(Un-)certainties in nuclear DFT

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UQNP-2024, Mainz, 29. June 2024

Outline

1. Statistical aspects of empirical calibration of nuclear DFT
2. Variation of model and data
3. Isovector observables: dipole polarizability, neutron radius
4. Isotopic radius differences
5. Conclusions

Acknowledgments:

J. Friedrich	Johannes Gutenberg University, Mainz/Germany
J. Erler, P. Klüpfel	formerly Friedrich-Alexander Univ., Erlangen/Germany
W. Nazarewicz, V. Kejzlar, L. Neufcourt	Michigan State University, Eeast Lansing
J. O'Neal	Argonne National Laboratory
S.M. Wild	Lawrence Livermore Laboratory
X. Roca-Maza	Universita degli Studi di Milano, Milano/Italy
J. Dobaczewski	University of York, York/GB

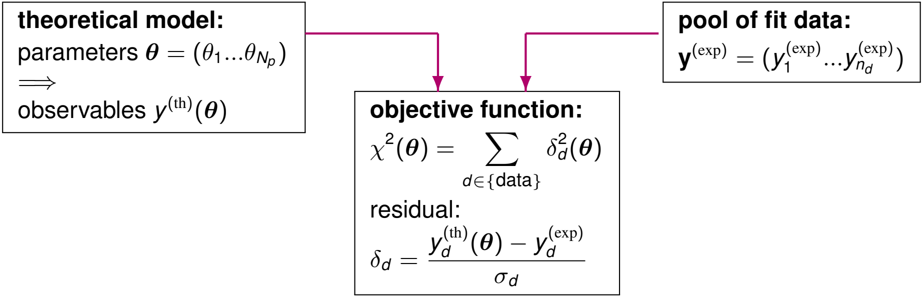
1) Statistical aspects of empirical calibration of nuclear DFT

Strategy for adjusting the model parameters to phenomenological data

theoretical model:
parameters $\boldsymbol{\theta} = (\theta_1 ... \theta_{N_p})$
$\Longrightarrow$
observables $y^{(\mathrm{th})}(\boldsymbol{\theta})$

pool of fit data:
$\mathbf{y}^{(\mathrm{exp})} = (y_1^{(\mathrm{exp})} ... y_{n_d}^{(\mathrm{exp})})$

Strategy for adjusting the model parameters to phenomenological data



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objective function:

$$\chi^2(\boldsymbol{\theta}) = \sum_{d \in \{\mathrm{data}\}} \delta_d^2(\boldsymbol{\theta})$$

residual:

$$\delta_d = \frac{y_d^{(\mathrm{th})}(\boldsymbol{\theta}) - y_d^{(\mathrm{exp})}}{\sigma_d}$$

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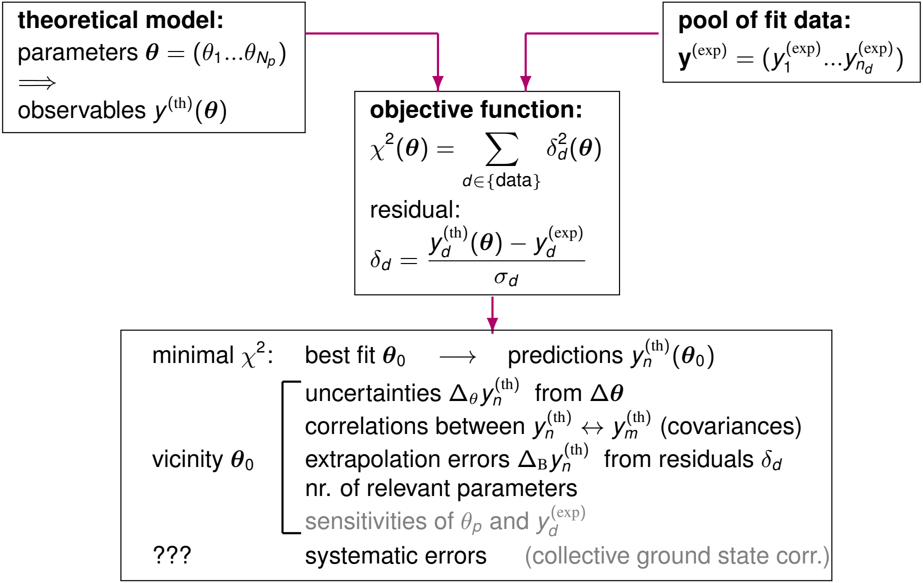

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minimal χ^2: best fit $\boldsymbol{\theta}_0$ $\longrightarrow$ predictions $y_n^{(\mathrm{th})}(\boldsymbol{\theta}_0)$

vicinity $\boldsymbol{\theta}_0$

- uncertainties $\Delta_\theta y_n^{(\mathrm{th})}$ from $\Delta\boldsymbol{\theta}$
- correlations between $y_n^{(\mathrm{th})} \leftrightarrow y_m^{(\mathrm{th})}$ (covariances)
- extrapolation errors $\Delta_{\mathrm{B}} y_n^{(\mathrm{th})}$ from residuals δ_d
- nr. of relevant parameters
- sensitivities of θ_p and $y_d^{(\mathrm{exp})}$

??? systematic errors (collective ground state corr.)

