MINISTERIO DE CIENCIA, INNOVACIÓN Y UNIVERSIDADES

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AGENCIA ESTATAL DE INVESTIGACIÓN

INFN

MOdeling Nuclear STructure and REactions

Bayesian inference on nuclear ground state and giant resonance data

Xavier Roca-Maza

TRIP use case Transmutation of elements 2025

RIKEN, March 10th - 12th

UNIVERSITAT DE BARCELONA

UNIVERSITAS STUDIORUM MEDIOLANENSIS

Motivation:
General aspects

Energy Density Functional (EDF) Theory $\Rightarrow$ suitable theoretical framework for the study of ground and some properties of collective excitations (E_x, sum rules)

New EDFs with **better capabilities**, **accuracy**, and **predictive power** have been reported [Energy Density Functional Methods for Atomic Nuclei, edited by N. Schunck (IOP, Bristol, 2019), pp. 2053–2563]

Exist **indications** that **current EDFs** have **reached their limits**.

[M. Kortelainen et al. PRC 89, 054314 (2014) for Skyrme EDF]

Extending Skyrme EDF (up to fourth-order derivative terms) did **not** lead to very **significant improvements** [P. Becker et al. PRC 96, 044330 (2017)]

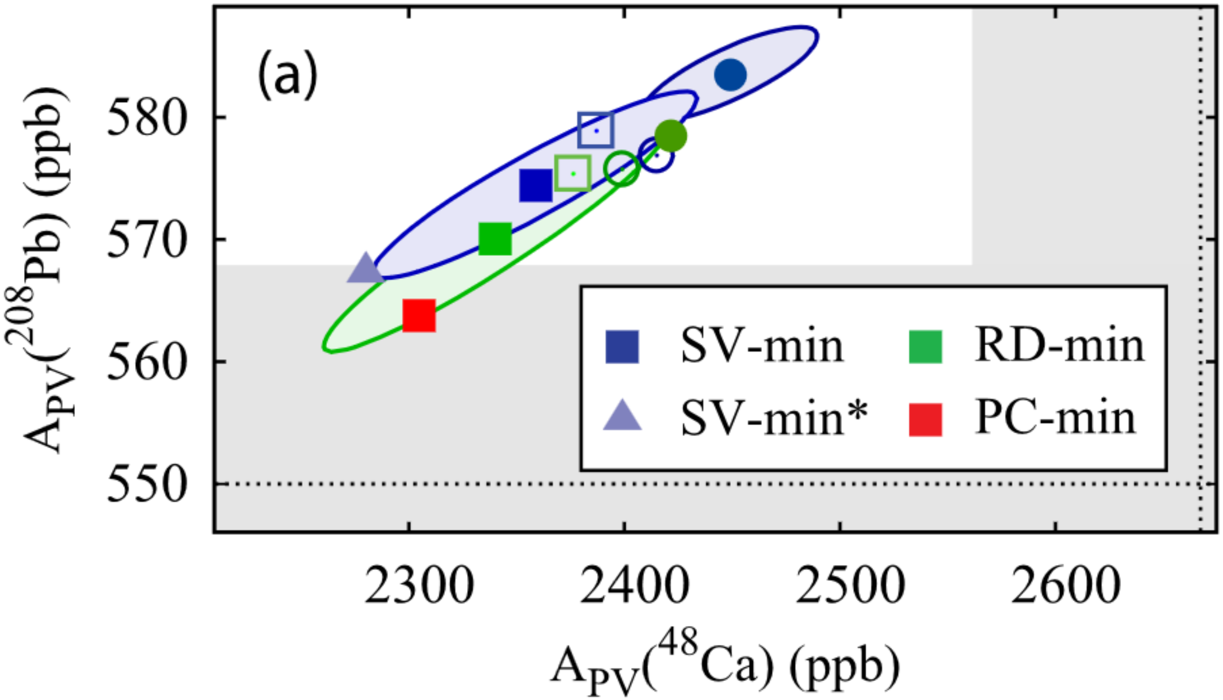
A symptom of the obstacles in further improving functionals can be found in the **difficulty** of **reproducing new, different observables**.

Motivation:

Recent example: parity violating elastic e$^-$ scattering by nuclei

See, e.g., **theoretical studies:** P.-G. Reinhard et al. PRL127, 232501 (2021); R. Essick et al. PRL127, 192701 (2021); P.-G. Reinhard et al. PRL129, 232501 (2022); E. Yüksel et al., PLB 836, 137622 (2023)]

Experimental studies: D. Adhikari (CREX Collaboration) et al., PRL129, 042501 (2022); D. Adhikari (PREX Collaboration) et al., PRL126, 172502 (2021)].



Other examples of current problems can be found in the literature (see, e.g., [L. Neufcourt et al. PRC 101, 044307 (2020); R. Navarro Pérez et al. and N. Schunck, PLB 833, 137336 (2022)]).

What it is actually measured?

Parity Violating Asymmetry

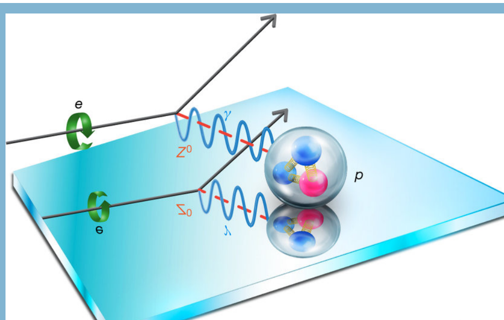
Elastic electron scattering by nuclei:

→ **Parity conserving**

Exchange of γ that essentially couples to protons $\mathbf{Q_p^{\,c}=1;\ Q_n^{\,c}=0}$

→ **Parity violating**

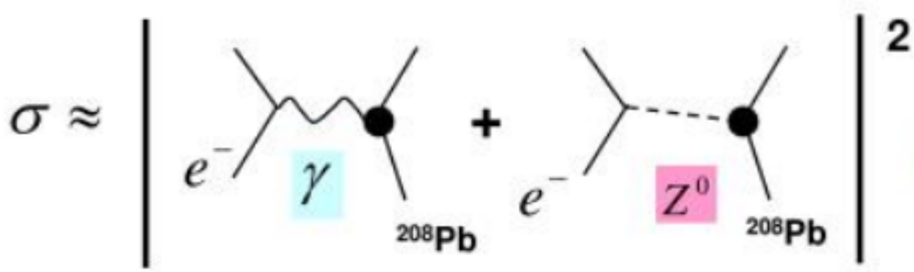
Exchange Z_0 that essentially couples to neutrons $\mathbf{Q_p^{\,W}=0.07;\ Q_n^{\,W}=-0.99}$



Nature **557**, 207–211 (2018)

Ultra-relativistic electrons ($m_e \to 0$) with spin **aligned** (+) or **anti-aligned** (-) to the beam line, in approaching the nucleus:

$$\left[\vec{\alpha}\cdot\vec{p} + V_{\mathrm{Coulomb}}(\vec{r}) \pm V_{\mathrm{Weak}}(\vec{r})\right]\Psi_\pm = E\Psi_\pm$$



One can get **advantage** form this **interference pattern** between **electromag.** and **weak** interact.

$$A_{PV} = \frac{\frac{d\sigma_+}{d\Omega} - \frac{d\sigma_-}{d\Omega}}{\frac{d\sigma_+}{d\Omega} + \frac{d\sigma_-}{d\Omega}} \approx \frac{\mathrm{Weak}}{\mathrm{Coulomb}}$$

Parity Violating Asimmetry:
simple model & correlations (neutron skin thickness $\Delta r_{\rm np}$ or L)

The **parity violating asymmetry** within the **PWBA:**

$$A_{PV}^{\rm PWBA} = \frac{G_F Q^2}{4\sqrt{2}\pi\alpha}\left[\underbrace{4\sin^2\theta_W}_{\approx 1} + \frac{F_n(Q)-F_p(Q)}{F_p(Q)}\right]$$

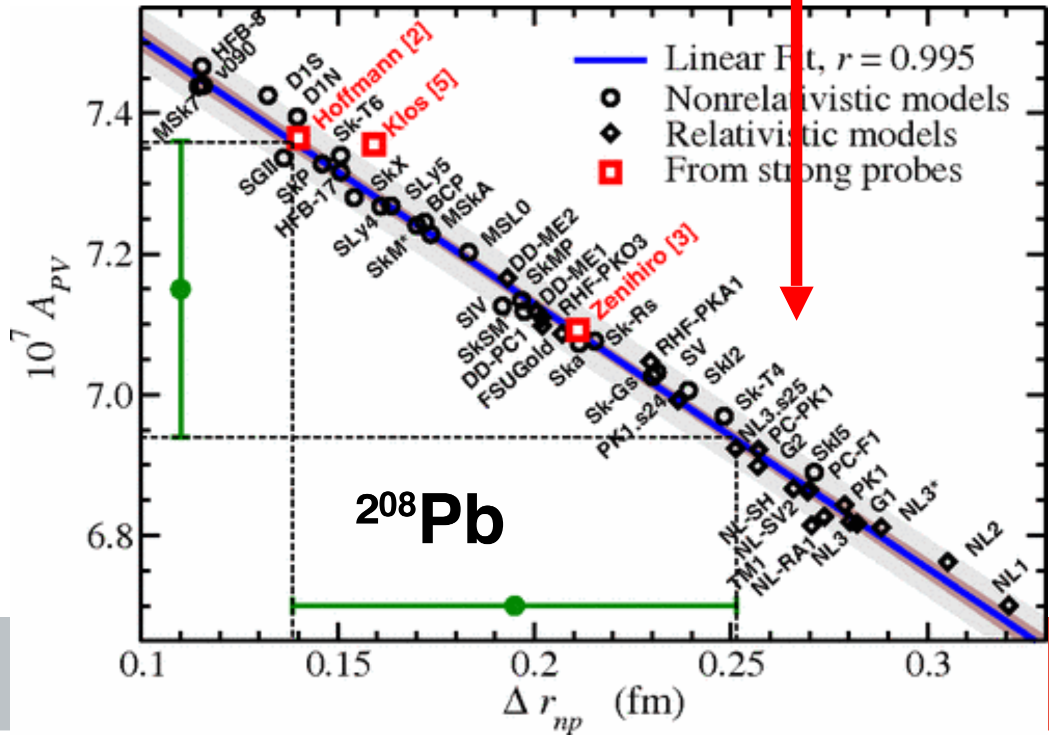
$$\xrightarrow{Q\to 0} \frac{G_F Q^2}{4\sqrt{2}\pi\alpha}\left[1 - \frac{Q^2\langle r_p^2\rangle}{3}\frac{\Delta r_{np}}{\langle r_p^2\rangle^{1/2}}\right]$$

