The impact of radius data on nuclear density functional theory

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Outline

Acknowledgments:

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exp. data	MAMI/Mainz, ISOLDE/CERN, NSCL/MSU, JLAB

1) Statistical aspects of empirical calibration of nuclear density functionals

Nuclear density functional theory (DFT)

nuclear energy-density functional: $E = E(\underbrace{\boldsymbol{p}}_{\text{params.}})[\underbrace{\rho(\mathbf{r}), \tau(\mathbf{r}), \mathbf{J}(\mathbf{r}), \xi(\mathbf{r})}_{\text{densities:local,kinetic,spin-orbit,pairing}}]$

eqs. of motion by variation of s.p. wavefunction & occupation amplitudes

typically a dozen free model parameters $\mathbf{p} \longleftrightarrow \chi^2$ fit to empirical data

$\Longrightarrow$ optimal $\mathbf{p}$, uncertainties of predictions, stat. correlations between observables

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2 functionals: Skyrme: density dependence, kinetic, surface, l*s, pairing
Fayans: " + gradient term in pairing & surface energy

Fayans pairing energy density $\mathcal{E} = \rho^2_{\text{pair}}(\mathbf{r})\Big(\underbrace{V_{\text{pair}} + V'_{\text{pair}}\rho^{\gamma}(\mathbf{r})}_{\text{volume\&surface pairing}} + \underbrace{V^{(\nabla)}_{\text{pair}}(\nabla\rho(\mathbf{r}))^2}_{\text{gradient term}}\Big)$

Strategy for adjusting the model parameters to phenomenological data

model ← parameters p

$$\chi^2(\mathbf{p}) = \sum_{\mathcal{O}\in\{\text{obs.}\}} \frac{\left(\mathcal{O}(\mathbf{p}) - \mathcal{O}^{(\text{exp})}\right)^2}{\Delta\mathcal{O}^2}$$

quality measure – to be minimized

$\mathcal{O}(\mathbf{p})$ = computed observable

$\mathcal{O}^{(\text{exp})}$ = experimental value for $\mathcal{O}$

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bulk properties of finite nuclei:

energy E_B,

radii R_c, r_c, surface th. σ_c,

l·s splitting $\Delta\varepsilon_{ls}$,

odd-even staggering of $E_B \to$ gap

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more detailed: differences of r_c

Probabilistic interpretation of the space of model parameters

probability distribution for model parameters $\boldsymbol{p}$:

$$\boxed{P(\boldsymbol{p}) \propto \exp\left(-\chi^2(\boldsymbol{p})\right)\,,\ \chi^2 = \sum_{\mathcal{O}\in\{\text{obs.}\}} \frac{\left(\mathcal{O}(\mathbf{p}) - \mathcal{O}^{(\exp)}\right)^2}{\Delta\mathcal{O}^2}}$$

$\Longrightarrow$ optimal parameter set $\boldsymbol{p}_0$: $\chi^2(\boldsymbol{p}_0) = \text{minimal}$

range of "reasonable" parameters: $\boldsymbol{p}$ such that $\chi^2(\boldsymbol{p}) \leq \chi^2(\boldsymbol{p}_0) + 1$

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statistical properties of the space of reasonable parameters:

average of an observable $A(\boldsymbol{p})$: $\overline{A} = \int d\boldsymbol{p}\, P(\boldsymbol{p}) A(\boldsymbol{p})$

variance (uncertainty of prediction): $\overline{\Delta^2 A} = \int d\boldsymbol{p}\, P(\boldsymbol{p})(A(\boldsymbol{p}) - \overline{A})^2.$

covariance: $\overline{\Delta A \Delta B} = \int d\boldsymbol{p}\, P(\boldsymbol{p})\,(A(\boldsymbol{p}) - \overline{A})(B(\boldsymbol{p}) - \overline{B})\ .$

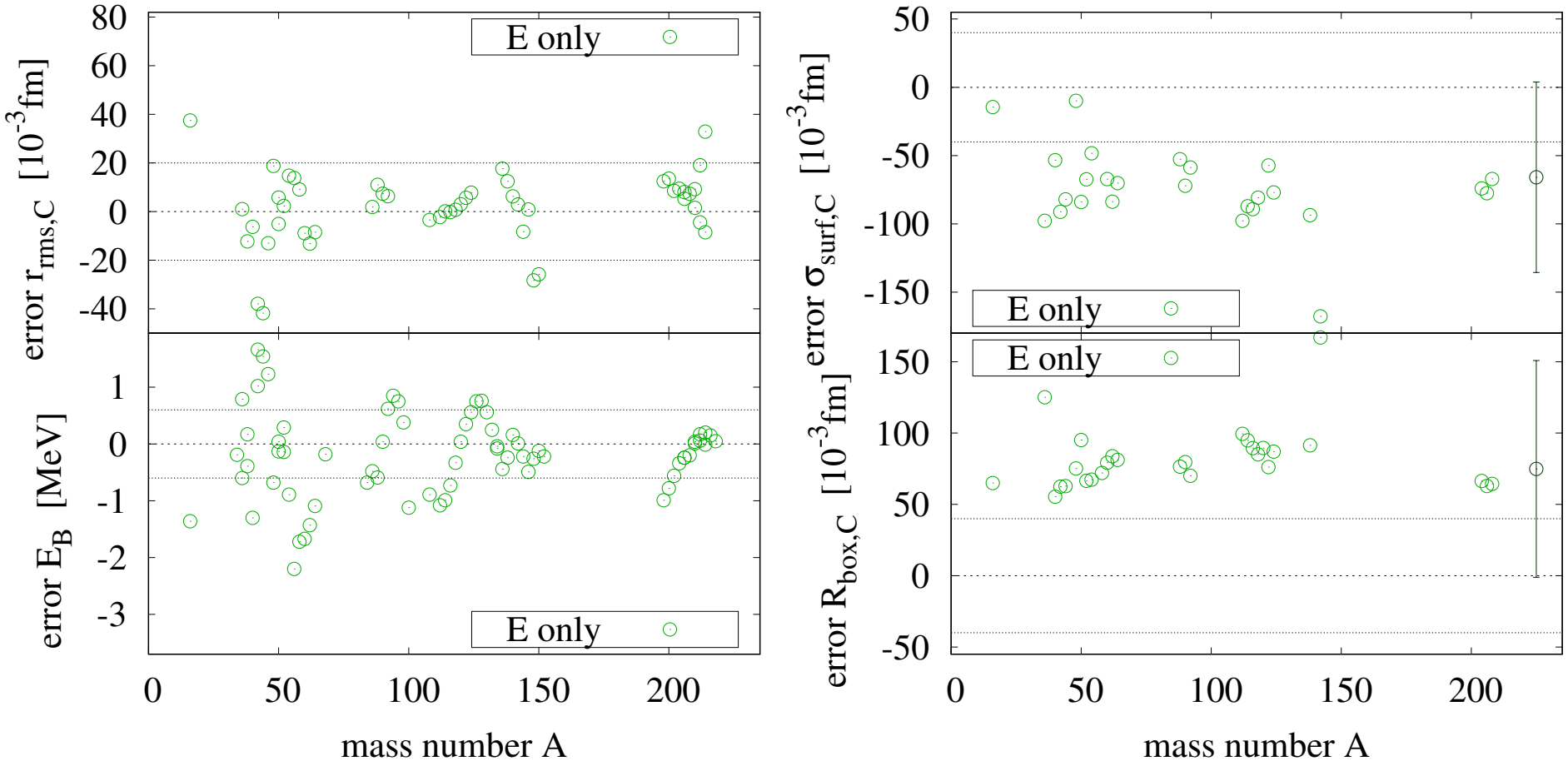
coefficient of determination (CoD): $r^2_{AB} = \dfrac{|\overline{\Delta A \Delta B}|^2}{\overline{\Delta^2 A}\,\overline{\Delta^2 B}}$ (statistical correlation)

$r^2_{AB} = 1 \leftrightarrow$ correlated, $r^2_{AB} = 0 \leftrightarrow$ uncorrel.

