DFT for high-lying giant resonances and prospects for ab initio-based energy density functionals

Gianluca Colò
Dep. of Physics and INFN, Milano (Italy)

- A DFT-based model for an accurate description of excited states: **QRPA plus particle-vibration coupling**

Starting from natural orbits, correlations up to 2p-2h (or 4 quasi-particles) seem to be sufficient for an accurate description of the nuclear response

- Bayesian inference of **nuclear matter parameters**

It would be interesting to study carefully the probability distributions for NM parameters within **different frameworks**

- An attempt for ***ab initio* based DFT**

Highly desirable!

Nuclear response using QRPA plus particle-vibration coupling (PVC)

We start from a Hartree-Fock-Bogoliubov (HFB) set of states obtained with a Skyrme EDF.

First step: **diagonalize *H* on a two quasi-particle basis (QRPA).**

This produces a set of "vibrational quanta" or "phonons" associated with the operators Γ_n and Γ_n^+.

$$\Gamma_n^\dagger = \sum_{\alpha\beta} X_{\alpha\beta}^{(n)} \alpha_\alpha^\dagger \alpha_\beta^\dagger - Y_{\alpha\beta}^{(n)} \alpha_\beta \alpha_\alpha$$

$$|n\rangle = \Gamma_n^\dagger |\tilde{0}\rangle = \left(\sum_{\alpha\beta} X_{\alpha\beta}^{(n)} \alpha_\alpha^\dagger \alpha_\beta^\dagger - Y_{\alpha\beta}^{(n)} \alpha_\beta \alpha_\alpha \right) |\tilde{0}\rangle$$

Connecting with CC

$$|\Phi\rangle = \exp[\chi^\dagger] |\Phi_0\rangle$$

$$\chi^\dagger = \frac{1}{2} \sum_{\alpha\beta} c_{\alpha\beta} \alpha_\alpha^\dagger \alpha_\beta^\dagger$$

QRPA can be obtained by looking at variations of the total energy at second order in the coefficients c [M. Waroquier *et al*., Phys. Rep. 148, 249 (1987)]

We wish to improve the structure of the excited states. We can go to the next order in the quasiparticle number in different ways.

$$|N\rangle = \left(\sum_{\alpha\beta} X^{(1)}_{\alpha\beta} \alpha^\dagger_\alpha \alpha^\dagger_\beta - Y^{(1)}_{\alpha\beta} \alpha_\beta \alpha_\alpha + \sum_{\alpha\beta\gamma\delta} X^{(2)}_{\alpha\beta\gamma\delta} \alpha^\dagger_\alpha \alpha^\dagger_\beta \alpha^\dagger_\gamma \alpha^\dagger_\delta - Y^{(2)}_{\alpha\beta\gamma\delta} \alpha_\delta \alpha_\gamma \alpha_\beta \alpha_\alpha \right) |\tilde{0}\rangle$$