30% due to Coulomb distortions (PREX) does not blur **the main physics**

The **parity violating asymmetry** within the **DWBA:**

○ ◇ → Energy Density Functionals

□ → Expeirmental ρ_n form hadronic probes + ρ_p from e$^-$ scattering



Neutron Skin of ^{208}Pb, Nuclear Symmetry Energy, and the Parity Radius Experiment
X. Roca-Maza, M. Centelles, X. Viñas, and M. Warda
Phys. Rev. Lett. **106**, 252501 – Published 21 June 2011

Recent experiments on $(\vec{p}, \vec{p}')$ scattering (RCNP)

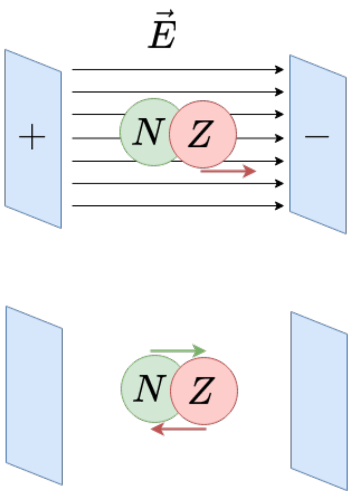
Electric Dipole Polarizability

The **electric dipole polarizability** measures the **tendency** of the nuclear **charge distribution** to be **distorted**

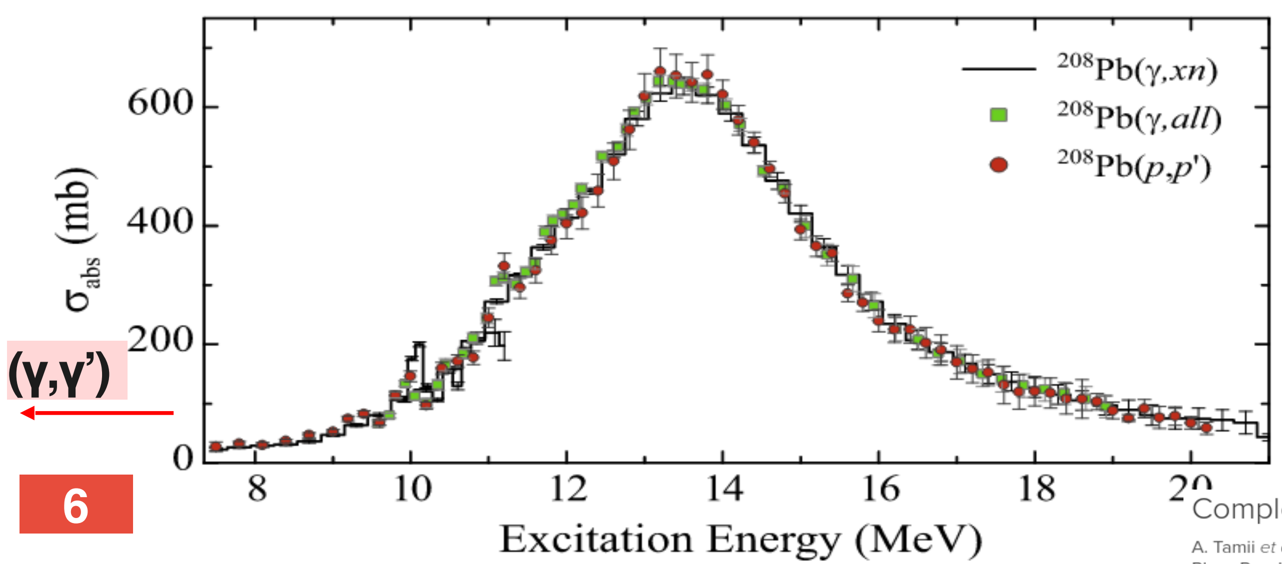
$$\alpha = \frac{\text{electric dipole moment}}{\text{external electric field applied}}$$

Microscopically, it relates with the **photo-absorption cross-section**

$$\alpha_D = \frac{\hbar c}{2\pi^2 e^2} \int \frac{\sigma_{\text{abs}}}{\omega^2} d\omega,$$



Measured using polarized proton scattering at very forward angles (dominated by E1 and M1 well separated)



$$\boxed{\alpha_D(^{208}\text{Pb}) = 19.6 \pm 0.6\ \text{fm}^3}$$

Complete Electric Dipole Response and the Neutron Skin in ^{208}Pb
A. Tamii *et al.*
Phys. Rev. Lett. **107**, 062502 – Published 3 August 2011

Electric Dipole Polarizability:
simple model & correlations (symmetry energy J and Δr_{np})

Applying the **dielectric theorem** to the **Droplet Model** Hamiltonian (first Migdal and latter on Meyer et al. NPA385, 269) one can find

$$\alpha_D \approx \frac{A\langle r^2\rangle}{12J}\left[1+\frac{5}{2}\frac{\Delta r_{np}+\sqrt{\frac{3}{5}\frac{e^2 Z}{70J}}-\Delta r_{np}^{\mathrm{surface}}}{\langle r^2\rangle^{1/2}(I-I_C)}\right]$$

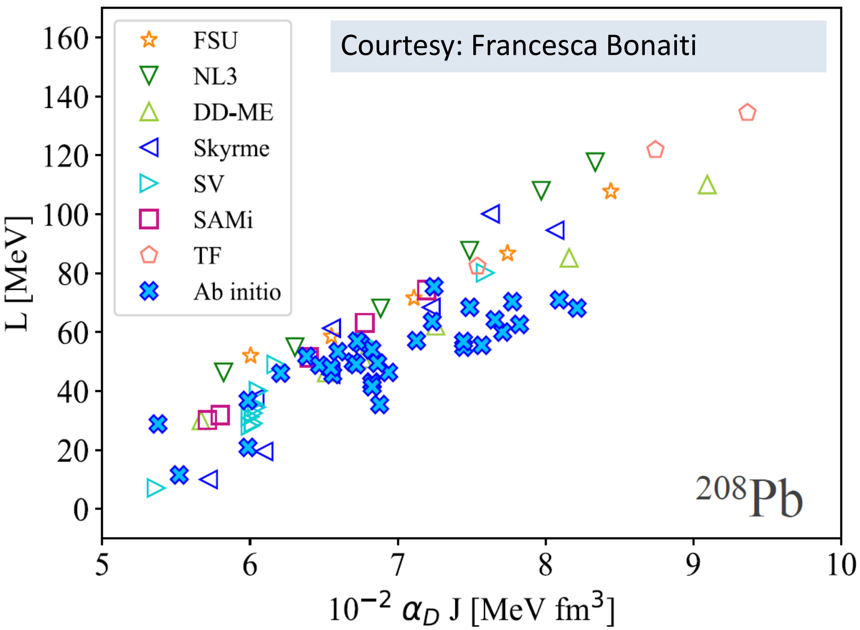
J = e(PNM)−e(SNM) → Symmetry energy at ρ_0

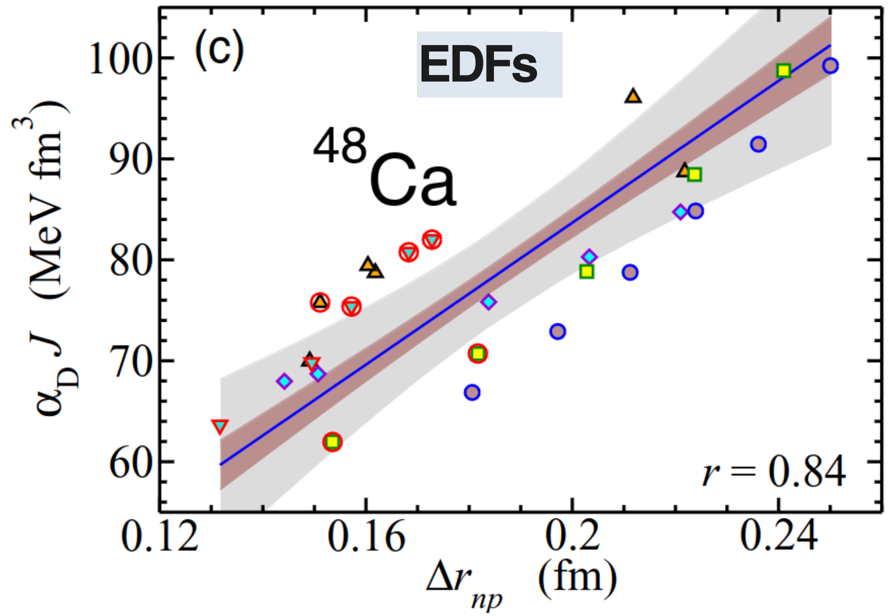
$\Delta r_{np} \equiv \langle r_n^2\rangle^{1/2} - \langle r_p^2\rangle^{1/2}$ → Neutron skin thickness

Using microscopic calculations (Energy Density Functionals & Ab initio)

DFT data from: Roca-Maza, Phys. Rev. C **88**, 024316 (2013)

Ab initio data from: Hu, Nat. Phys. **18**, 1196-1200 (2022)