2) Application examples

Example 1: Impact of radii in bulk ground state properties

Distribution of errors on E_B, $r_{\mathrm{rms,C}}$, $R_{\mathrm{box,C}}$, $\sigma_{\mathrm{surf,C}}$ – fit to E_B only

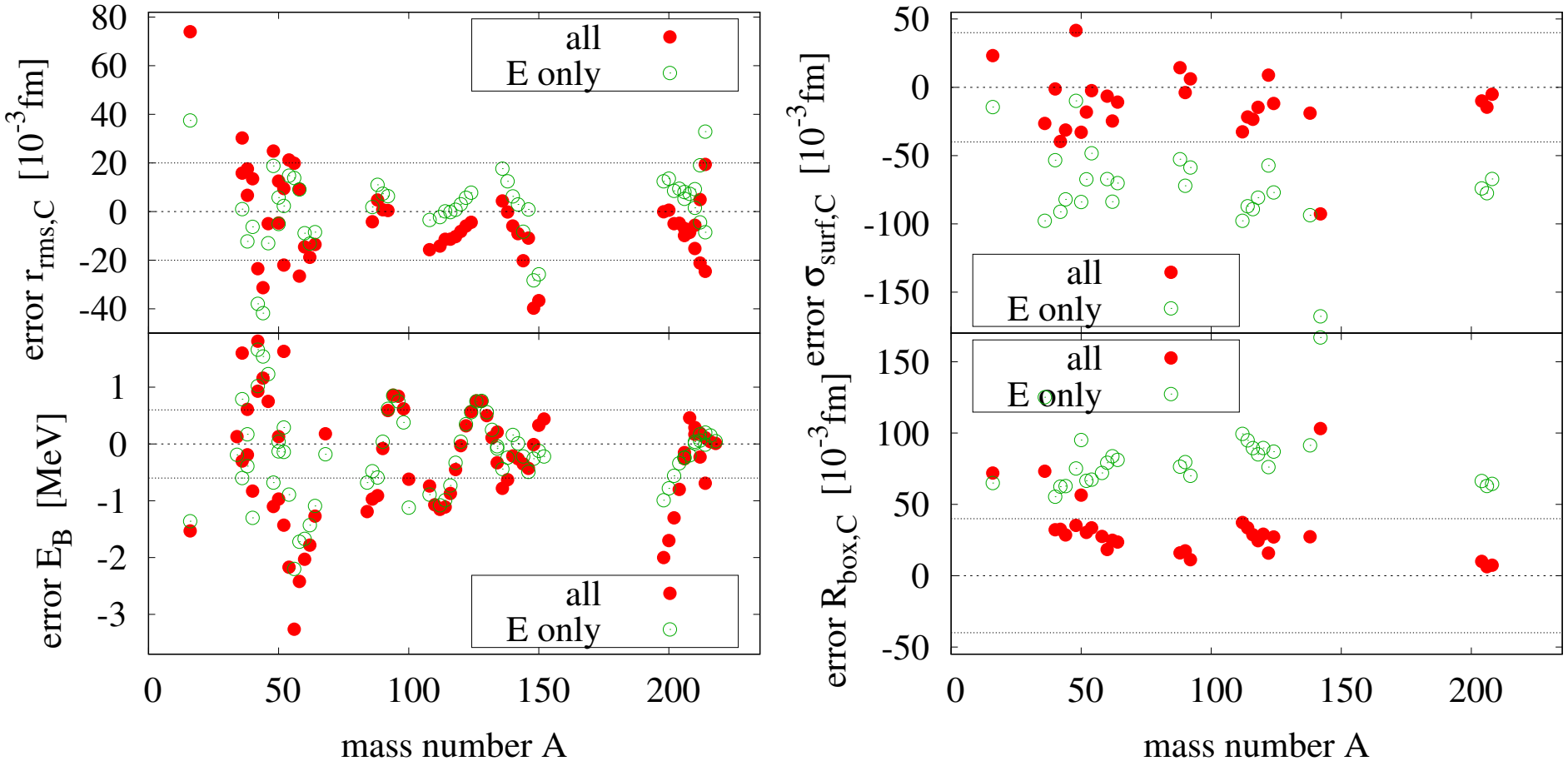


r.m.s. radius $r_{\mathrm{rms,C}}$ well predicted by E_B fit

box radius $R_{\mathrm{box,C}}$ and surface thickness $\sigma_{\mathrm{surf,C}}$ systematically off the goal

large extrapolation uncertainty for $R_{\mathrm{box,C}}$ and $\sigma_{\mathrm{surf,C}}$ $\Longrightarrow$ can be adjusted within model

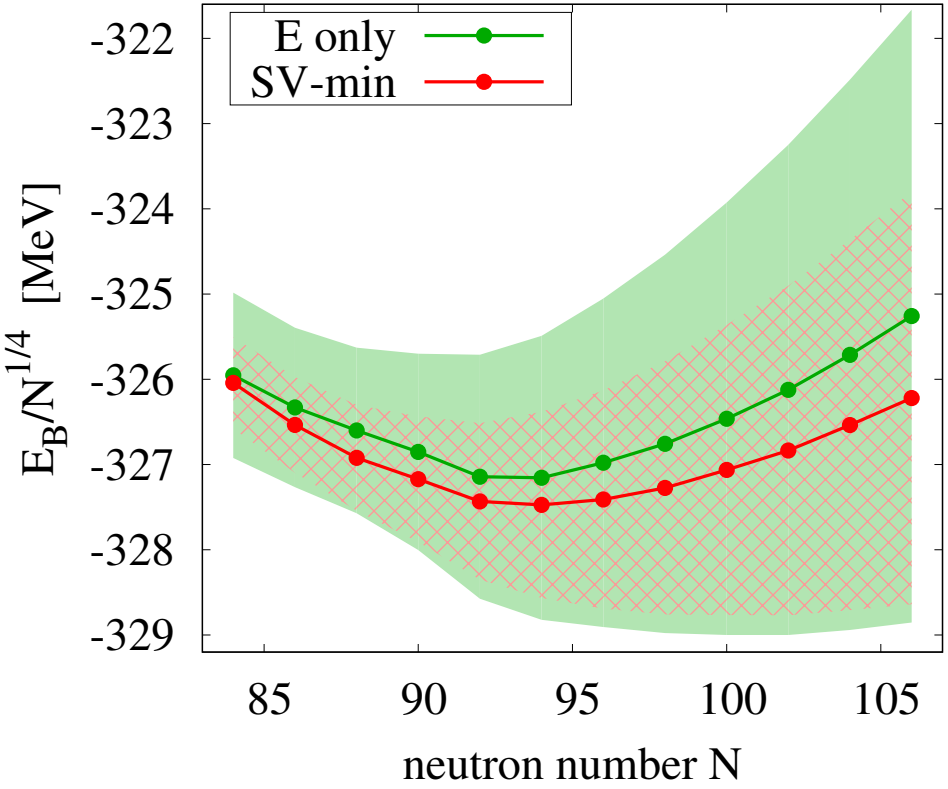
Distribution of errors on E_B, $r_{\mathrm{rms,C}}$, $R_{\mathrm{box,C}}$, $\sigma_{\mathrm{surf,C}}$ – fit to all

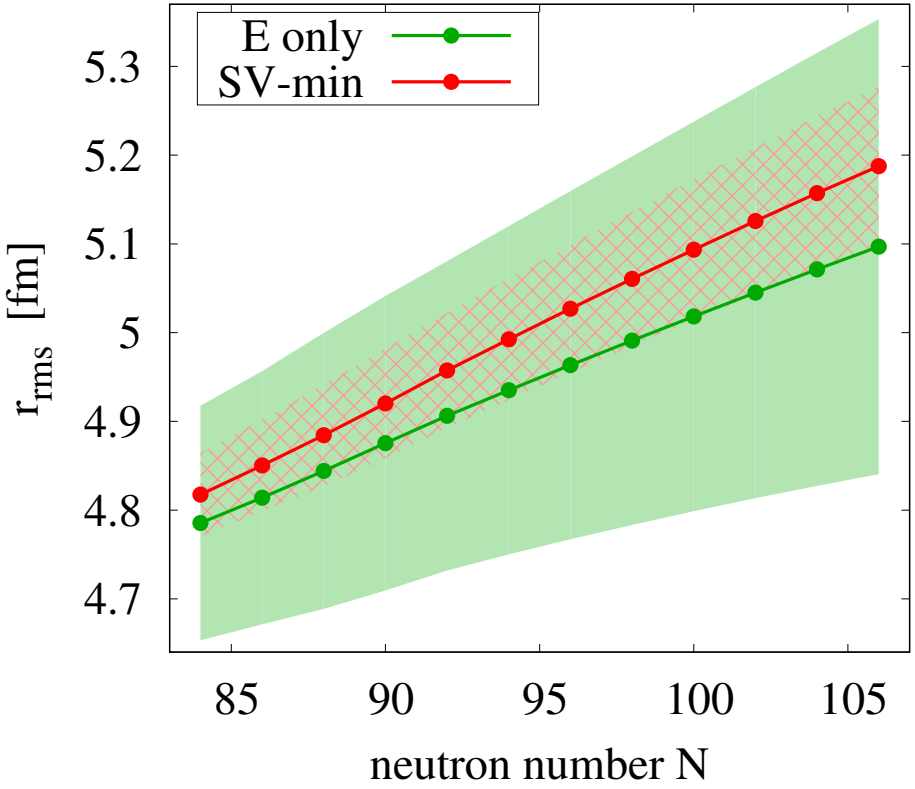


include also $r_{\mathrm{rms,C}}$, $R_{\mathrm{box,C}}$, $\sigma_{\mathrm{surf,C}}$ in the fit data

$\Longrightarrow$ accomodate box radius $R_{\mathrm{box,C}}$ and surf. thickn. $\sigma_{\mathrm{surf,C}}$ at only small sacrifices in E_B