Nuclear DFT models (e.g. non-relativistic)

variational formulation on the basis of a given energy functional

$$E_{\text{tot}} = E_{\text{kin}} + \int d^3r\,\mathcal{E}_{\text{model}}(\rho_0, \rho_1, \tau_0, \tau_1, \mathbf{J}_0, \mathbf{J}_1, \xi_p, \xi_n) + E_{\text{Coulomb}} - E_{\text{c.m.}} - E_{\text{rot}}$$

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$\mathcal{E}_{\mathrm{model}}$ is functional of local densities:

$\rho(r) =$ particle, $\tau(r) =$ kinetic, $\mathbf{J}(r) =$ l*s, $\xi(r) =$ pairing

indices: $T = 0 \equiv$ isoscalar, $T = 1 \equiv$ isovector, $p =$ proton, $n =$ neutron

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often point couplings:	$c_\rho\ \rho * \rho$	volume	$c_\rho = c_\rho(\rho)$ dens.dep.
	$c_\nabla\ \nabla\rho * \nabla\rho$	surface	
	$c_\tau\ \rho * \tau$	kinetic	
	$c_{ls}\ \rho * \nabla\mathbf{J}$	spin orbit	
	$c_{pair}\ \xi * \xi$	pairing	$c_{pair} = V_{\text{pair}} + V'_{\text{pair}}\rho$

$\longleftrightarrow$ low q expansion of effective interaction (T-matrix)

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typically 11–15 model parameters

volume by nuclear matter parameters: E/A, $\rho_{\rm eq}$, K, m^*/m, $\kappa_{\rm TRK} \equiv m_1^*/m$

surface $T = 0\&1$, kinetic $T = 0\&1$, spin-orbit $T = 0\&1$

pairing 1–4 parameters

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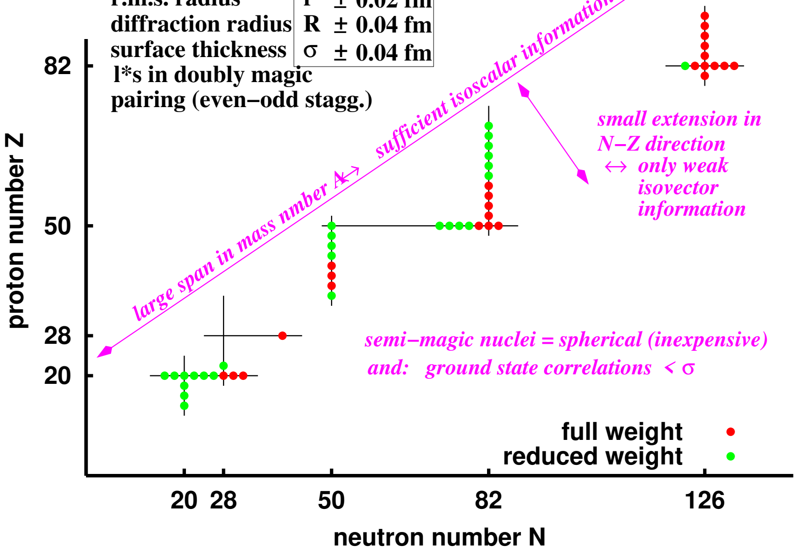
typically 11–15 model parameters ↔ tuned to empirical data on nuclear bulk properties

The pool of fit data – nuclear ground state properties

SV-min

Fit Observables:	y	σ
binding energy	E_B	± 1MeV
r.m.s. radius	r	± 0.02 fm
diffraction radius	R	± 0.04 fm
surface thickness	σ	± 0.04 fm
l*s in doubly magic		
pairing (even−odd stagg.)		



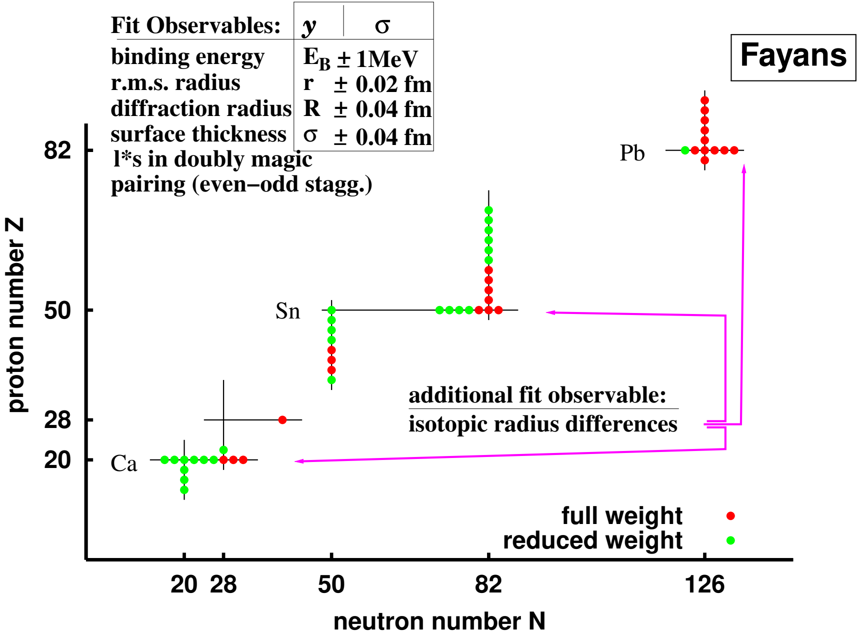
large span in mass nmber A ↔ sufficient isoscalar information

small extension in N−Z direction ↔ only weak isovector information

semi−magic nuclei = spherical (inexpensive)

and: ground state correlations < σ

The pool of fit data – nuclear g.s. properties & radius differences



Fayans

Fit Observables:	***y***	**σ**
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diffraction radius	**R**	**± 0.04 fm**
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l*s in doubly magic		
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additional fit observable:
isotopic radius differences