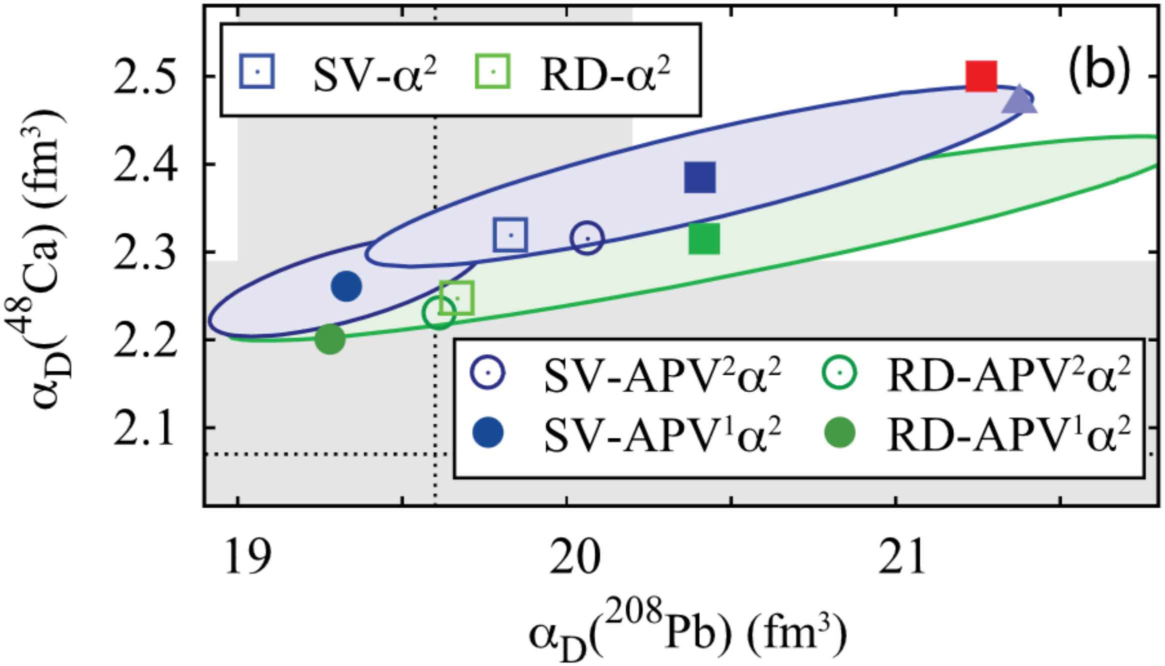




Phys. Rev. C **92**, 064304 – Published 8 December 2015

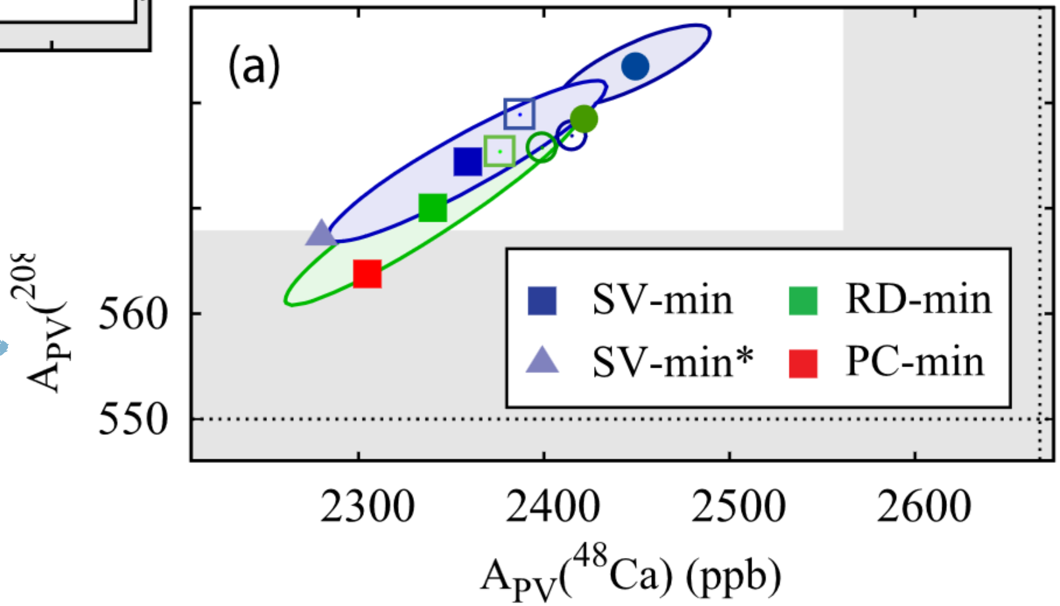
Summary:

A_{PV} (sensitive to Δr_{np}) and α_D (sensitive to J and Δr_{np}) in ^{48}Ca and ^{208}Pb



Simultaneous description of **dipole polarizabilities** → point to a **good understanding** of **symmetry energy (J)** and **neutron skins (Δr_{np})**

No simultaneous description of **parity violating asymmetries** (ground state observable) → point to a **deficient understanding** of **neutron skins**



Combined Theoretical Analysis of the Parity-Violating Asymmetry for ^{48}Ca and ^{208}Pb

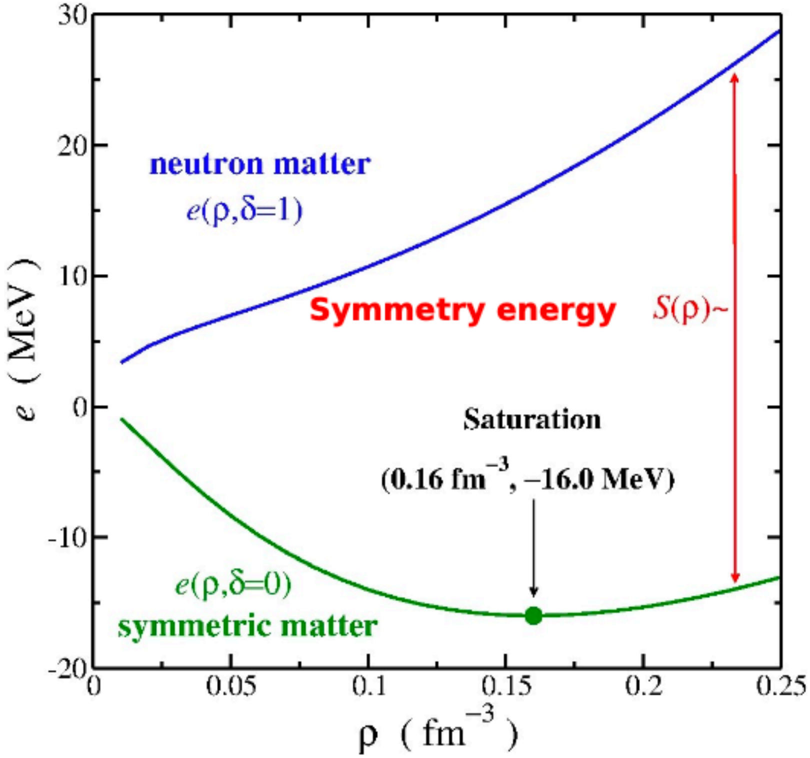
Paul-Gerhard Reinhard, Xavier Roca-Maza, and Witold Nazarewicz

Phys. Rev. Lett. **129**, 232501 – Published 2 December 2022

Nuclear Equation of State
Definition of some useful parameters

Unpolarized **nuclear matter** at zero temperature (10^{10}K→1MeV) is defined as the **energy** per **nucleon** (e) as a function of the **neutron** (ρ_n) and **proton** (ρ_p) **densities** as (*isospin conserving* $V_{nn} = V_{pp} = V_{np}$):

$$\boxed{e(\rho,\delta) = e(\rho,0) + S(\rho)\delta^2} + \mathcal{O}[\delta^4] \quad \text{where } \rho = \rho_n + \rho_p \text{ and } \delta = \frac{\rho_n - \rho_p}{\rho}$$



It is customary to **expand $e(\rho,\delta)$** around nuclear **saturation density** $\rho_0 \sim 0.16$ fm^{-3}

$$e(\rho,0) = e(\rho_0,0) + \frac{1}{2}K_0 x^2 + \mathcal{O}[\rho^3] \text{ where } x = \frac{\rho-\rho_0}{3\rho_0}$$

$$S(\rho) = J + Lx + \frac{1}{2}K_{sym}x^2 + \mathcal{O}[\rho^3,\delta^4]$$

K_0 → how **compressible** is symmetric matter at ρ_0

J → **penalty energy** for converting all **protons into neutrons** in symmetric matter at ρ_0

L → **neutron pressure** in neutron matter at ρ_0

Bayesian inference:

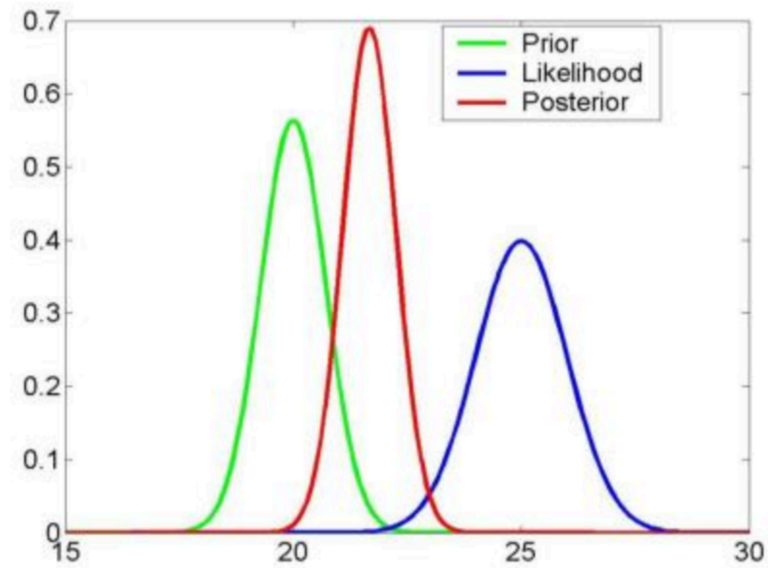
Statistical tool to test model on the basis of observation

new data: $\boxed{p(y\,|\,\theta)}$

prior knowledge: $\boxed{p(\theta)}$

$$\boxed{p(\theta\,|\,y) \propto p(y\,|\,\theta)\,p(\theta)}$$

posterior $\propto$ likelihood · prior



We can include **prior knowledge** into computing statistical **probabilities** of an **observable** given a **set of data** (in the present case assuming a Skyrme EDF)