Extrapolation *r*-process nuclei – neutron rich Sn chain





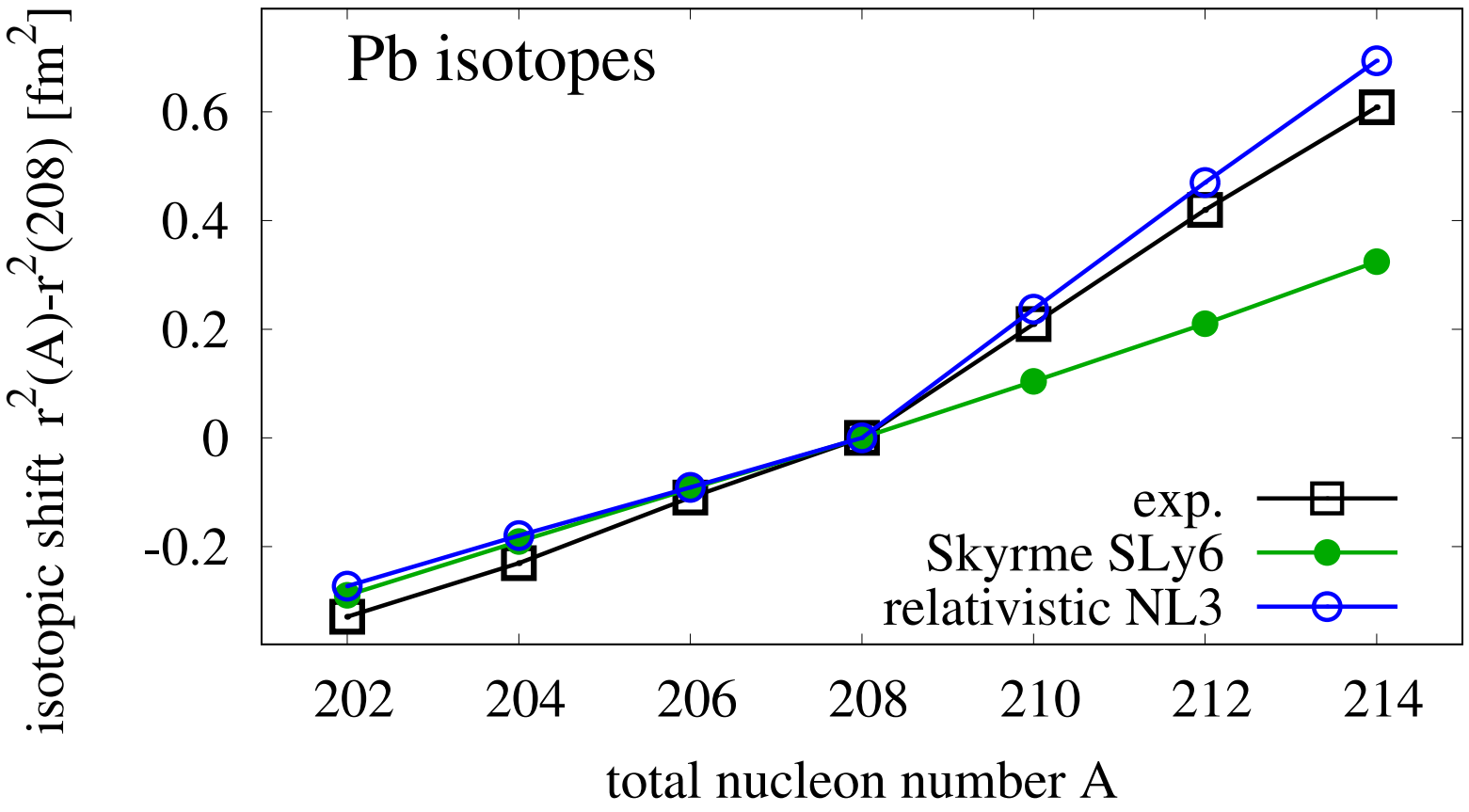
fit to E_B only fixed model parameters too weakly $\Rightarrow$ lousy extrapolation errors

large fit pool E_B, $r_{\mathrm{rms,C}}$, $R_{\mathrm{box,C}}$, $\sigma_{\mathrm{surf,C}}$ $\Longrightarrow$ more reliale extrapolations

still demand for improvement $\longleftrightarrow$ can more detailed radius data help?

Example 2: Kink of r.m.s. radii at ^{208}Pb and spin-orbit term

Isotopic shifts $r^2_{\mathrm{rms,C}}(^A\mathrm{Pb}) - r^2_{\mathrm{rms,C}}(^{208}\mathrm{Pb})$ – problem with kink at ^{208}Pb



all Skyrme models up to year 1995 failed at the kink – RMF reproduced it at once

statistical analysis indicated sensitivity to pairing and spin-orbit term

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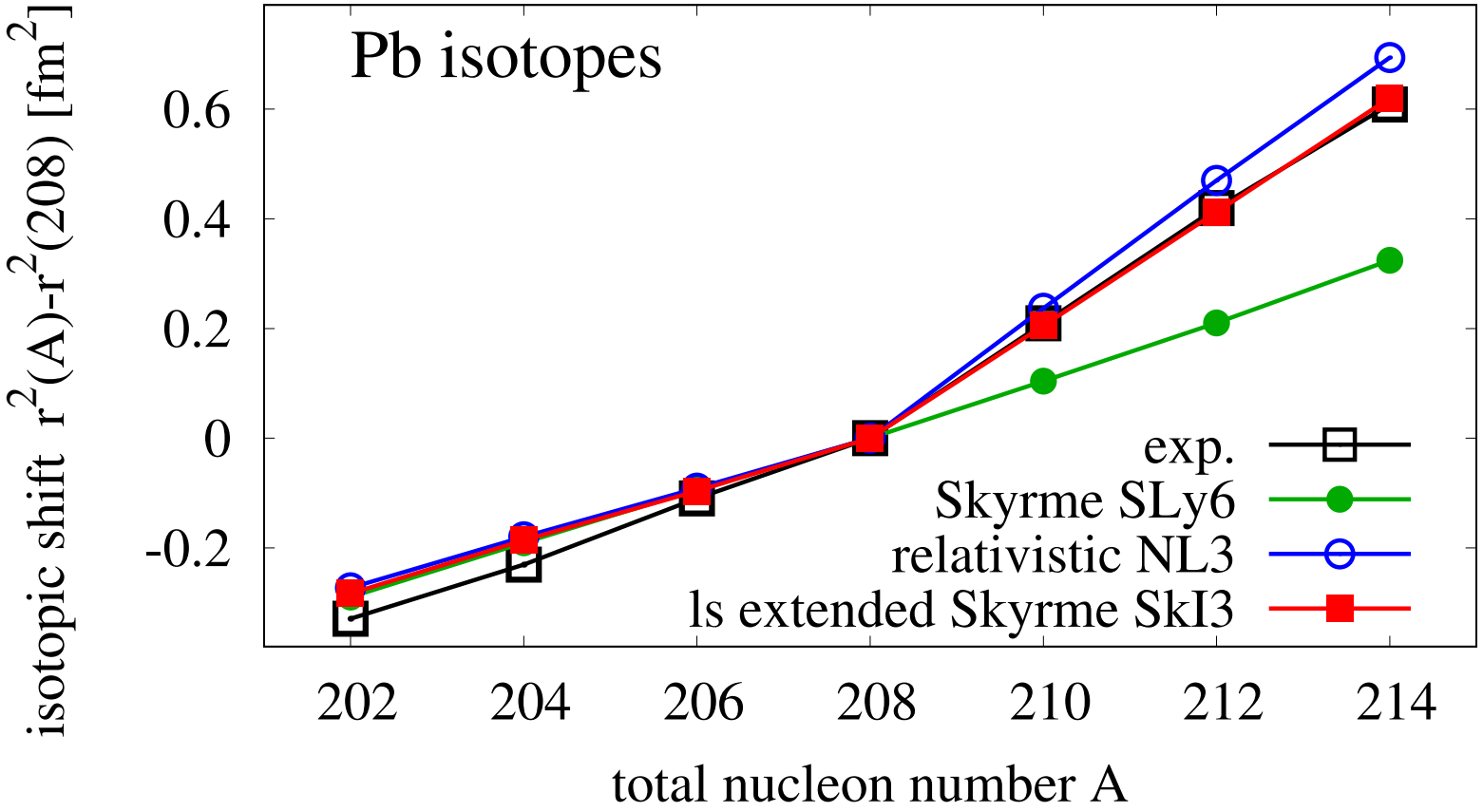
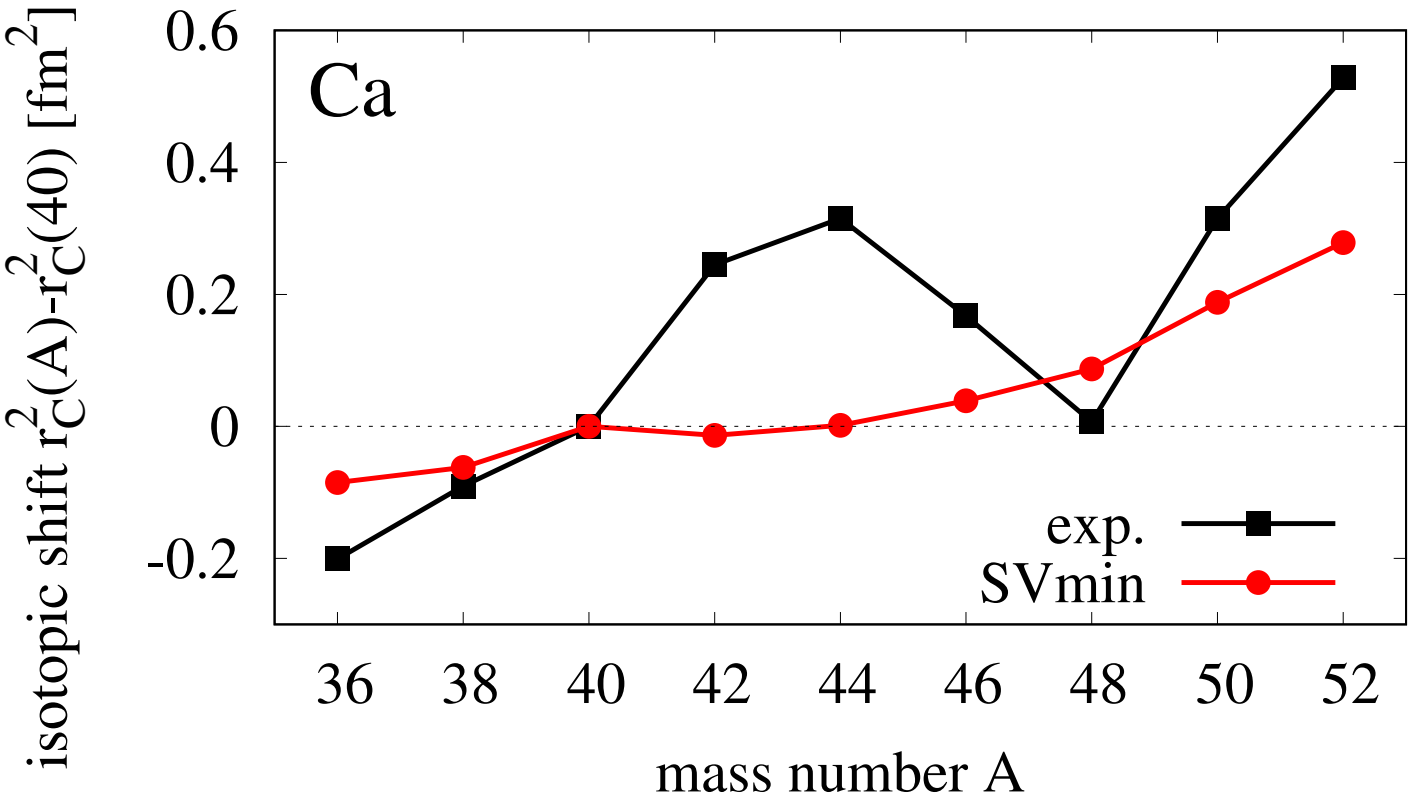