The basic probability distribution

$$p(\boldsymbol{\theta}\sigma|\mathbf{y}) \quad = \exp\left(-\frac{\chi^2(\boldsymbol{\theta}|\mathbf{y})}{\sigma^2}\right) \quad \approx \quad \exp\left(-\frac{(\boldsymbol{\theta}-\boldsymbol{\theta}_0)\hat{H}(\boldsymbol{\theta}-\boldsymbol{\theta}_0)}{2\sigma^2}\right)$$

Gaussian process

$\boldsymbol{\theta}$ = model parameters

$\boldsymbol{\theta}_0$ = model parameters at the best fit point

$\mathbf{y}$ = fit data

σ = global scaling parameter, used in Bayesian formula

$H_{\alpha\beta}$ $= \partial_{\theta_\alpha}\partial_{\theta_\beta}\chi^2\Big|_{\boldsymbol{\theta}_0} = \sum_d \frac{\partial\delta_d}{\partial_{\theta_\alpha}}\frac{\partial\delta_d}{\partial_{\theta_\beta}}$ = Hessian matrix

$C_{\alpha\beta}$ $= \left(H^{-1}\right)_{\alpha\beta}$ = covariance matrix

Distribution of model parameters (or: leeway of the model)

$\sigma=1 \Rightarrow$ **probability of $\boldsymbol{\theta}$:** $\mathcal{P}(\boldsymbol{\theta}|\mathbf{y}) \propto \exp\left(-\chi^2(\boldsymbol{\theta}|\mathbf{y})\right) \approx \exp\left(-\frac{(\boldsymbol{\theta}-\boldsymbol{\theta}_0)\hat{H}(\boldsymbol{\theta}-\boldsymbol{\theta}_0)}{2}\right)$

Various statistical quantities can be deduced from that:

$$
\begin{aligned}
\overline{A} \quad &= \int d\boldsymbol{\theta}\mathcal{P}(\boldsymbol{\theta})A(\boldsymbol{\theta}) = \text{expectation value of observable } A \\
\Delta A \quad &= \sqrt{\int d\boldsymbol{\theta}\mathcal{P}(\boldsymbol{\theta})(A(\boldsymbol{\theta}) - \overline{A})^2} = \text{variance of } A \\
\overline{\Delta A \Delta B} \quad &= \int d\boldsymbol{\theta}\mathcal{P}(\boldsymbol{\theta})(A(\boldsymbol{\theta}) - \overline{A})(B(\boldsymbol{\theta}) - \overline{B}) = \text{covariance } A \leftrightarrow B \\
r_{AB} \quad &= \frac{\overline{\Delta A \Delta B}^2}{\Delta A \Delta B} = \text{Coefficient of Determination (CoD)} \\
\mathcal{P}(A, B) \quad &\propto \exp\left(-(A - \overline{A})\frac{d\boldsymbol{\theta}}{dA}\hat{H}\frac{d\boldsymbol{\theta}}{dB}(B - \overline{B})\right) = \text{probability distr. for } A \text{ and } B \\
&\longrightarrow \text{error ellipsoid in plane of } A \text{ and } B \equiv \text{correlated uncertainties} \\
\delta\theta_\alpha \quad &= \sqrt{H_{\alpha\alpha}} = \text{uncorrelated uncert. of } \theta_\alpha \leftrightarrow \text{vary } \theta_\alpha \text{ for all other } \theta_\beta \text{ fixed} \\
\Delta\theta_\alpha \quad &= \sqrt{C_{\alpha\alpha}} = \text{correlated uncert. of } \theta_\alpha \leftrightarrow \text{vary } \theta_\alpha \text{ for other } \theta_\beta \text{ re-optimized}
\end{aligned}
$$

leeway of $\boldsymbol{\theta} \longleftrightarrow$ model & data exploration and development

Error estimates from Bayesian calculus

probability distribution for an observable y^* outside the given data $\mathbf{y}$:

$$\boxed{p(y^*|\mathbf{y}) \propto \int d\sigma\, d\boldsymbol{\theta}\, p(y^*|\boldsymbol{\theta}\sigma)p(\boldsymbol{\theta}\sigma|\mathbf{y})\pi(\boldsymbol{\theta})}$$

$$\begin{aligned}
\pi(\boldsymbol{\theta}) &= \text{prior} \\
p(\boldsymbol{\theta}\sigma|\mathbf{y}) &= e^{-\chi^2} = \text{model likelihood function} \\
p(y^*|\boldsymbol{\theta}\boldsymbol{\sigma}) &= \exp\left(-\frac{(y^*(\boldsymbol{\theta})-y^*(\boldsymbol{\theta}_0))^2}{\overline{\Delta_\theta {y^*}^2}\,\sigma^2}\right) = \text{probab. distribution of } y^* \text{ for given } \boldsymbol{\theta},\sigma \\
\Delta_\theta y^* &= \text{variance} \quad \sqrt{\int d\boldsymbol{\theta}\mathcal{P}(\boldsymbol{\theta})(y^*(\boldsymbol{\theta})-\overline{y^*})^2} =
\end{aligned}$$

for Gaussian processes evaluate σ integration by saddle-point approximation ($N_d \gg 1$)

Error estimates from Bayesian calculus

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for Gaussian processes evaluate σ integration by saddle-point approximation ($N_d \gg 1$)

having $p(y^*|\mathbf{y})$ one can compute:

average $\overline{y^*}$ and Bayesian extraploated error $\Delta_B y^* = \sqrt{\int dy^* p(y^*|\mathbf{y})(y^* - \overline{y^*})^2}$