In **previous works**, either using χ^2-test or Bayesian inference to find the **optimal** parameters θ of the model, **never** used **only observable** quantities and **both ground** and **excited** state **properties** of nuclei

Prior knowledge input in parameters of the model

Pietro Klausner, et al. PRC 111 014311 (2025)

Skyrme EDF parameters

$(t_0, t_1, t_2, t_3, x_0, x_1, x_2, x_3, \alpha, W_0)$

↕

7 **bulk** parameters from EoS $(E_0, K_0, \rho_0, J, L, m_0^*, m_1^*)$

Plus 2 **surface** (G_0, G_1) and 1 **spin-orbit** (W_0) parameter

Possibility to input physically motivated priors

Prior (uniform) distribution

Par.	Units	Lower limit	Upper limit
ρ_0	[fm^{-3}]	0.150	0.175
E_0	[MeV]	-16.50	-15.50
K_0	[MeV]	180.00	260.00
J	[MeV]	24.00	40.00
L	[MeV]	-20.00	120.00
G_0	[MeV fm^5]	90.00	170.00
G_1	[MeV fm^5]	-90.00	70.00
W_0	[MeV fm^5]	60.00	190.00
m_0^*/m		0.70	1.10
m_1^*/m		0.60	0.90

Observables employed (define Likelihood)

Pietro Klausner, et al. PRC 111 014311 (2025)

Skyrme calculations with HFBCS-QRPA code [1]:

- Ground state Skyrme **Hartree-Fock** (HF) calculation
- Excited state **self-consistent RPA** with the HF ground state

* An estimate of the **Skyrme model** (<u>based on experience</u>) **theoretical error** must be taken into account for the inference:

- B.E. accurate within about 2 MeV
- R_{ch} about 0.05 fm
- E_x in Giant Resonances about 0.5 MeV

Ground-state properties

	$B.E.$ [MeV]	R_{ch} [fm]	ΔE_{SO} [MeV]
^{208}Pb	1636.4 ± 2.0*	5.50 ± 0.05*	2.02 ± 0.50*
^{48}Ca	416.0 ± 2.0*	3.48 ± 0.05*	1.72 ± 0.50*
^{40}Ca	342.1 ± 2.0*	3.48 ± 0.05*	-
^{56}Ni	484.0 ± 2.0*	-	-
^{68}Ni	590.4 ± 2.0*	-	-
^{100}Sn	825.2 ± 2.0*	-	-
^{132}Sn	1102.8 ± 2.0*	4.71 ± 0.05*	-
^{90}Zr	783.9 ± 2.0*	4.27 ± 0.05*	-

Isoscalar resonances

	E^{IS}_{GMR} [MeV]	E^{IS}_{GQR} [MeV]
^{208}Pb	13.5 ± 0.5*	10.9 ± 0.5*
^{90}Zr	17.7 ± 0.5*	-

Isovector properties

	α_D [fm^3]	$m(1)$ [MeV fm^2]	A_{PV} (ppb)
^{208}Pb	19.60 ± 0.60	961 ± 22	550 ± 18
^{48}Ca	2.07 ± 0.22	-	2668 ± 113

[1]Code available G. Colò, X. Roca-Maza, arXiv:2102.06562v1

Skyrme model emulator

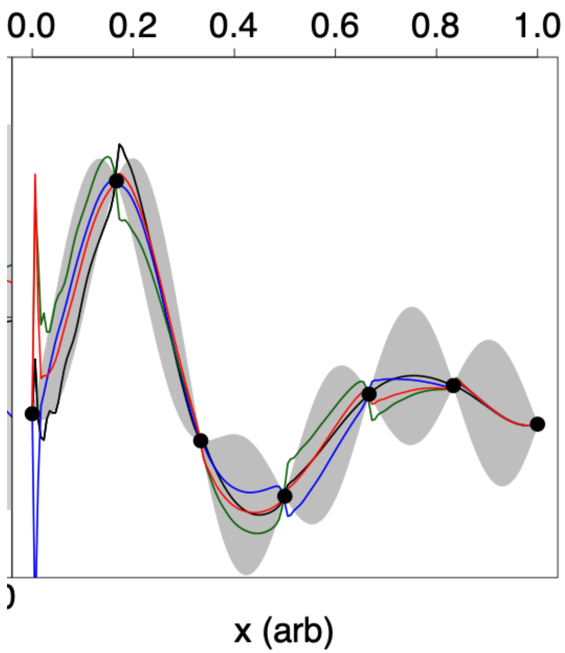
The **calculation** of all the **observables** take ~**hour**

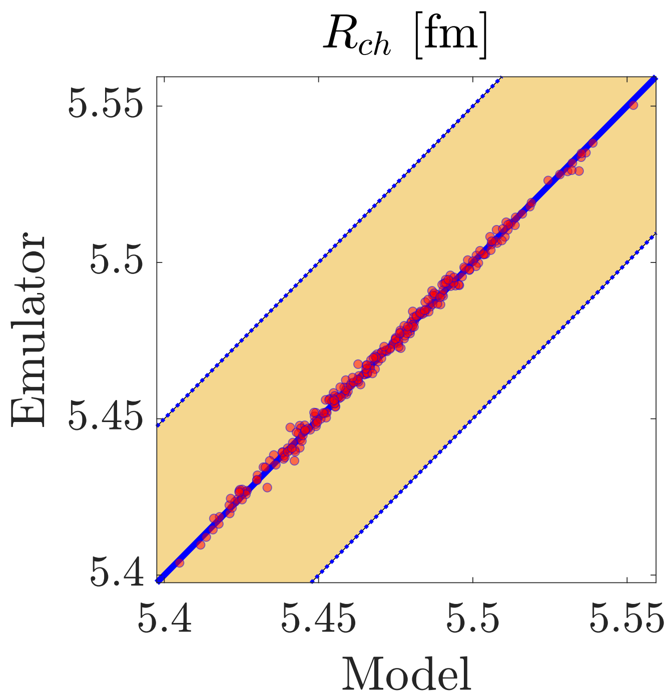
Inference need 10^{6-7} **model evaluations**

[to reasonably cover the full model space (Metropolis Hastings Sampling)]

To save time: use of gaussian process **emulator** needed [1] to estimate **Skyrme** calculations

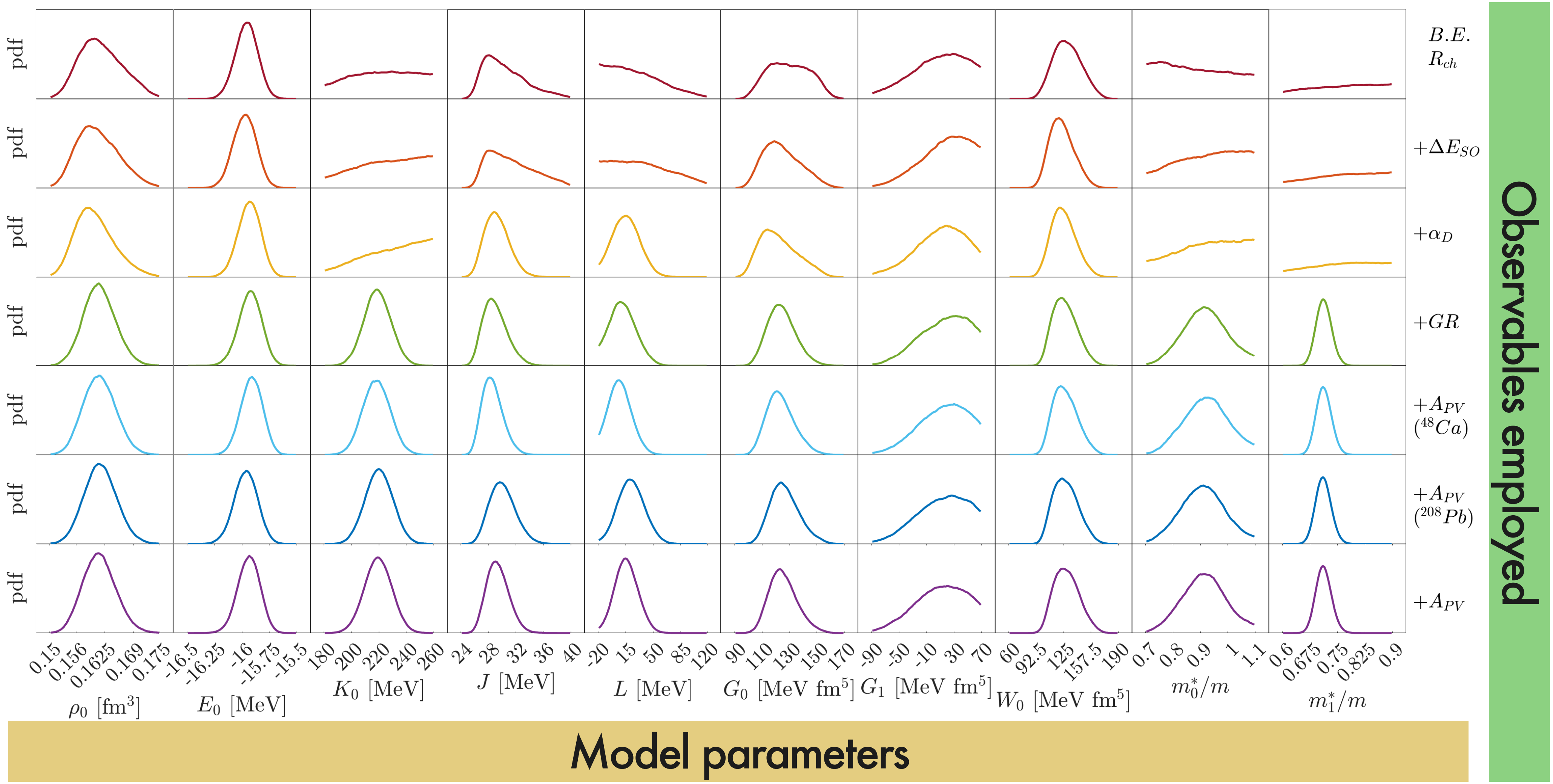
(multidimensional interpolation on the basis of a training grid of actual model calculations)