non-relativistic limit of RMF revealed different isospin structure of spin-orbit term

extend Skyrme functional by isovector spin-orbit term $\Longrightarrow$ kink also reproduced

Example 3: Isotopic shifts and odd-even staggering in Ca isotopes

The problem: trend of charge r.m.s. radii in Ca chain

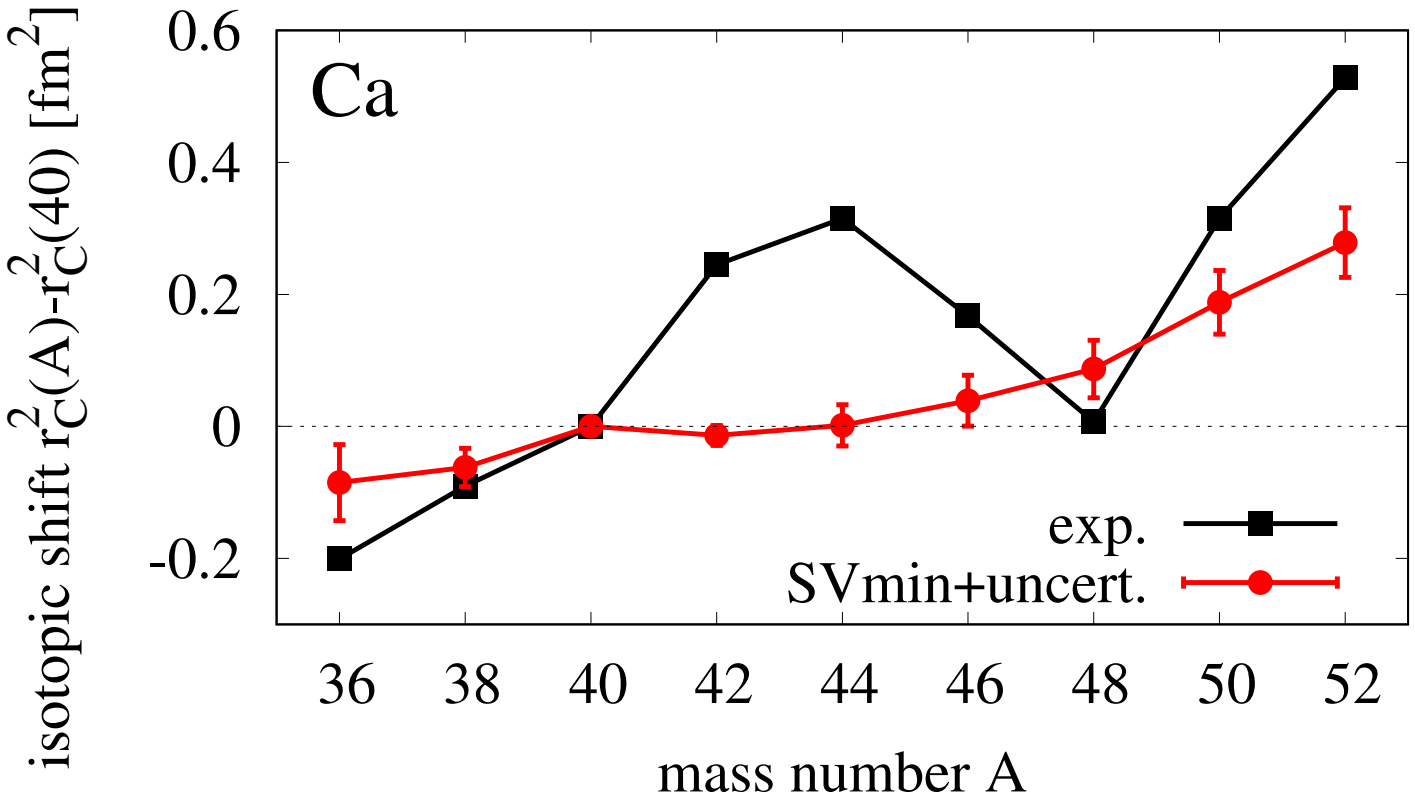


SVmin = fit of Skyrme functional with “traditional pairing” (contact force & density dep.)

$\Longrightarrow$ theory averages nicely, but fails to reproduce the trend

Statistical uncertainty ↔ explore leeway of the Skyrme functional

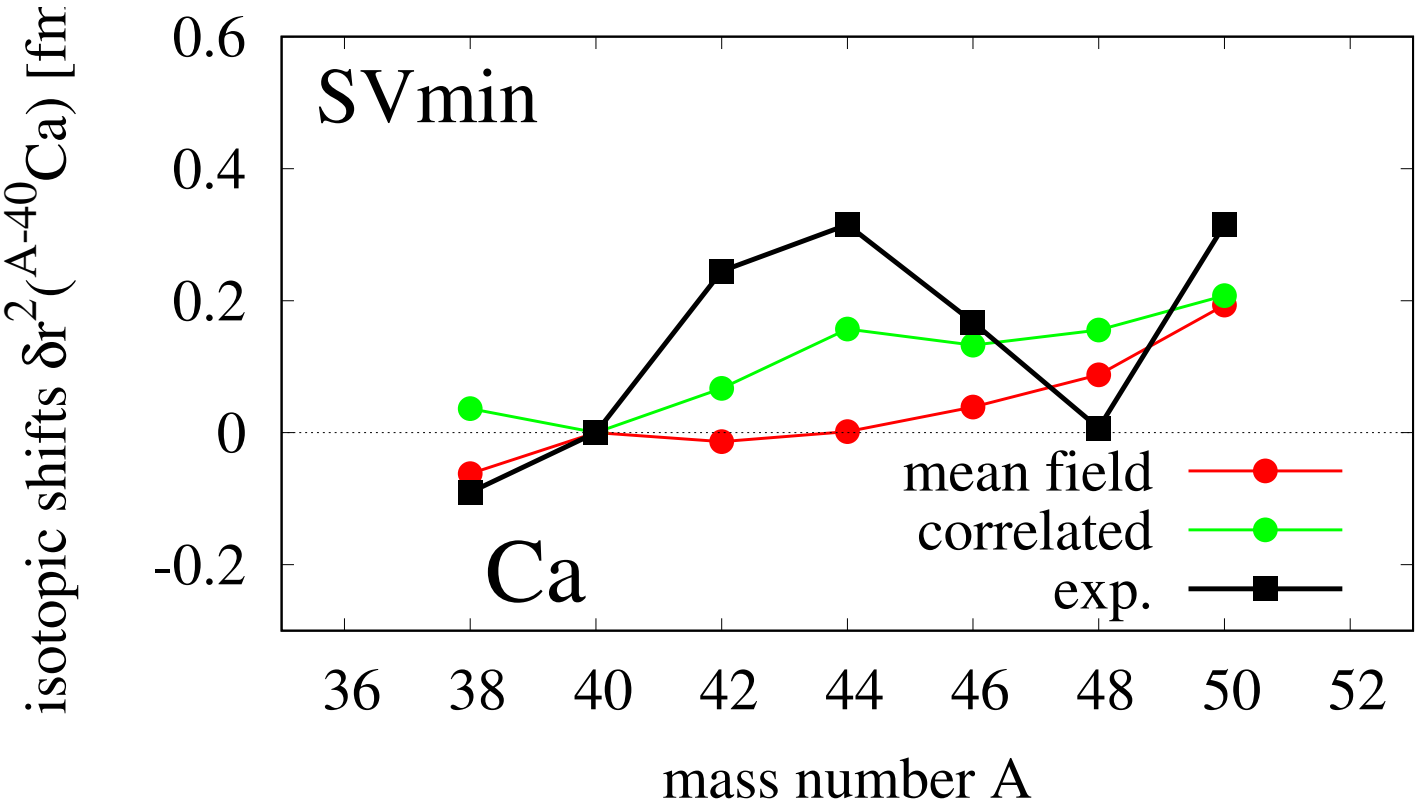
look at error bands to check chances for fitting the trend