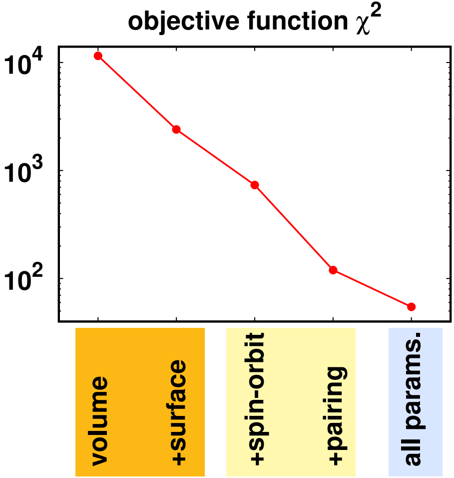
used here for extrapolations (e.g. exotic nuclei)

2) Variation of model and data

Impact of model parameters

Evolution of quality with size of model (Skyrme functional)

number of DFT parameters		
	isoscalar	isovector
volume	3	1 + 1
vol. kinetic	1	1
surface	1	1
spin-orbit	1	1
pairing	1 + 1-2	



7 parameters (volume...pairing) ⟹ already quality model

all 14 parameters ⟹ fine tuning, precision model (isovector weakness)

Singular Value Decomposition (SVD) of the Hessian matrix

dimensionles Hessian:

$$\boxed{\tilde{H}_{ij} = \frac{H_{ij}}{\sqrt{H_{ii}H_{jj}}}}$$

diagonalize $\tilde{H}_{ii'}$:

eigenvectors $\equiv$ effective parameters

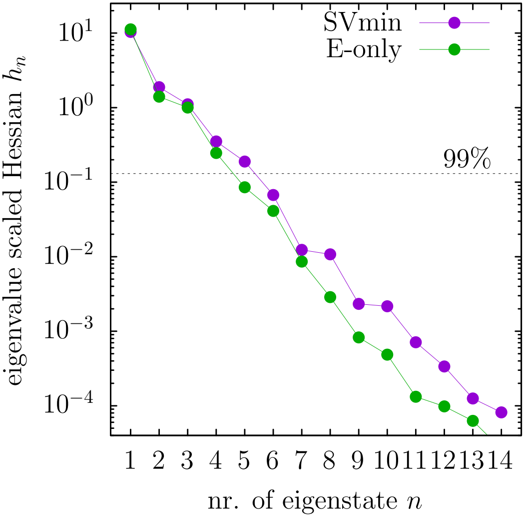
eigenvalues $\tilde{h}_n$

$\leftrightarrow$ impact of "eigen-parameter" n

spans 5 order of magnitude

only 4-5 relevant parameters

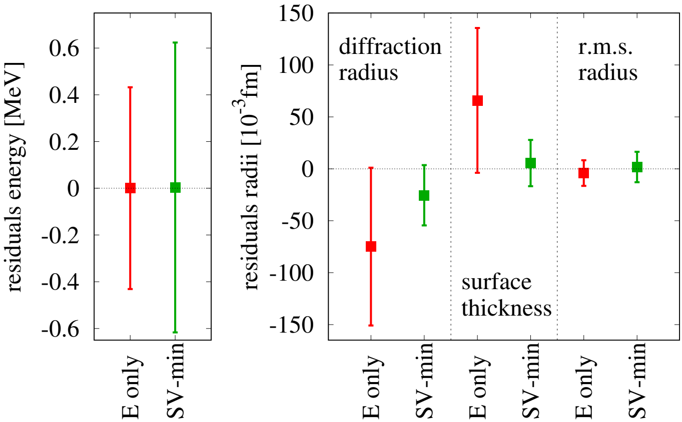
more data $\Rightarrow$ more relev. parameters



The impact of fit data

The impact of fit data

compare: fit to E_B only ("E only") $\longleftrightarrow$ fit to all = E_B, $r_{\mathrm{rms,C}}$, $R_{\mathrm{box,C}}$, $\sigma_{\mathrm{surf,C}}$ ("SV-min")



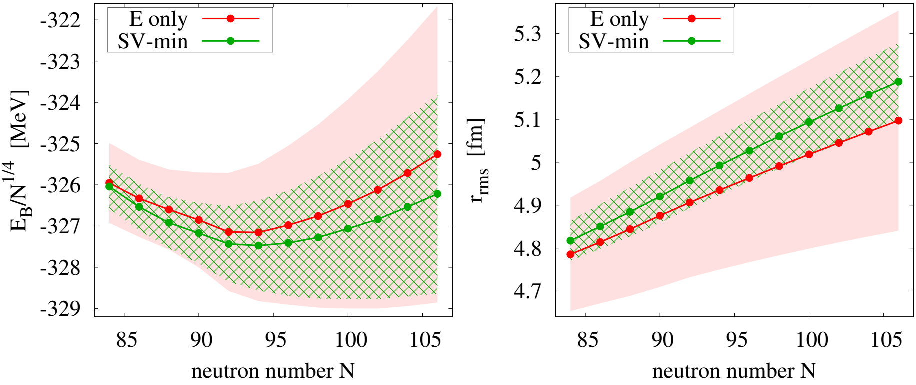
center symbol
↔ average error

error bar
↔ r.m.s. error

"E only": fit only to E_B data $\Longrightarrow$ surprisingly good also for other observables
Δr, ΔR, $\Delta\sigma$ large $\longleftrightarrow$ leeway to accomodate radii

SV-min: fit with radius data $\Longrightarrow$ improved radii, small sacrifice E_B