[1] MADAI software https://madai.phy.duke.edu/

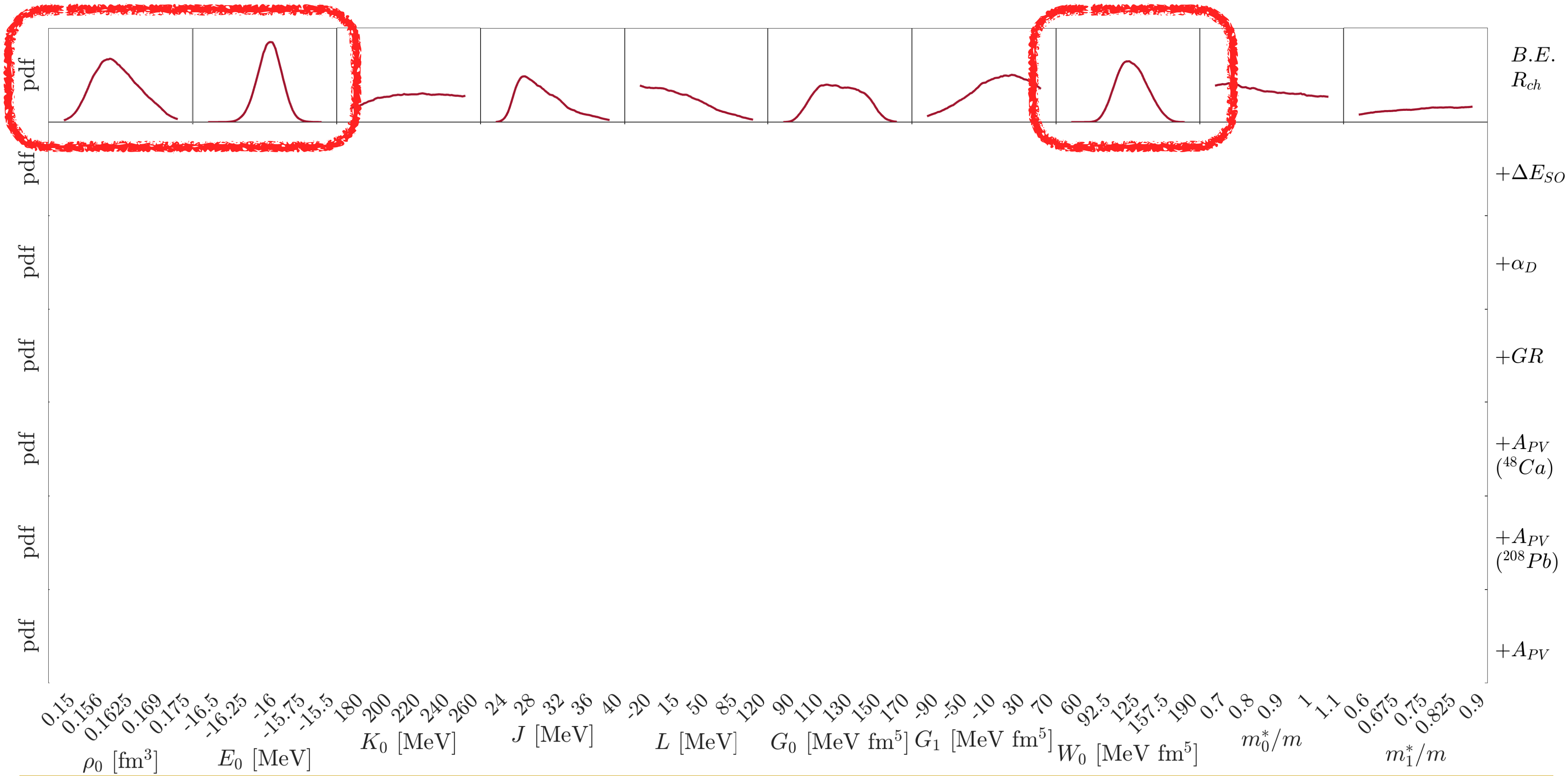
Progressive posterior distributions:
Each type of observable included sequentially



Pietro Klausner, et al. PRC 111 014311 (2025)

Only binding energies included:

ρ_0, E_0 and W_0 posteriors rather well determined, some bias for J



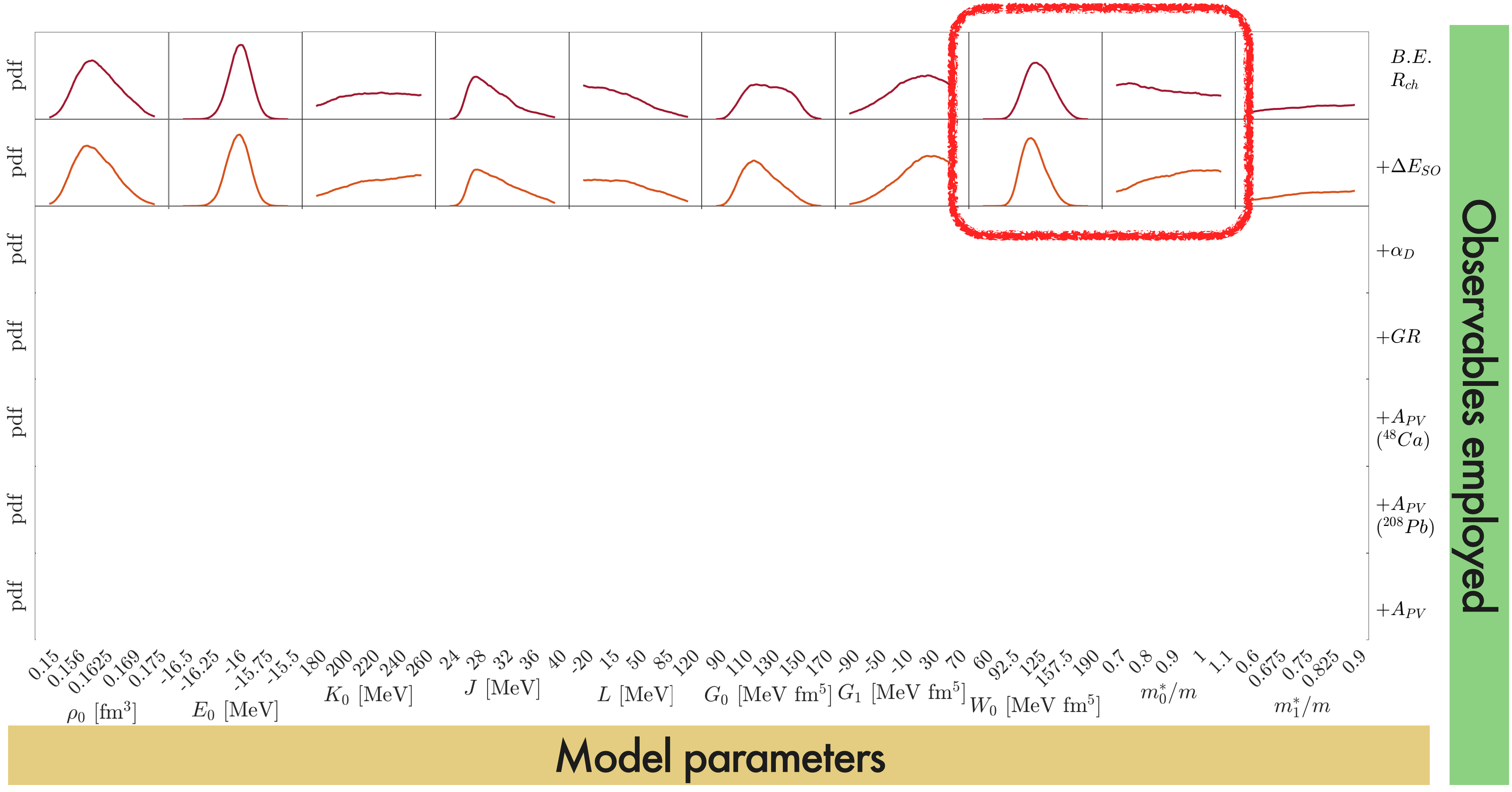
Model parameters

Observables employed

Pietro Klausner, et al. PRC 111 014311 (2025)