extrapolation error too small $\Longrightarrow$ enforcing isotopic shifts will destroy overall quality

Impact of collective ground-state corrrelations

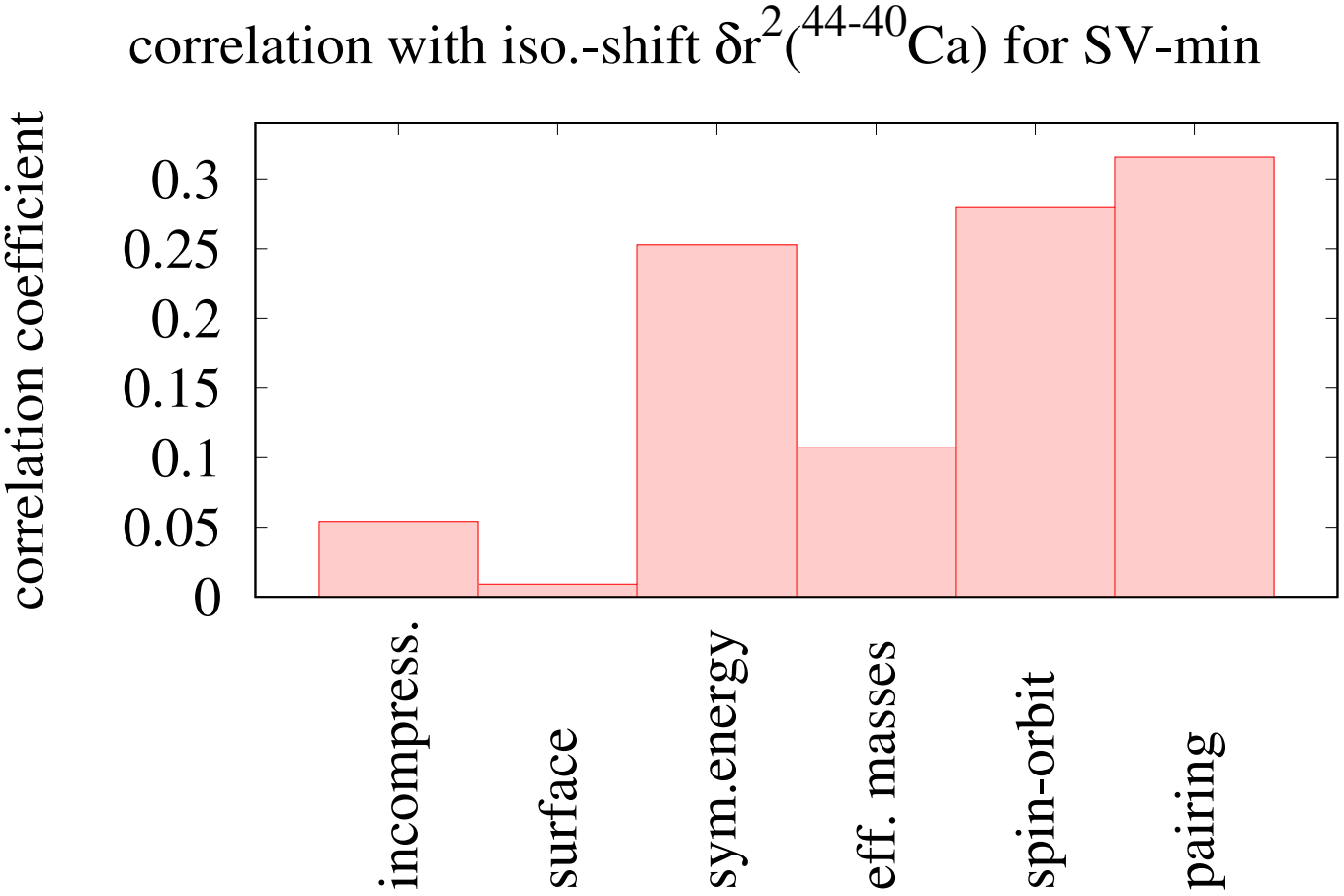
g.s. vibrations from low-lying 2^+ states contribute to radii



the effect is visible, but too small ⇒ the problem is the functional

Find most promising feature of functional

look at statistical correlations to find strongest lever



symmetry energy:	fixed by polarizability	⇒ no!
spin-orbit splittings:	conceivable but limited changeability	⇒ unlikely!
pairing:	least well known, least well fixed	⇒ try that!

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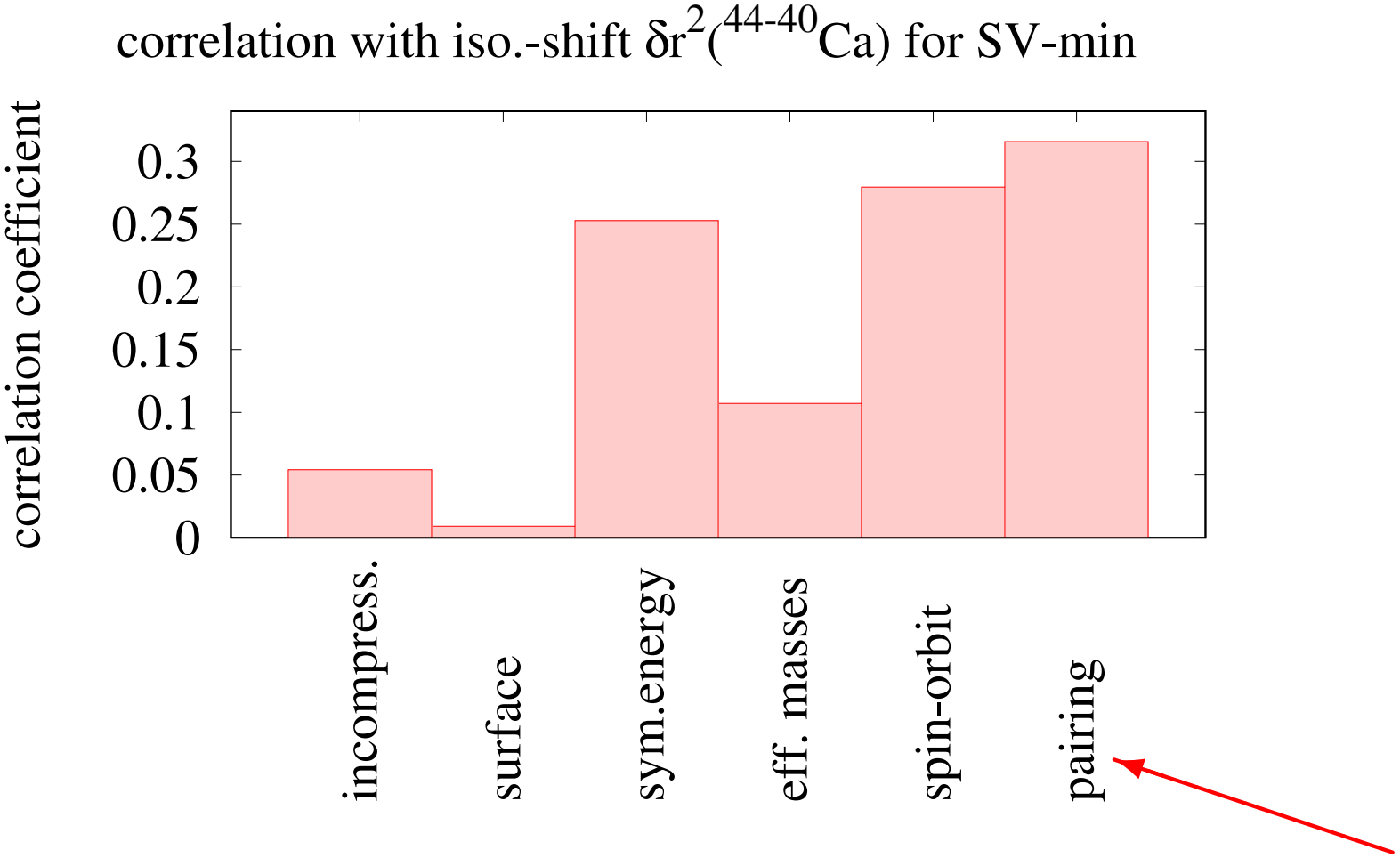