Test: extrapolation to *r*-process nuclei – neutron rich Sn chain

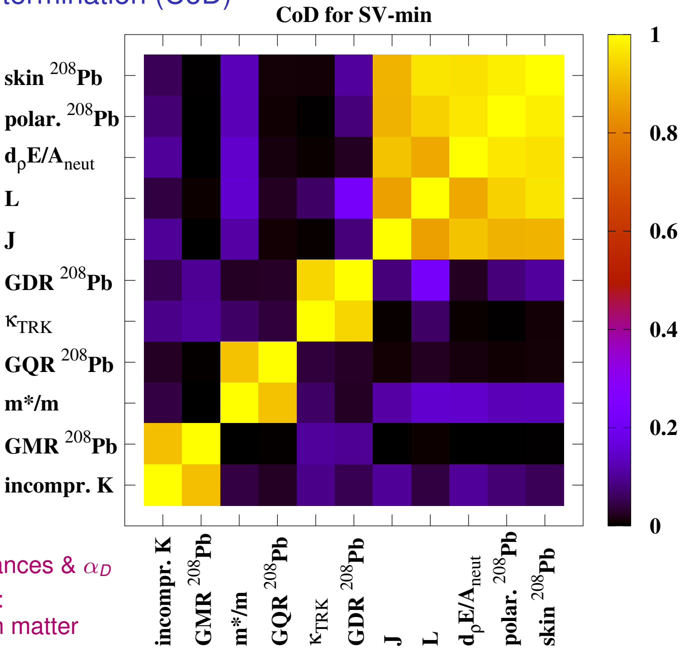


"E only":	large extrapolation errors
SV-min:	more fit data $\Longrightarrow$ more reliable extrapolations, particularly radii
???	more data for smaller extrapolation errors, systematic errors

3) Isovector observables: dipole polarizability, neutron radius

Correlations between model paramaters and observables

Coefficients of Determination (CoD)



static isovector

dynamic isovector

dynamic isoscalar

static isoscalar

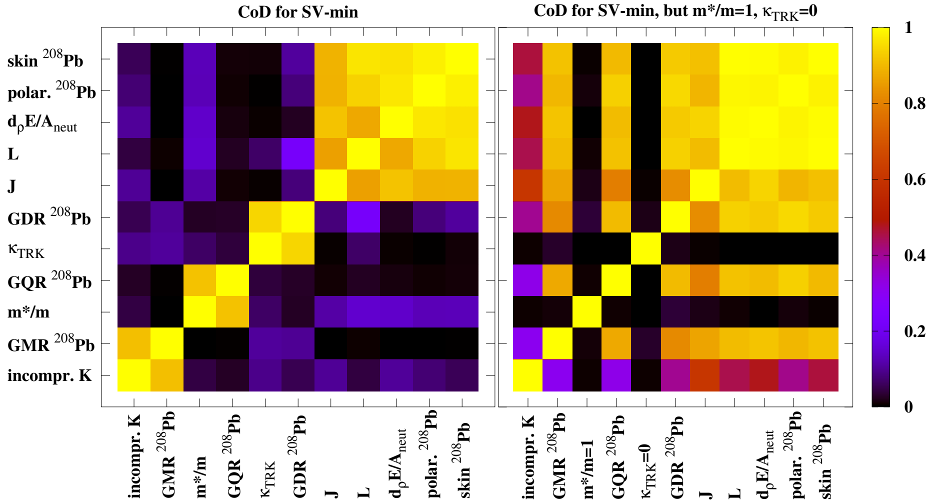
$\Longrightarrow$

NMP ↔ giant resonances & α_D

large isovector block:

$r_{\mathrm{neut}} \leftrightarrow \alpha_D \leftrightarrow$ neutron matter

CoD: impact of model – frozen m^*/m

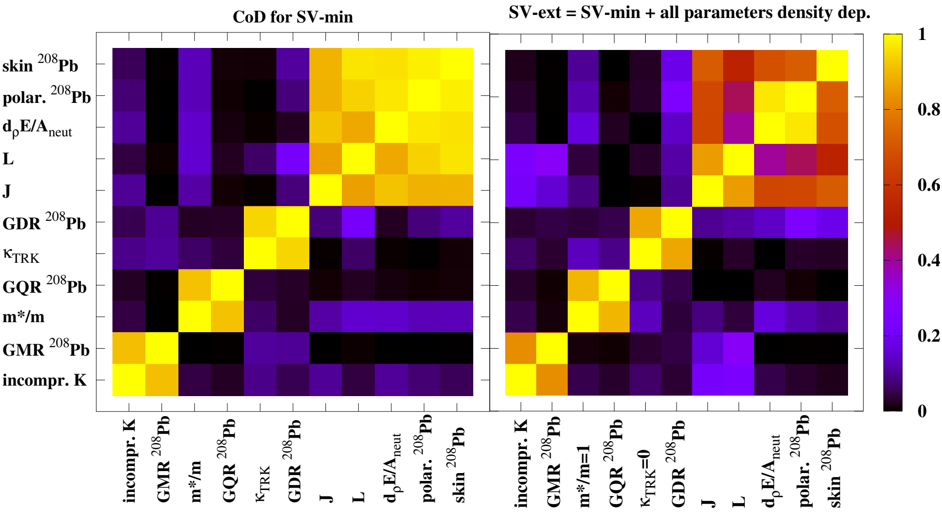


$\Longrightarrow$

less model flexibility $\longleftrightarrow$ more correlations

rigid m^*/m overestimates correlations ($\leftrightarrow$ RMF)