+ spin-orbit

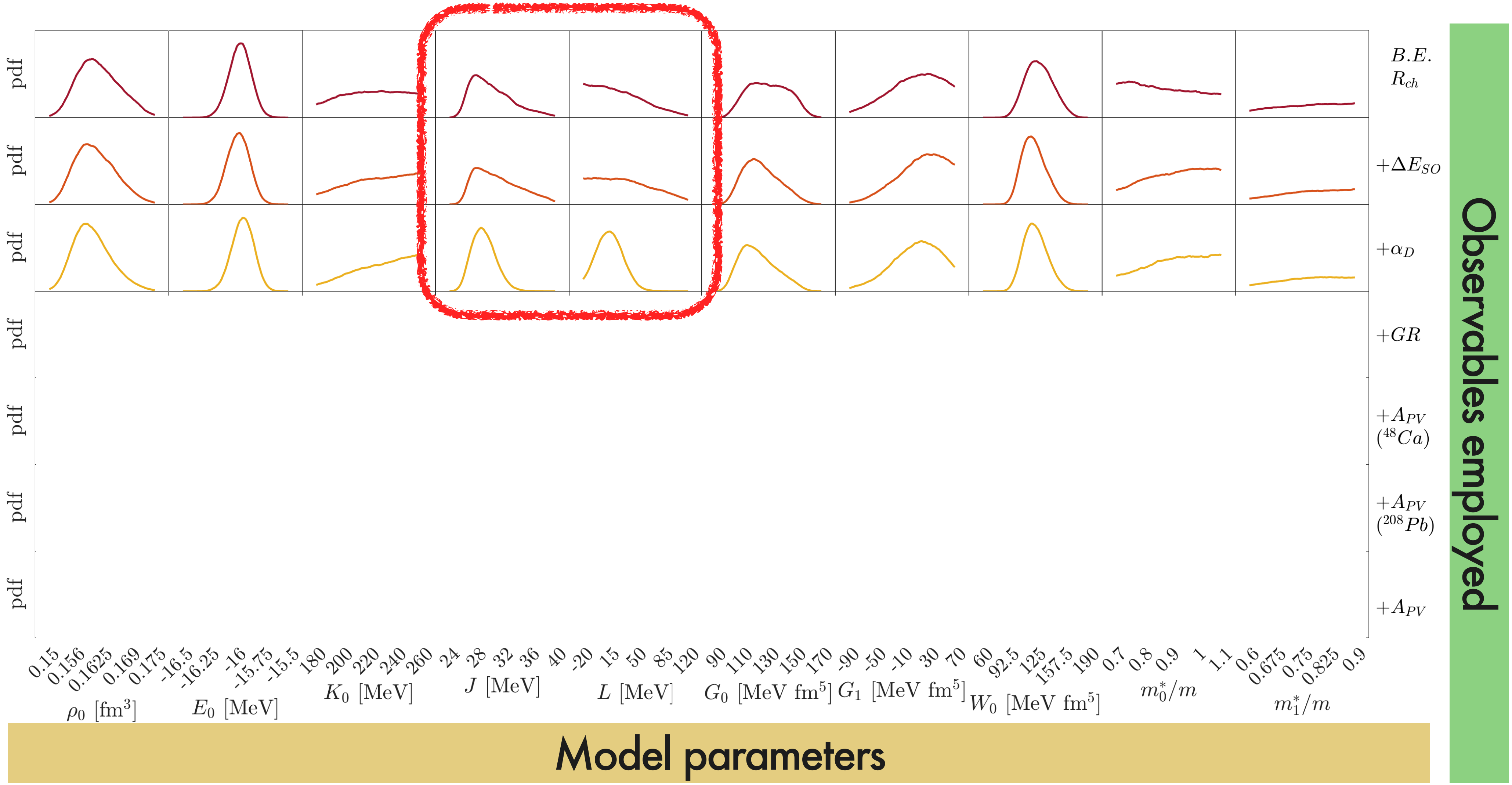
narrower posterior for W_0



Pietro Klausner, et al. PRC 111 014311 (2025)

+ α_D in ^{48}Ca and ^{208}Pb

Symmetry energy parameters J and L well constrained



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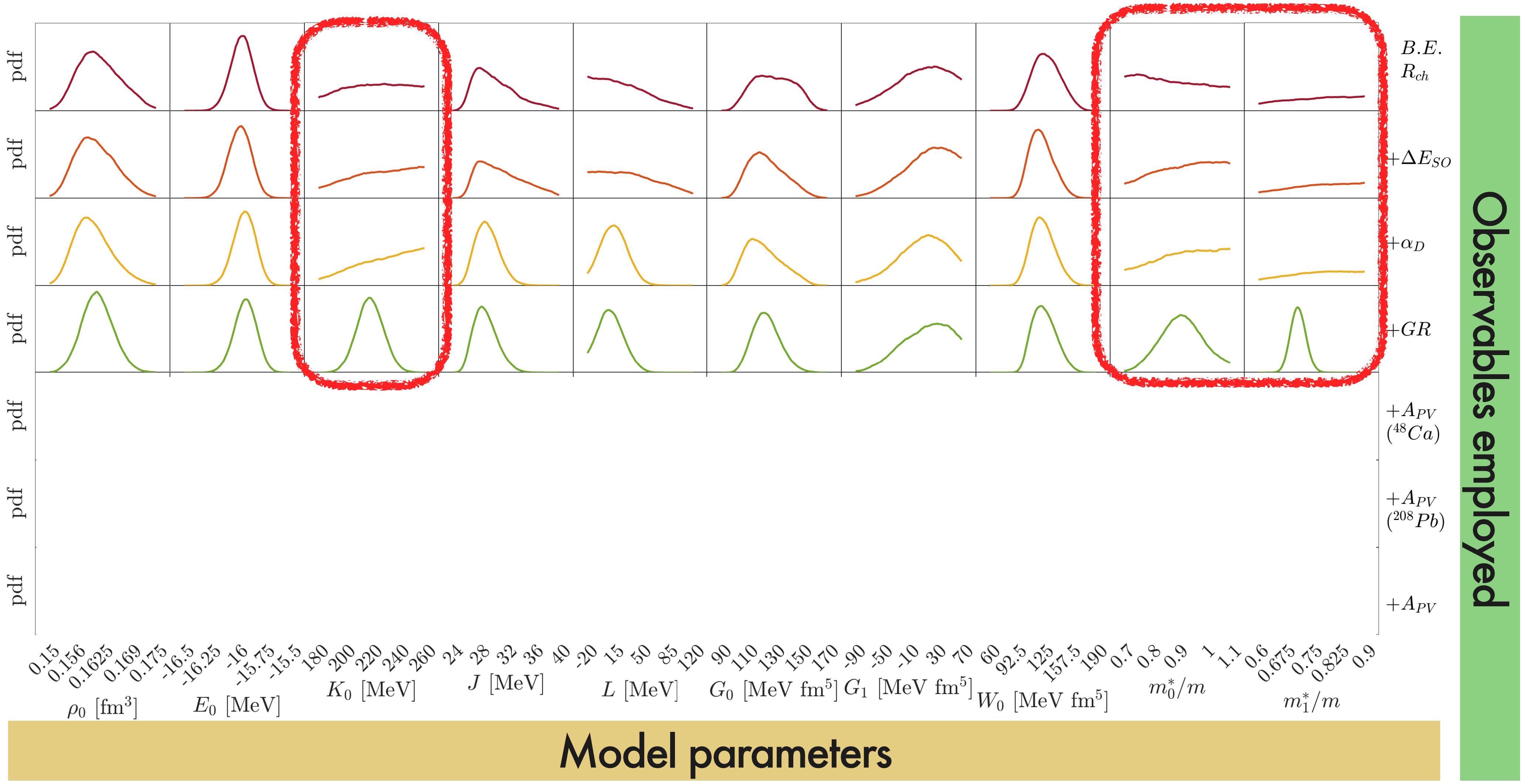
+ E_x of IS Giant Monopole and Quadrupole Resonances
+ energy weighted sum rule of IV Giant Dipole Resonance

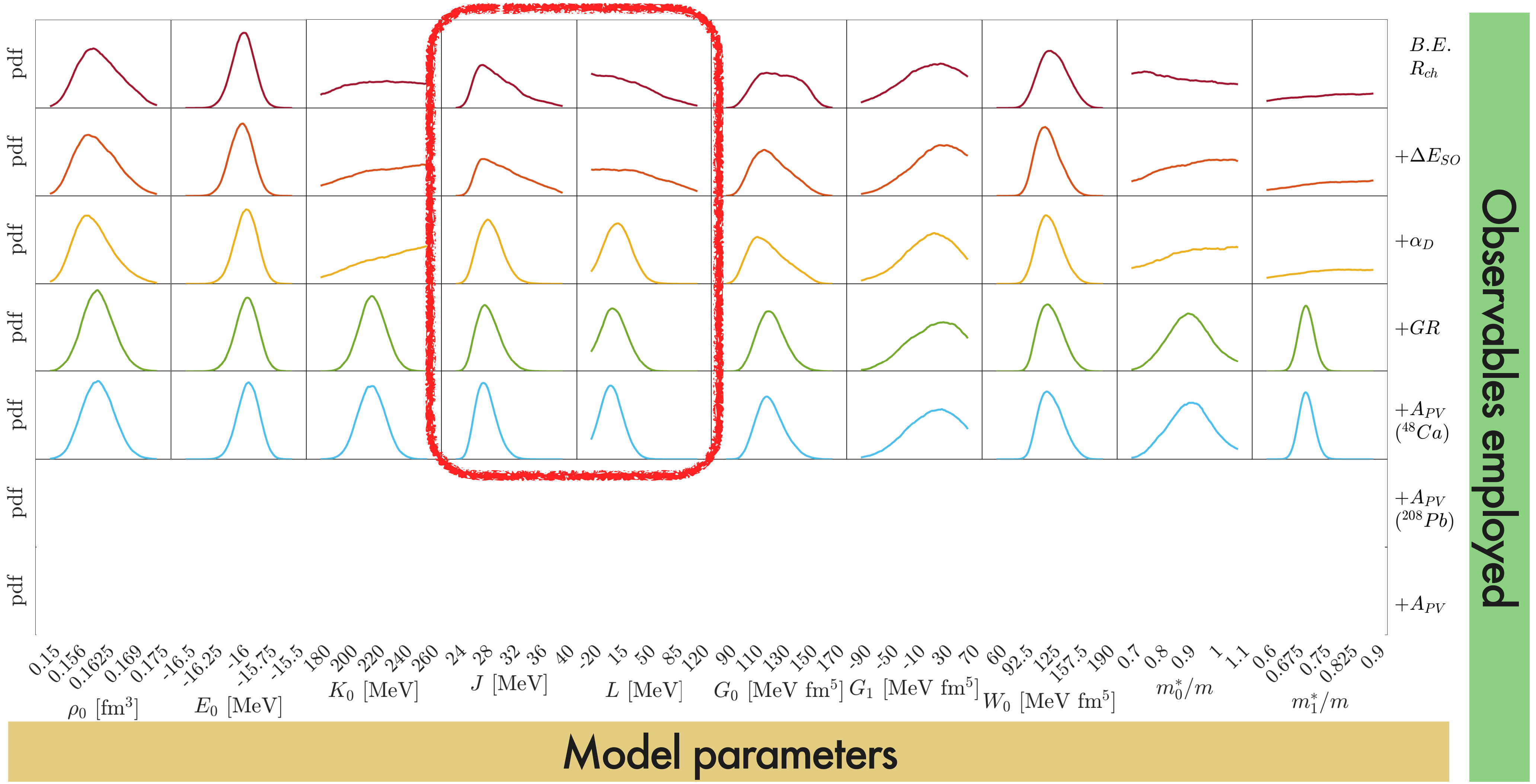
Incompressibility K_0 and effective masses (IV and IS) well determined