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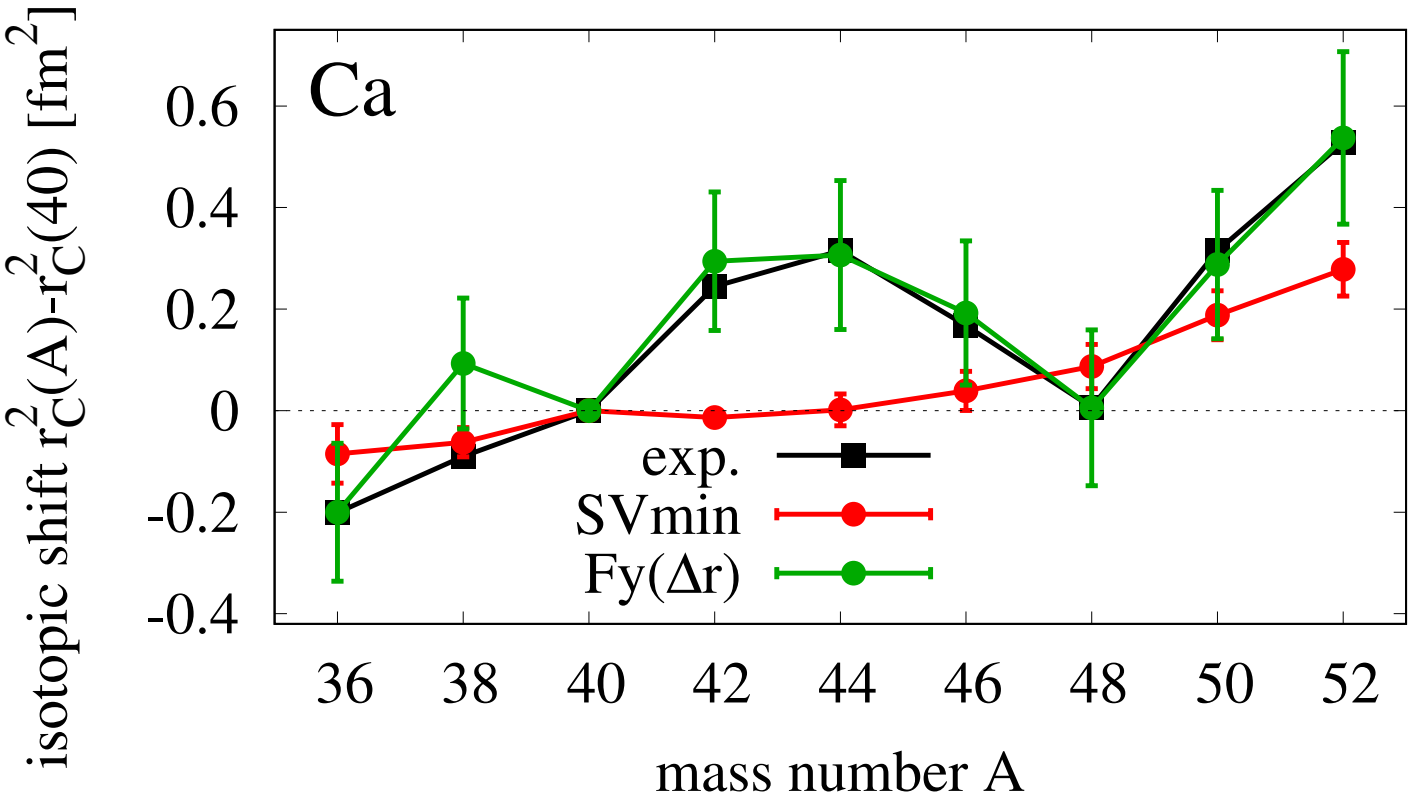
Fit isotopic trend with Fayans functional: Fy(Δr,HFB) the solution