CoD: impact of model – more ρ-dependence



$\Longrightarrow$

more model flexibility $\longleftrightarrow$ less correlations

L almost decoupled from $r_{\rm neut}$, α_D

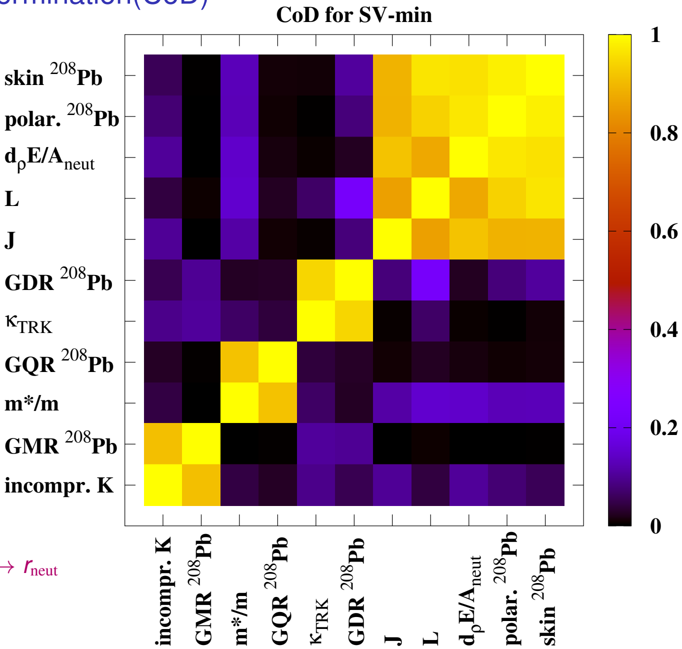
Coefficient of Determination(CoD)

static isovector

dynamic isovector

dynamic isoscalar

static isoscalar



$\Longrightarrow$

check relation $\alpha_D \longleftrightarrow r_{\text{neut}}$

Neutron radii and Pb/Ca Radius EXperiment (PREX/CREX)

Measuring the neutron radius

(ignore here proton and α scattering)

PREX = Pb Radius EXperiment / CREX = Ca Radius Experiment:

scattering of high-energy polarized electrons (beam energy $E_{\rm in} = 953$ MeV / 2182 MeV)

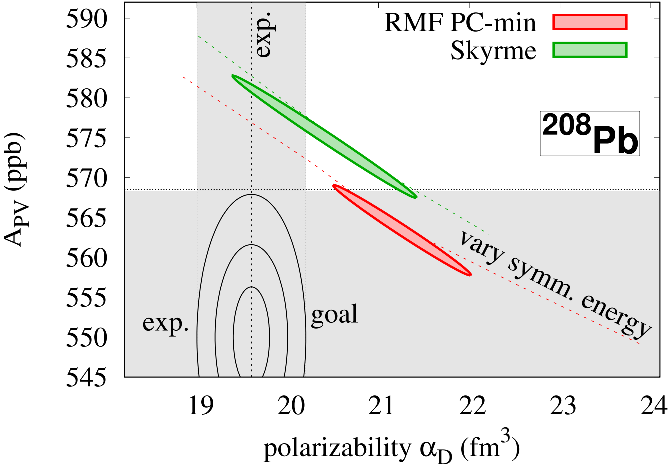
$\Longrightarrow$ Parity-Violating Asymmetry $A_{\rm PV}(q) \propto (\sigma_\uparrow - \sigma_\downarrow)/\sigma_{\rm total}$
at transfered momentum $q = 0.39$/fm / 0.873/fm

isovector dipole polarizability α_D:

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

$\Longrightarrow$ measuring $A_{\rm PV} \equiv$ measuring $r_{\rm neut}$ formally equivalent
measuring $r_{\rm neut}$ close to measuring α_D statistical correlation

Compatibility of A_{PV} and α_D measurements in ^{208}Pb

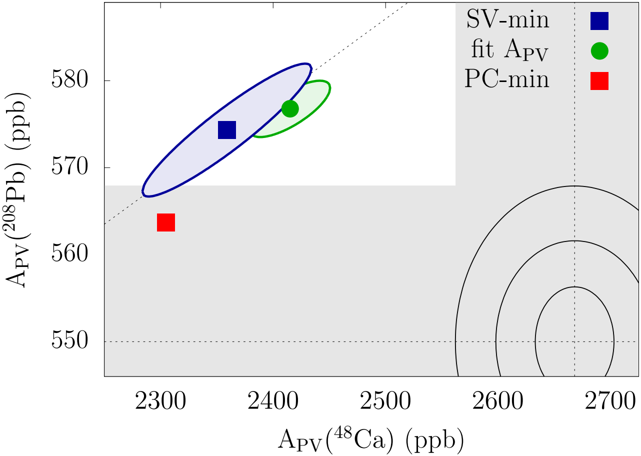


uncertainty ellipsoids follow the trends along variation of symmetry energy L

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

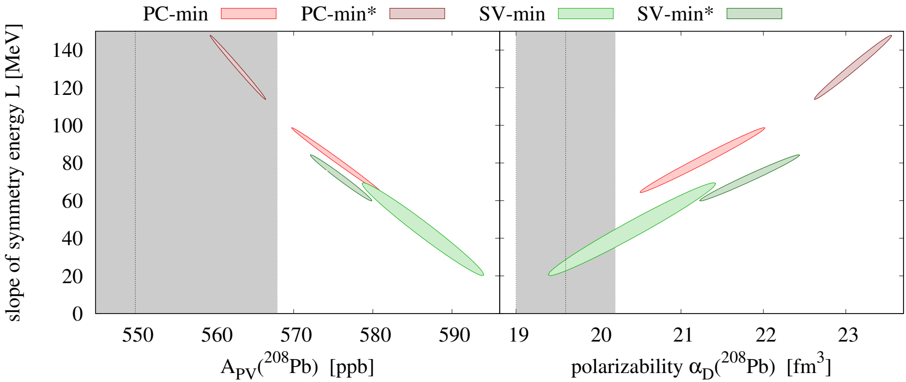
A_{PV} & α_D cannot be tuned simultaneously