Pietro Klausner, et al. PRC 111 014311 (2025)

+ $A_{\rm PV}$ in ^{48}Ca

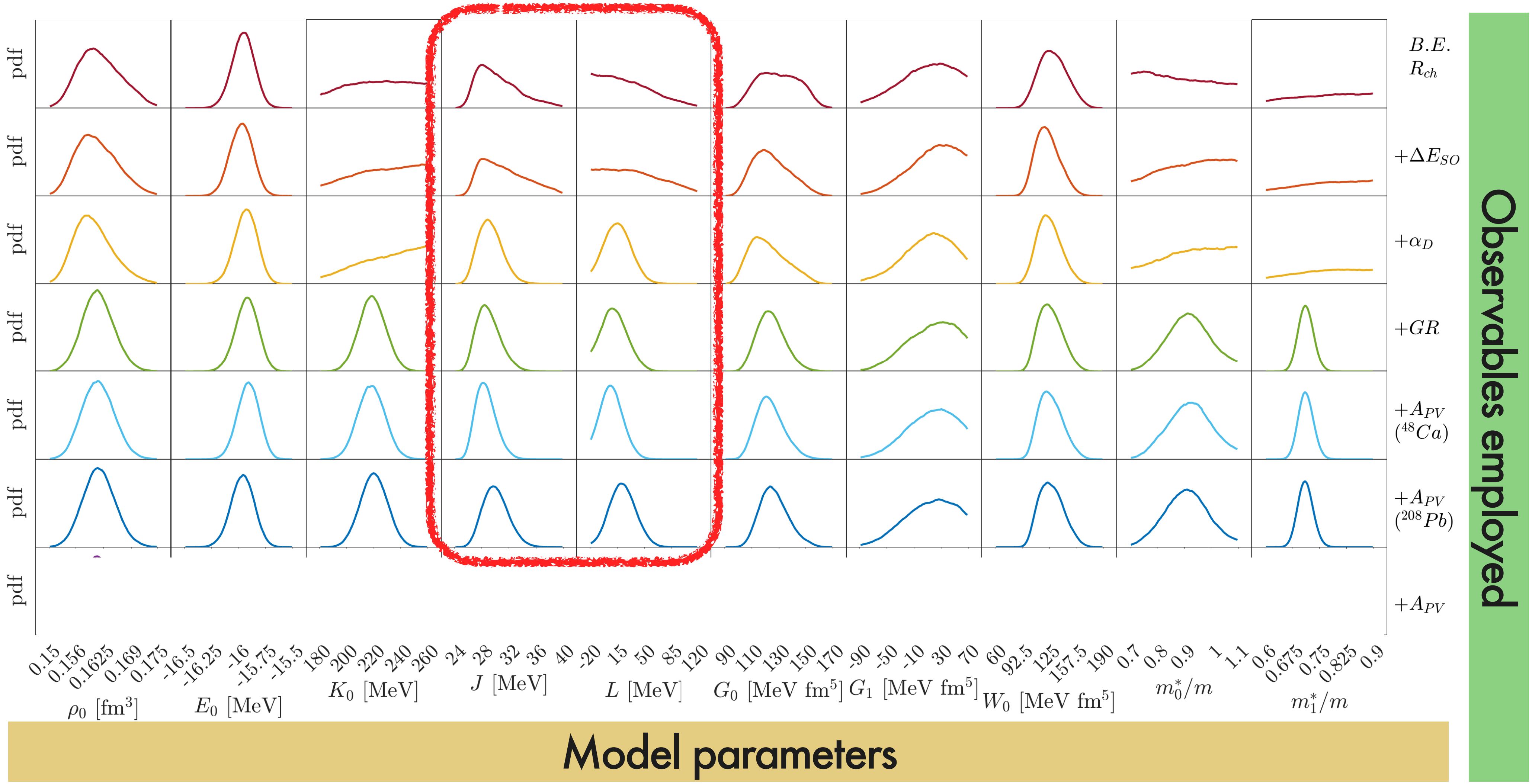
slight narrowing and decrease in the average values of J and L



Pietro Klausner, et al. PRC 111 014311 (2025)

+ $A_{\rm PV}$ in ^{208}Pb (NO $A_{\rm PV}$ in ^{48}Ca included)

slight widening and increase in the average values of J and L



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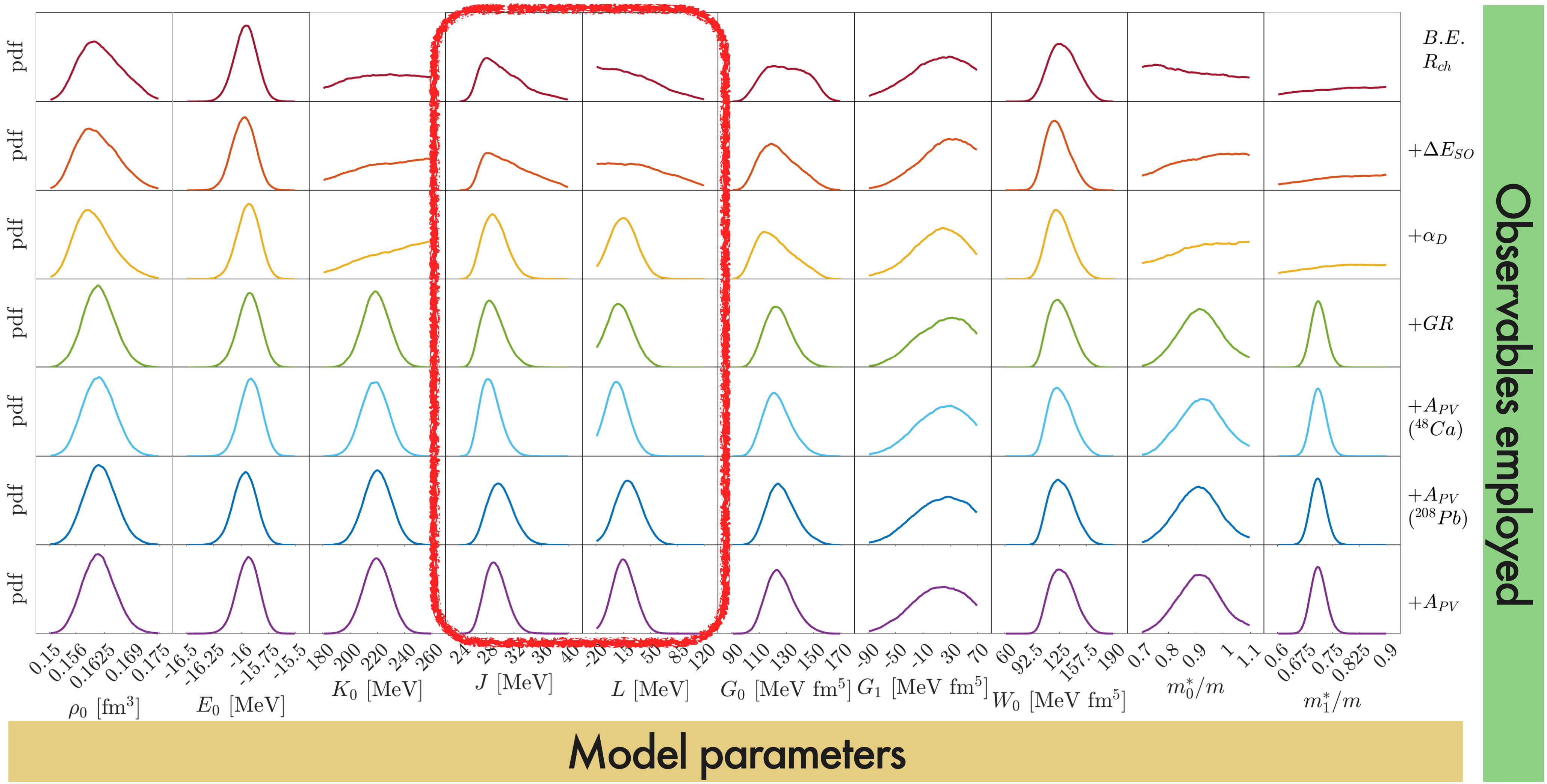
A_{PV} in ^{48}Ca and ^{208}Pb included