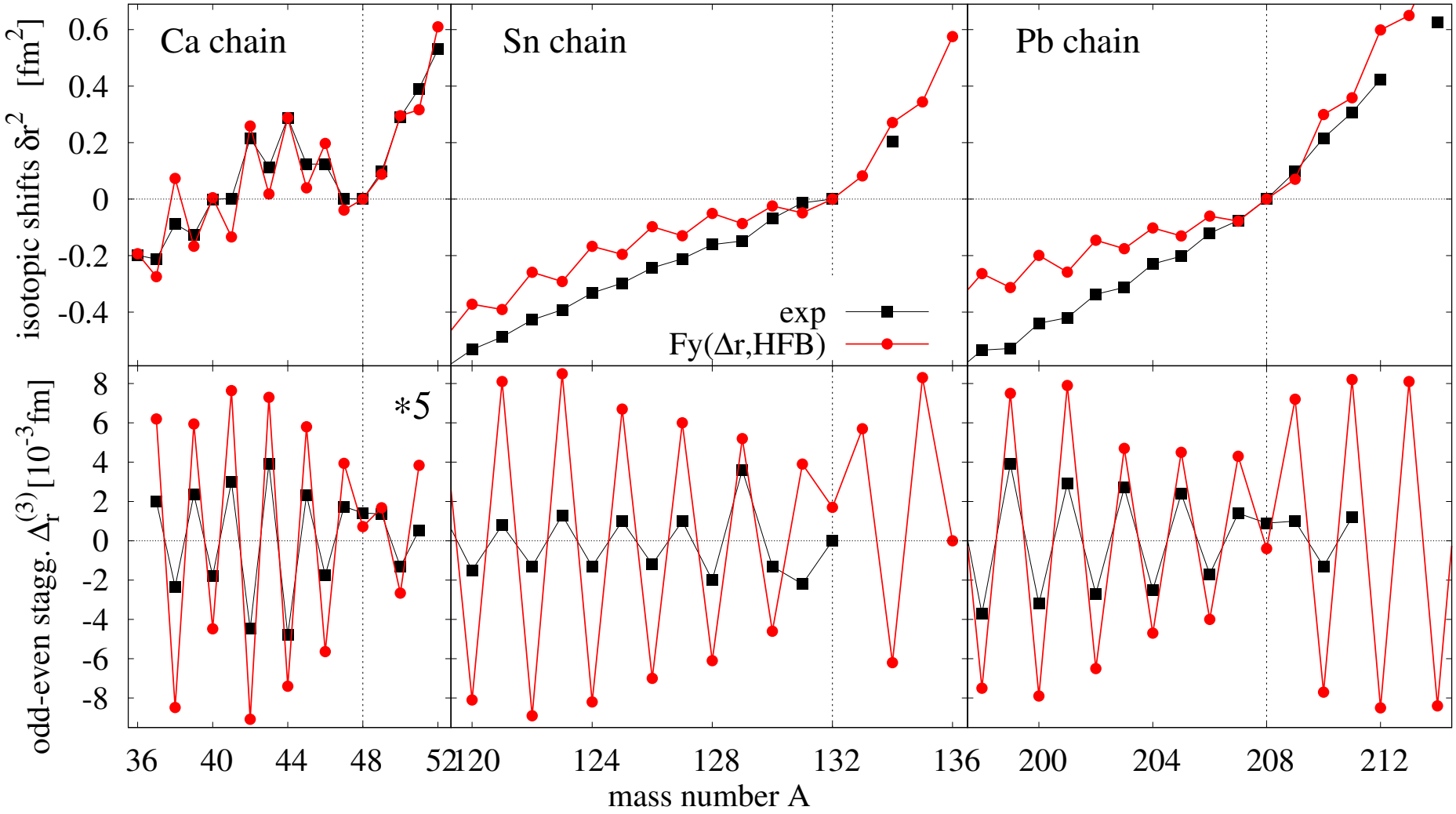


$\Longrightarrow$ Fy(Δr,HFB) reproduces trend for Ca isotopes almost perfectly

other isotopic chains? $\longrightarrow$ to be checked

Example 4: Isotopic shifts and odd-even staggering in Sn & Pb isotopes

The problem: trends in Sn & Pb isotopes, odd-even staggerings

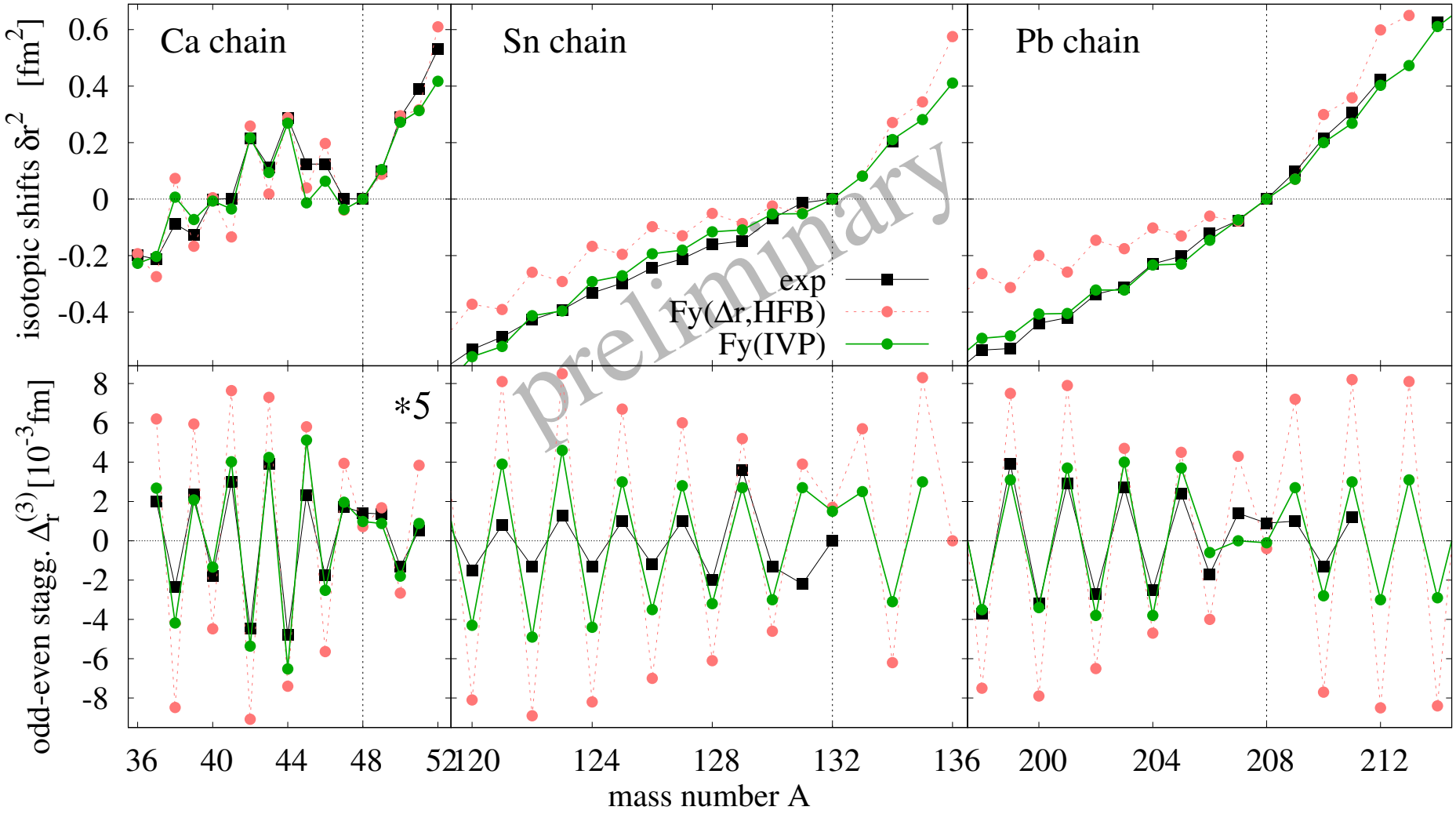


Fy(Δr,HFB) fails in: staggering $\Delta_r^{(3)}$, kinks at ^{132}Sn & ^{208}Pb, isot. trends Ca & Pb

statistical analysis: all these observables $\longleftrightarrow$ pairing

yet missing in Fayans functional: isovector pairing (IVP) $\Longrightarrow$ try!

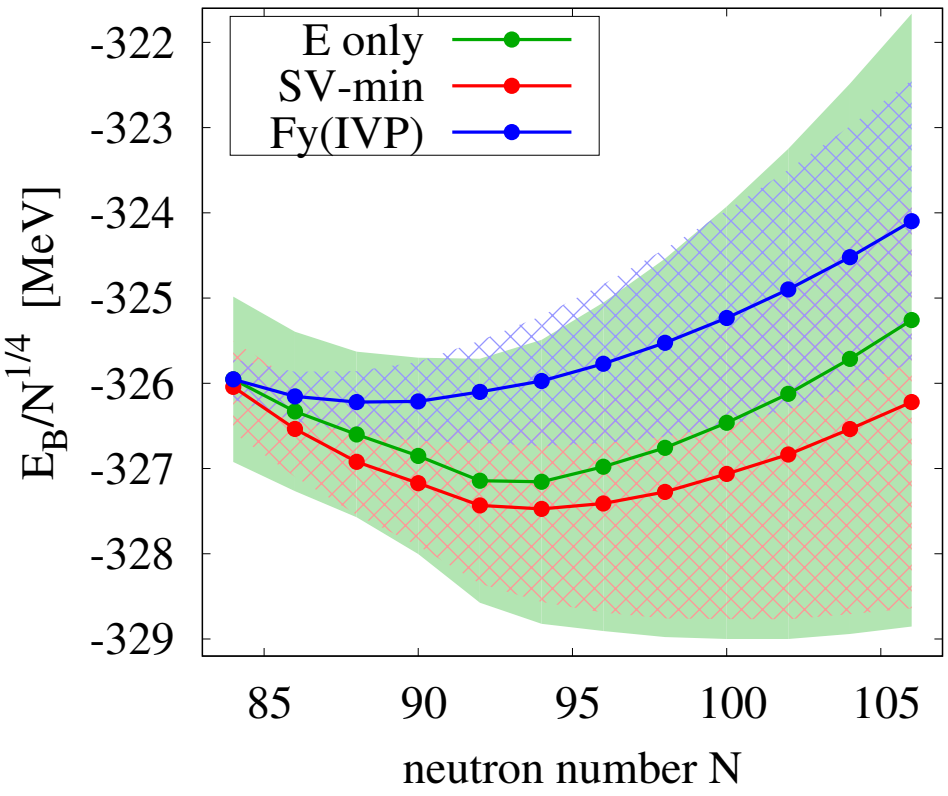
The problem: trends in Sn & Pb isotopes, odd-even staggerings

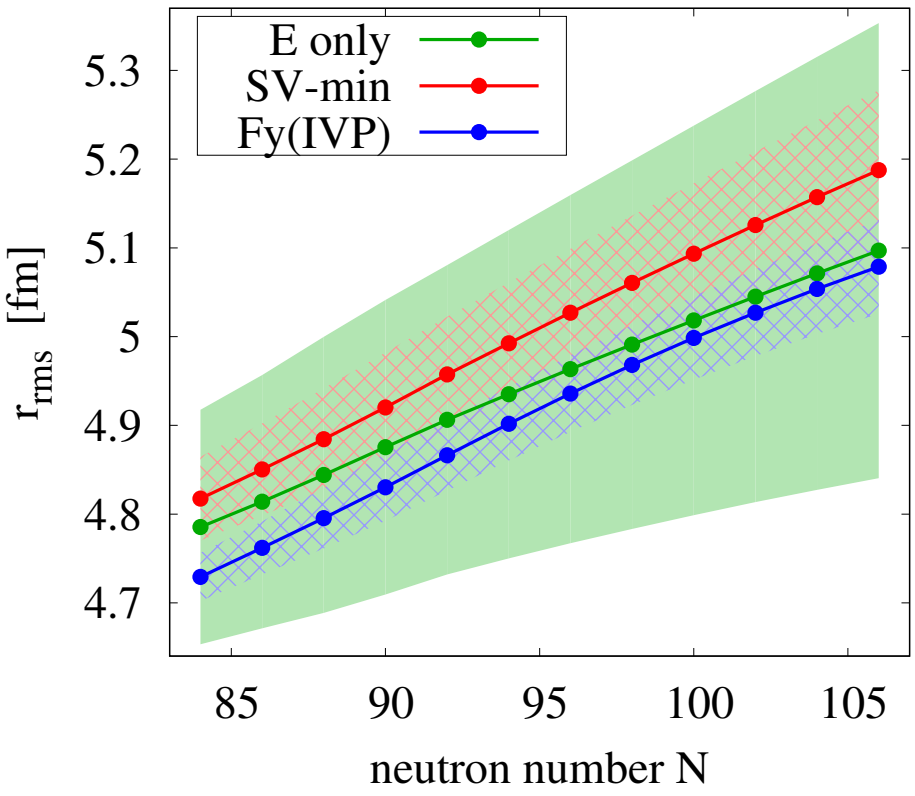


fit functional with IVP adding data on $\Delta_r^{(3)}$(Ca) and isot.trends Ca&Pb $\Longrightarrow$ Fy(IVP)

Fy(IVP): solves nearly all problems, still slightly to large $\Delta_r^{(3)}$(Sn)

Extrapolation *r*-process nuclei – neutron rich Sn chain





data on isotopic shifts & odd-even staggerings + extended model (Fayans)
$\Longrightarrow$ somewhat more reduction of errors

r-process $\equiv$ neutron rich nuclei $\Longrightarrow$ better information from neutron radius r_n?

