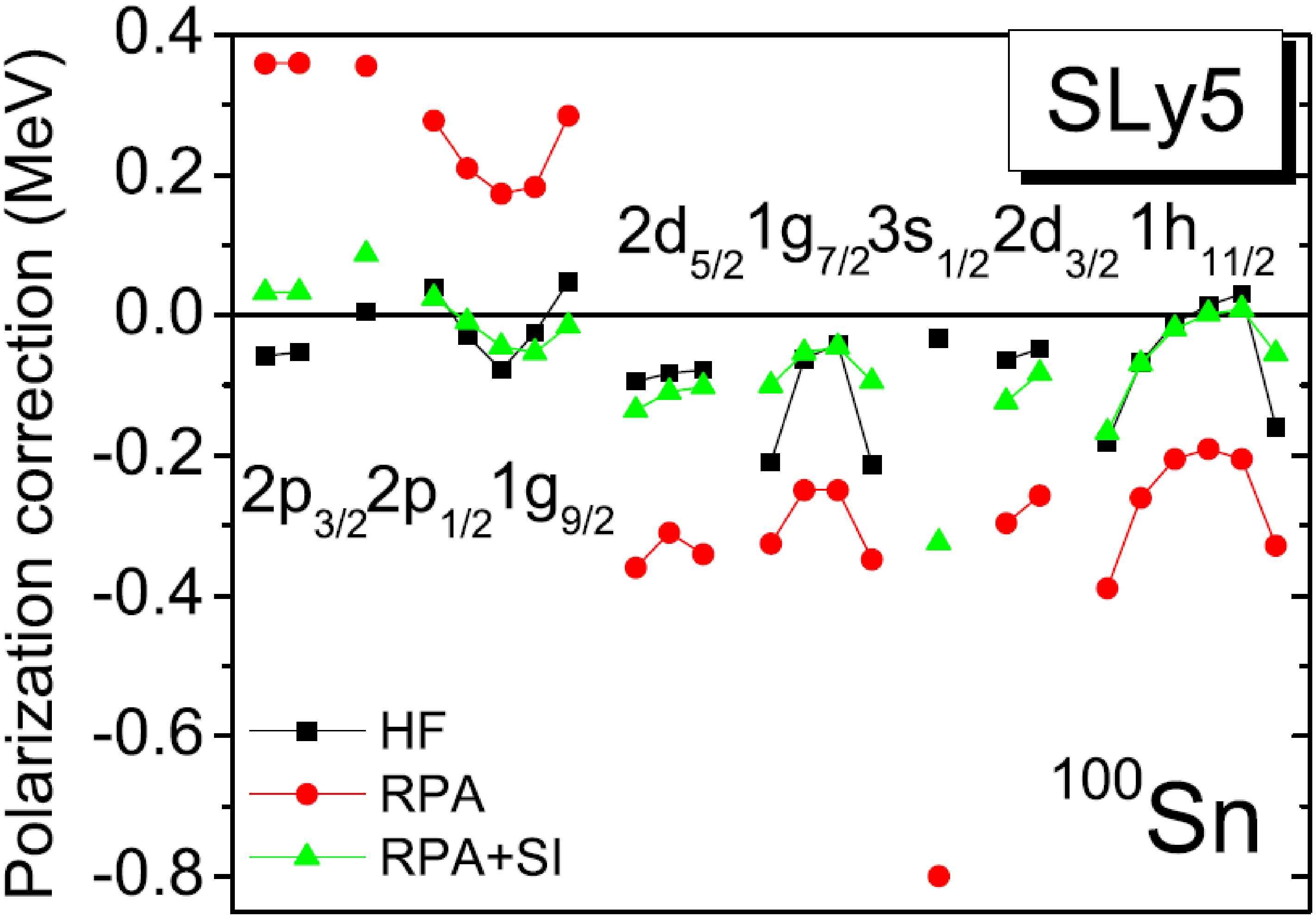
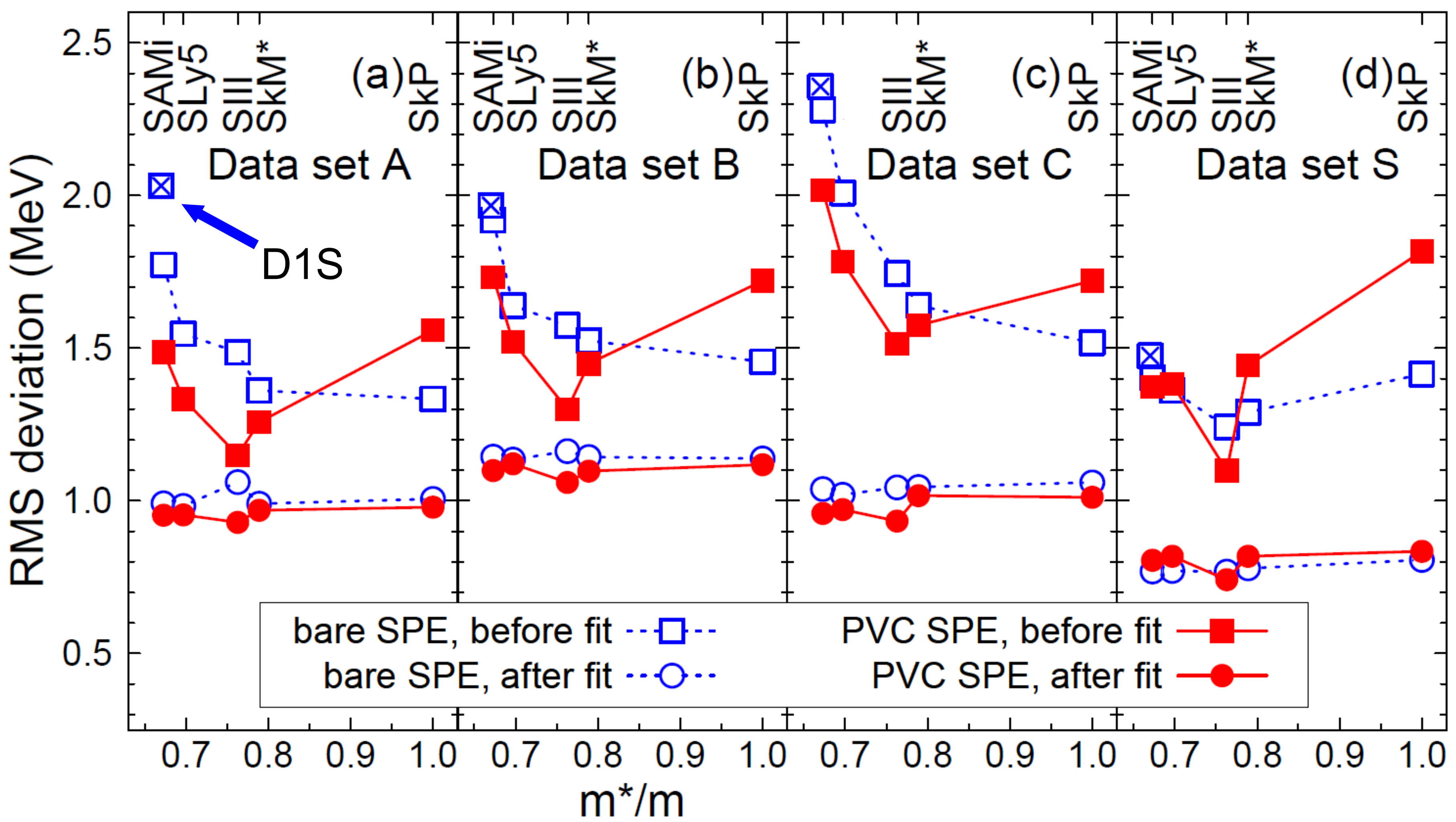


FIG. 5. (Color online) Same as in Fig. 1, but for the Skyrme EDF SLy5 [49]. The RPA results correspond to the SIF terms in Eq. (46), whereas RPA + SI denotes both SIF and SI contributions combined.

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

Particle-vibration-coupling (PVC) corrections



D. Tarpanov *et al*, Phys. Rev. Lett. 113, 252501 (2014)