^{48}Ca dominates the posterior on J and L with respect to ^{208}Pb



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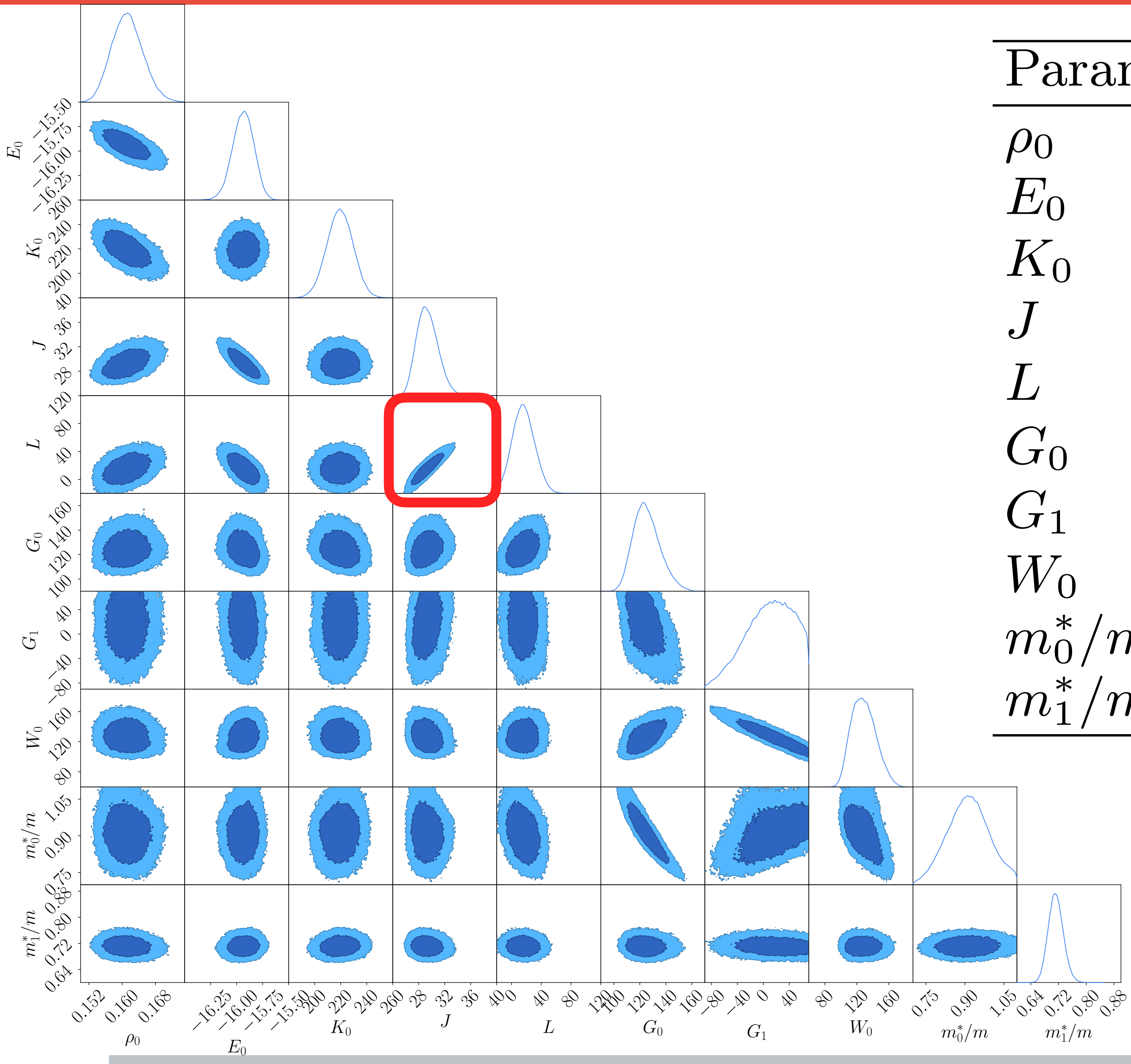
Corner plot and mean parameter values

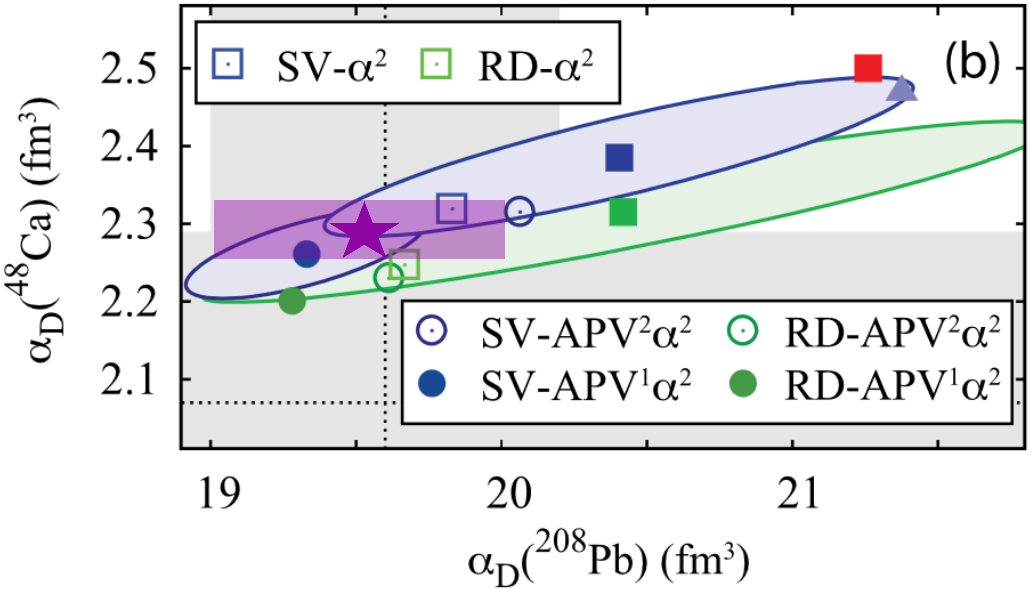
Pietro Klausner, et al. PRC 111 014311 (2025)



Parameter		μ	σ
ρ_0	[fm^3]	0.161	0.004
E_0	[MeV]	-15.938	0.102
K_0	[MeV]	219.483	10.007
J	[MeV]	29.378	1.626
L	[MeV]	16.136	14.732
G_0	[MeV fm^5]	125.470	10.210
G_1	[MeV fm^5]	9.439	35.735
W_0	[MeV fm^5]	128.719	14.848
m_0^*/m		0.913	0.079
m_1^*/m		0.712	0.021

Can we accommodate α_D and A_{PV} without compromising other observables?

Pietro Klausner, et al. PRC 111 014311 (2025)



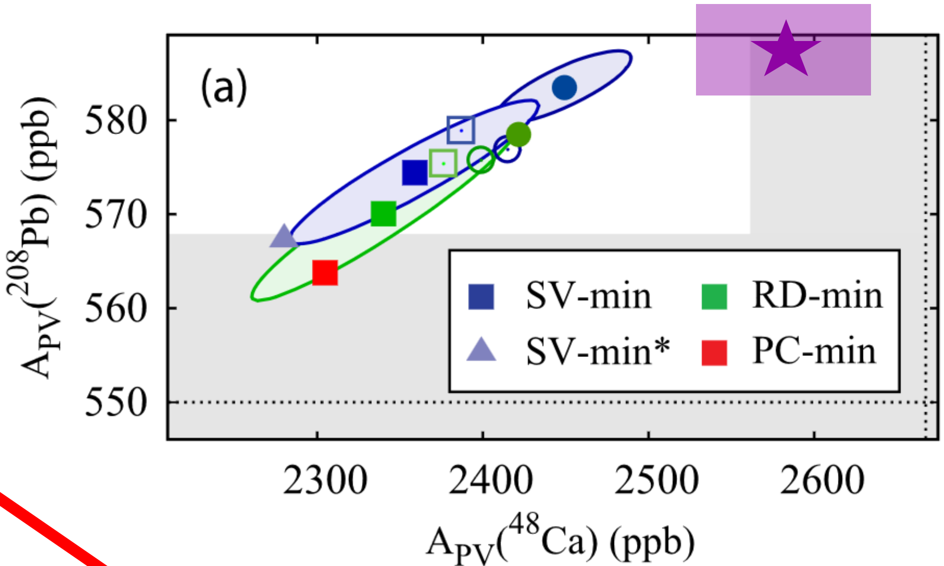
New results ★

	α_D (fm^3)	$m(1)$ (MeV fm^2)	A_{PV} (ppb)
^{208}Pb	19.5 ± 0.5	958 ± 22	589 ± 5
^{48}Ca	2.30 ± 0.08	–	2591 ± 54

	B.E. (MeV)	R_{ch} (fm)	ΔE_{SO} (MeV)
^{208}Pb	1636 ± 1.8	5.49 ± 0.03	2.34 ± 0.16
^{48}Ca	417 ± 1.2	3.51 ± 0.02	1.92 ± 0.20
^{40}Ca	342 ± 1.6	3.50 ± 0.02	–
^{56}Ni	482 ± 1.4	–	–
^{68}Ni	590 ± 1.0	–	–
^{100}Sn	826 ± 1.6	–	–
^{132}Sn	1103 ± 1.7	4.71 ± 0.03	–
^{90}Zr	784 ± 1.3	4.27 ± 0.02	–

Isoscalar resonances

	E^{IS}_{GMR} (MeV)	E^{IS}_{GQR} (MeV)
^{208}Pb	13.5 ± 0.3	10.8 ± 0.4
^{90}Zr	17.8 ± 0.4	–



Keeping ground and excited state **properties** within typical **Skyrme-EDF accuracy**

Conclusions

Bayesian inference performed for **observable** quantities only, taking into account **ground state** properties and **Giant Resonances**

Well **known correlations reproduced/confirmed**

Polarizability determines symmetry energy parameters

Large **errors** on A_{PV} do **not** allow for a **strong bias** on the results

Low values of J and L due to a **posterior** distribution from **masses biased** by $N = Z$ nuclei. **Work on progress in this direction**

Use of **other nuclear models** to **repeat** the same **inference** (model dependence of the results) **envisaged.**

Collaborators

→ Gianluca **Colò** (University of Milan)

→ Pietro **Klausner** (University of Milan)

→ Enrico **Vigezzi** (INFN Milan)