Example 5: Neutron radii and Pb Radius EXperiment (PREX)

Measuring the neutron radius

PREX = Pb Radius EXperiment:

scattering of high-energy polarized electrons (beam energy $E_{\rm in} = 953$ MeV)
$\Longrightarrow$ Parity-Violating Asymmetry $A_{\rm PV}(q) \propto (\sigma_\uparrow - \sigma_\downarrow)/\sigma_{\rm total}$
at transfered momentum $q = 0.39$/fm

isovector dipole polarizability α_D:

from photo-absorption strength σ_γ as $\alpha_D = \int_0^{\infty(E_{\rm max})} dE\, E^{-2}\, \sigma_\gamma(E)$

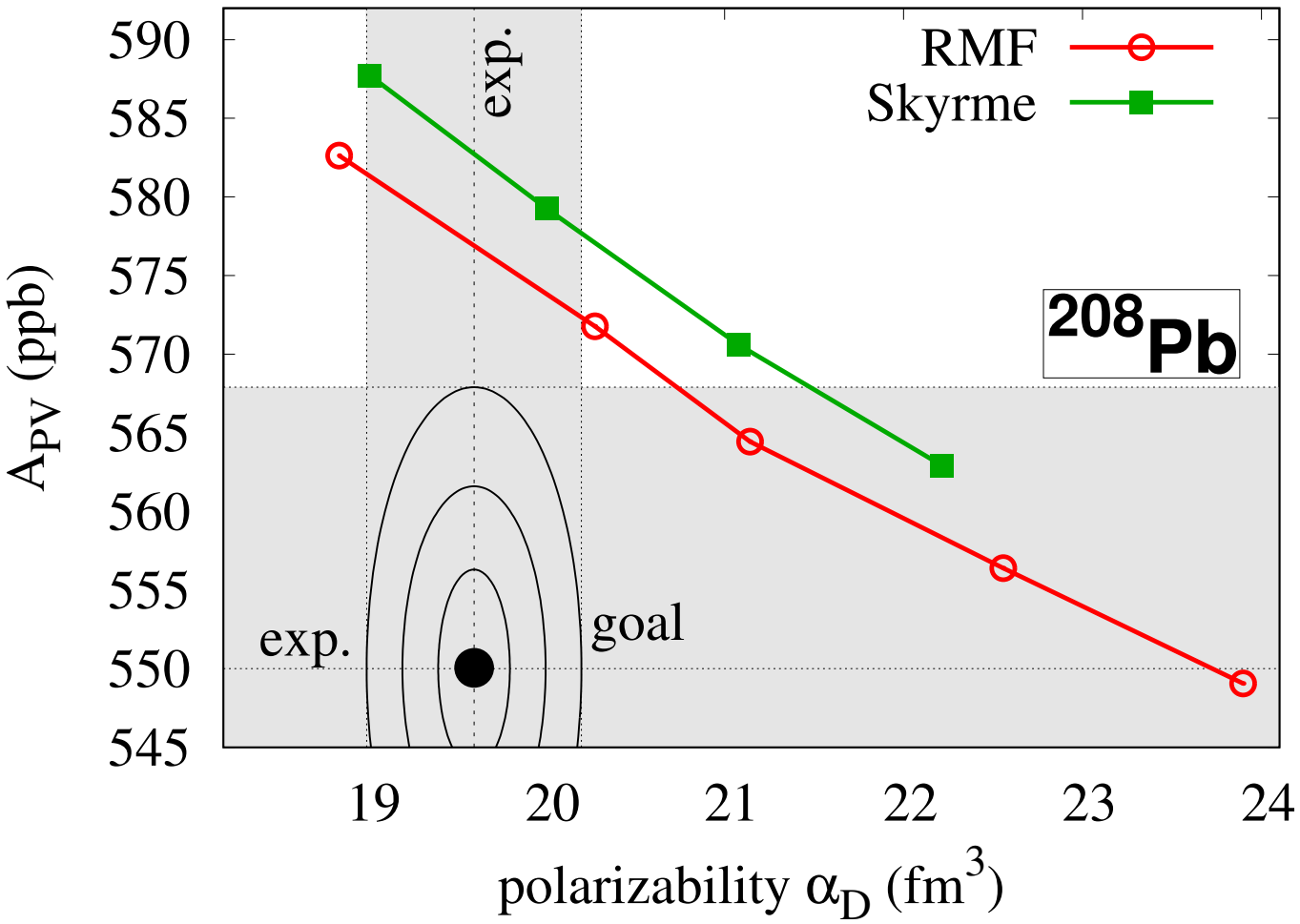
correlations α_D**,** $A_{\rm PV}$**, neutron radius** $r_{\rm neut}$:

Coefficient of Determination (CoD):

	$A_{\rm PV}$	α_D	$r_{\rm neut}$
$A_{\rm PV}$	1	0.99	0.99
α_D	0.99	1	0.98
$r_{\rm neut}$	0.99	0.98	1

$\Longrightarrow$ $A_{\rm PV}$ & α_D equivalent, model assisted measurement of $r_{\rm neut}$

Fy(IVP) and extrapolation uncertainty to neutron matter



collection of Skrme and RMF parametrizations line up to a linear trend

the trend avoids the matching point in plane of α_D and A_{PV}

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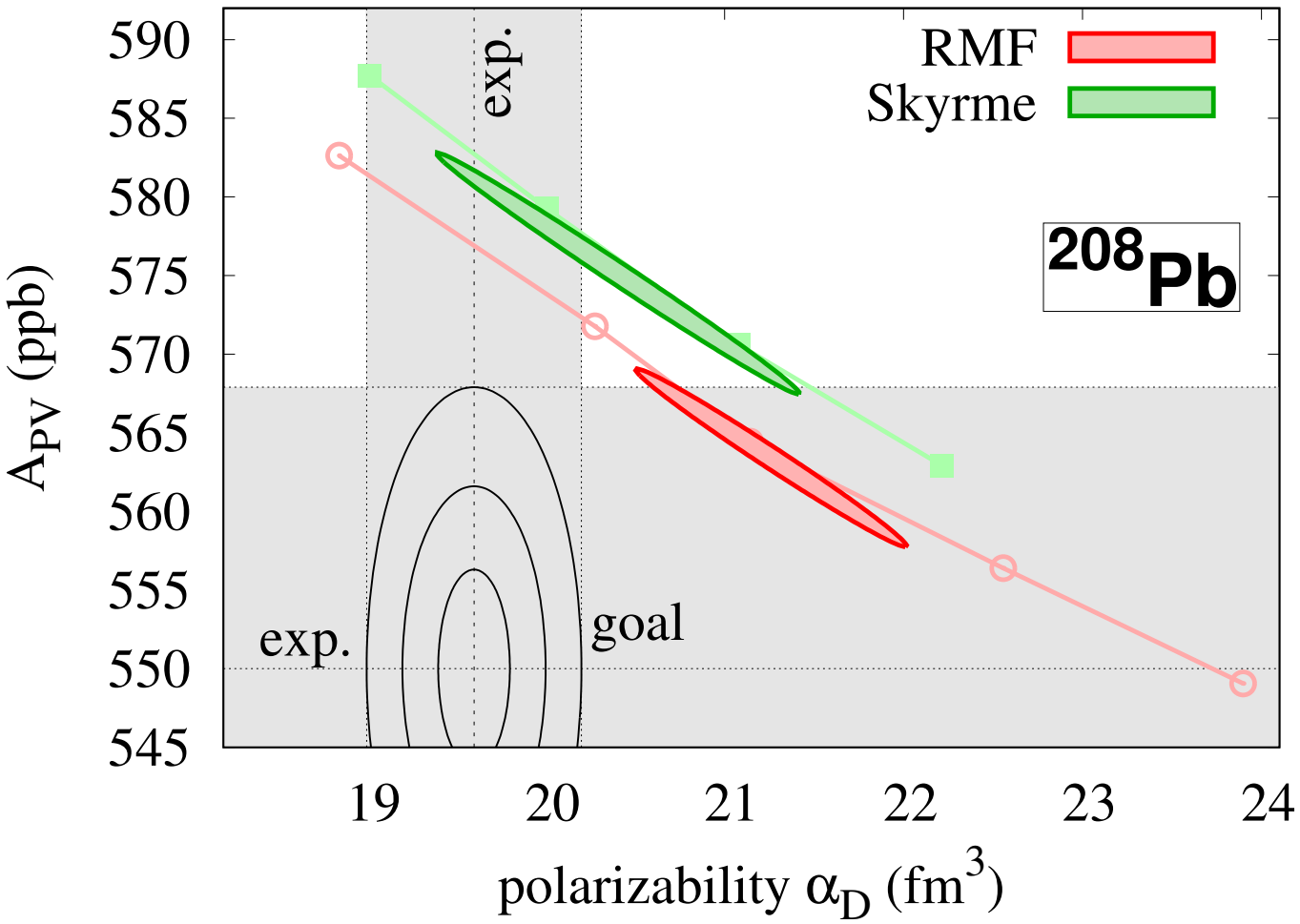

the (1σ) uncertainty ellipsoids also follow the linear trends

incompatible data: either A_{PV} or α_D can be tuned in the given models

$\Longrightarrow$ put the data point on hold, work on resolving the dilemma

Conclusions

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1. deliver valuable data for better confining models
2. challenge models by revealing missing features
3. more info from exotic nuclei needed to improve extrapolations
4. info on neutron radius highly desirable, still an enigma