Compatibility of A_{PV} measurements in ^{208}Pb and ^{48}Ca



again: error ellipsoids avoid the goal
attempt to fit additionally both A_{PV} does not work

“Predictions” for slope of symmetry energy *L*

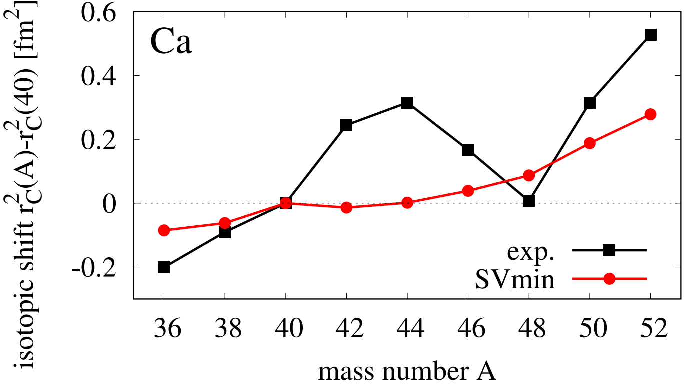


conflicting predictions:	A_{PV}	↔	$L \approx$ 120-... MeV
	α_D	↔	$L \approx$ 10-40 MeV
	mean-field	↔	$L \approx$ 20-90 MeV

4) Isotopic radius diferrences

Isotopic shifts in Ca isotopes

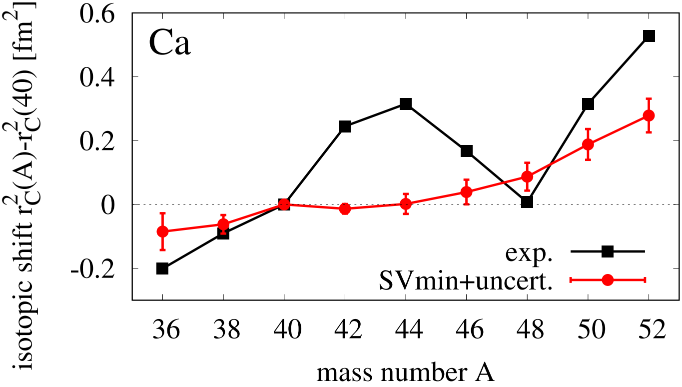
The problem: trend of r.m.s. radii (isotopic shifts) in Ca chain



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

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

The problem: trend of r.m.s. radii (isotopic shifts) in Ca chain



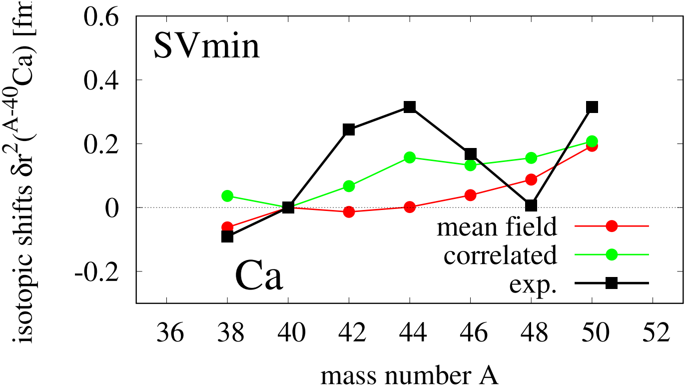
SVmin = fit of Skyrme functional with “traditional pairing” (contact force & density dep.)

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

deviation far outside uncertainty $\longleftrightarrow$ correlations or functional?

Impact of collective ground-state corrrelations

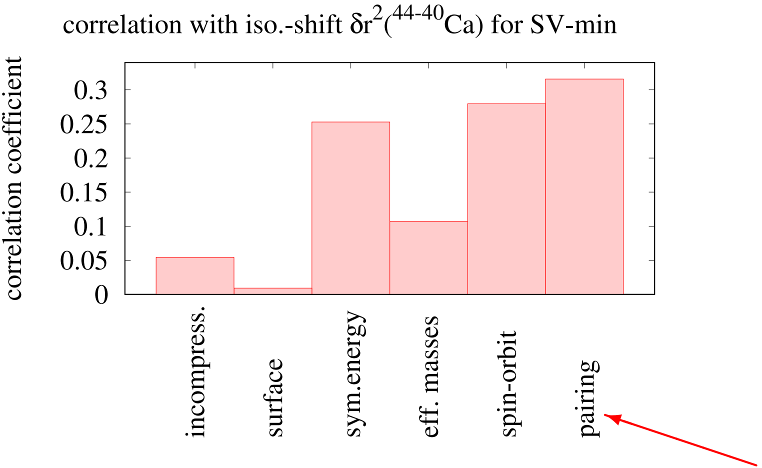
g.s. vibrations from low-lying 2^+ states contribute to radii



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

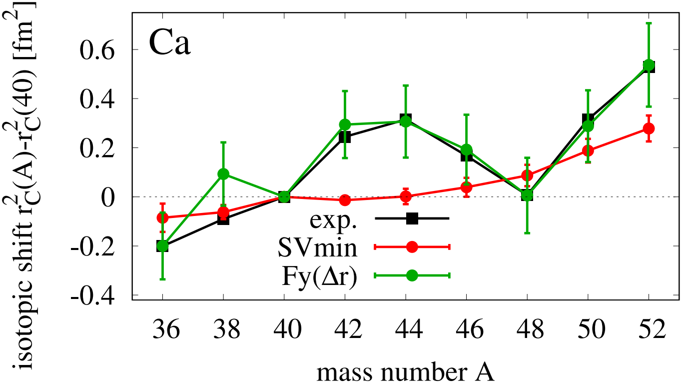


symmetry energy: fixed by polarizability

spin-orbit splittings: conceivable but limited changeability

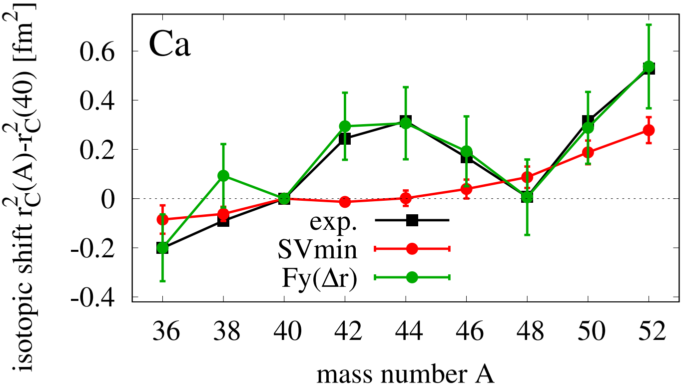
pairing: least well known, least well fixed ⇒ try Fayans pairing

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



Fayans pairing: $\mathcal{E}_{\text{pair}} = \xi^2 \left(V_{\text{pair}} + V'_{\text{pair}}\rho + V''_{\text{pair}}(\nabla\rho)^2 \right)$

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

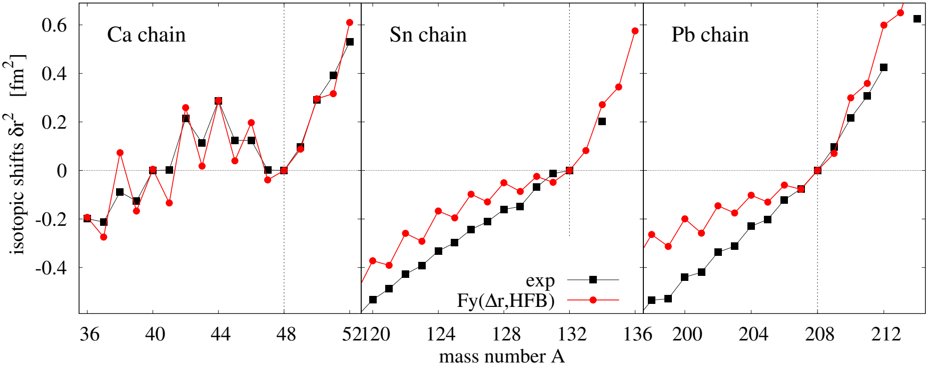


Fayans pairing: $\mathcal{E}_{\text{pair}} = \xi^2 \left(V_{\text{pair}} + V'_{\text{pair}}\rho + V''_{\text{pair}}(\nabla\rho)^2 \right)$

$\Longrightarrow$ Fy(Δr,HFB) reproduces trend for Ca isotopes almost perfectly
larger uncertainties $\leftrightarrow$ more flexible model

Isotopic shifts in Sn & Pb isotopes

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

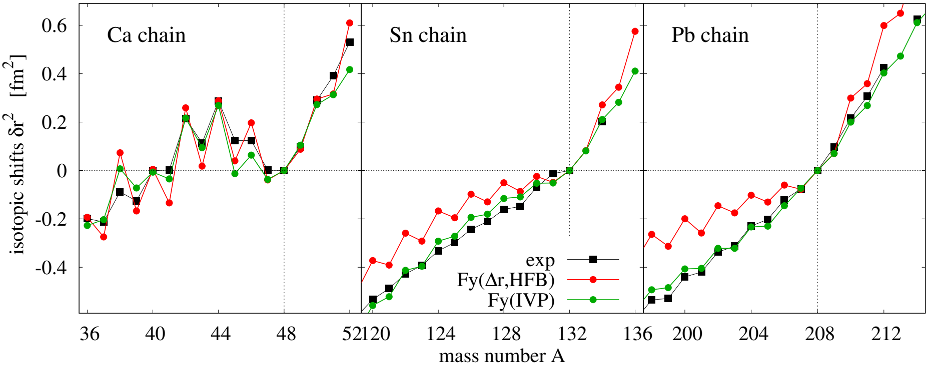


Fy(Δr,HFB) fails in: isotopic trends Sn & Pb, kinks at ^{132}Sn & ^{208}Pb, odd-even staggering

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

extend Fayans functional by isovector pairing (IVP)

add fit data on odd-even staggering and isotopic trends in Sn&Pb



$\Longrightarrow$ Fy(IVP): considerable improvement, fair isotopic differences over a wide range

Conclusions

Nuclear DFT uses empirical input ↔ statistical methods

⟶ simple methods (frequentists, Gaussian):
variances, co-variances, ... ⇒ model development, data selection

⟶ Bayesian calculus:
reliable extrapolation errors,...

Headaches

UQ:
non Gaussian regimes/observables – DFT emulators

DFT development:
systematic expansion $\mathcal{O}\{\nabla^2\}$,
what about density dependence? – no systematics, not enough data
decisive isovector observables?

extrapolation:
infer $\Delta_B E(\mathrm{exotic})$ from $\Delta_B E(\mathrm{known})$
infer $\Delta_B r(\mathrm{exotic})$ from $\Delta_B r(\mathrm{known})$
what about an observable A for which $A(\mathrm{known})$ does not exist? (e.g. r_{neut})

systematic errors:
which ground-state correlations are incorporated in DFT?
– e.g.: short-range = yes, long-range = no
effective operators? reliable mean-field operators?
formal structure of the functional (see above “density dependence”)