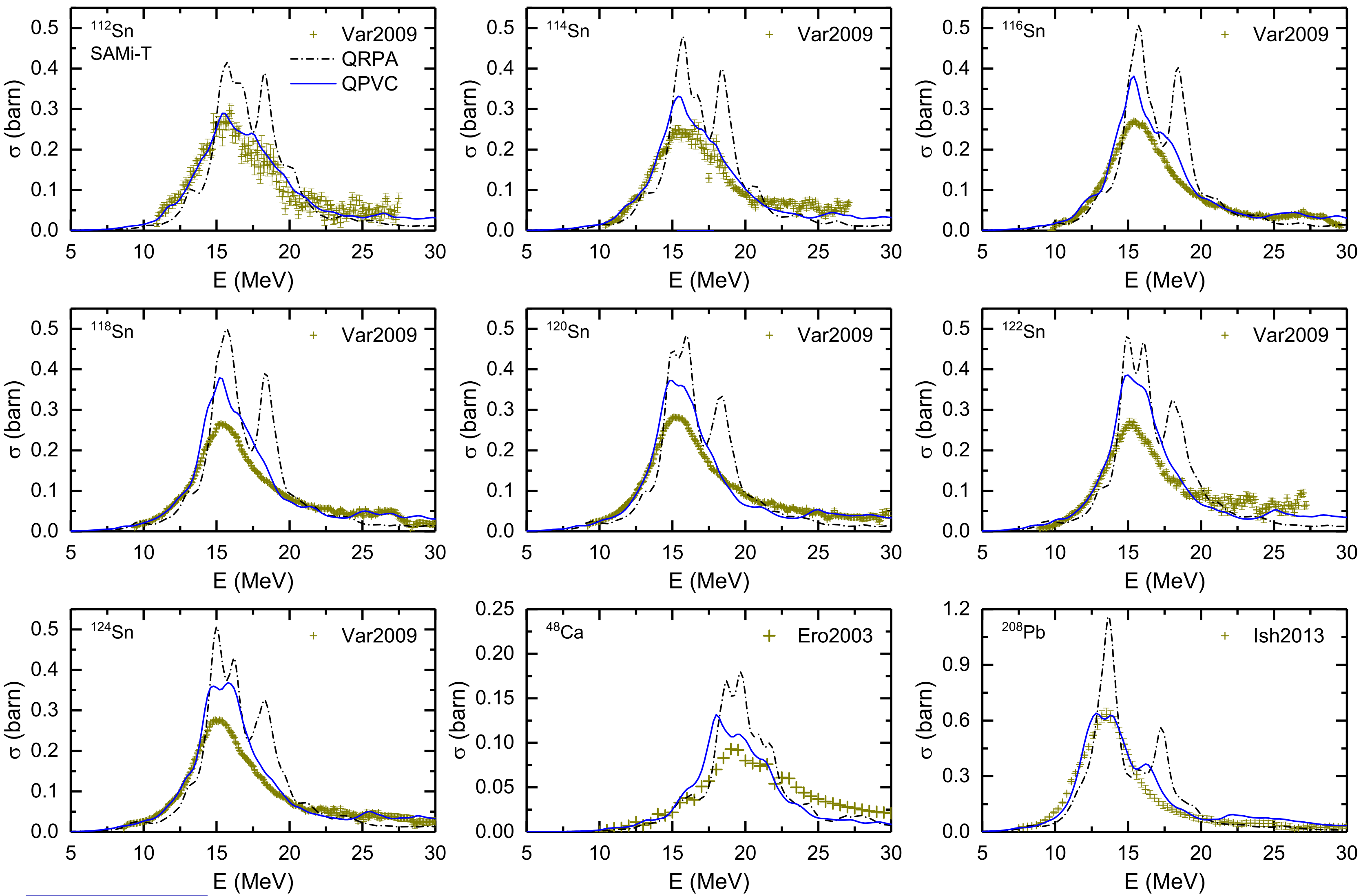
$$|N\rangle = \left(\sum_{\alpha\beta} X^{(1)}_{\alpha\beta} \alpha^\dagger_\alpha \alpha^\dagger_\beta - Y^{(1)}_{\alpha\beta} \alpha_\beta \alpha_\alpha + \sum_{\alpha\beta n} X^{(2)}_{\alpha\beta n} \alpha^\dagger_\alpha \alpha^\dagger_\beta \Gamma^\dagger_n - Y^{(2)}_{\alpha\beta n} \alpha_\delta \alpha_\gamma \alpha_\beta \Gamma_n \right) |\tilde{0}\rangle$$

We can now treat these components **explicitly**, although it is quite demanding. In most of the application we have included these components **implicitly** though a self-energy.

$$|\Phi\rangle = \exp[\chi^\dagger]|\Phi_0\rangle \qquad \chi^\dagger = \frac{1}{2}\sum_{\alpha\beta} c_{\alpha\beta}\alpha^\dagger_\alpha \alpha^\dagger_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta} c_{\alpha\beta\gamma\delta}\alpha^\dagger_\alpha \alpha^\dagger_\beta \alpha_\delta \alpha_\gamma$$

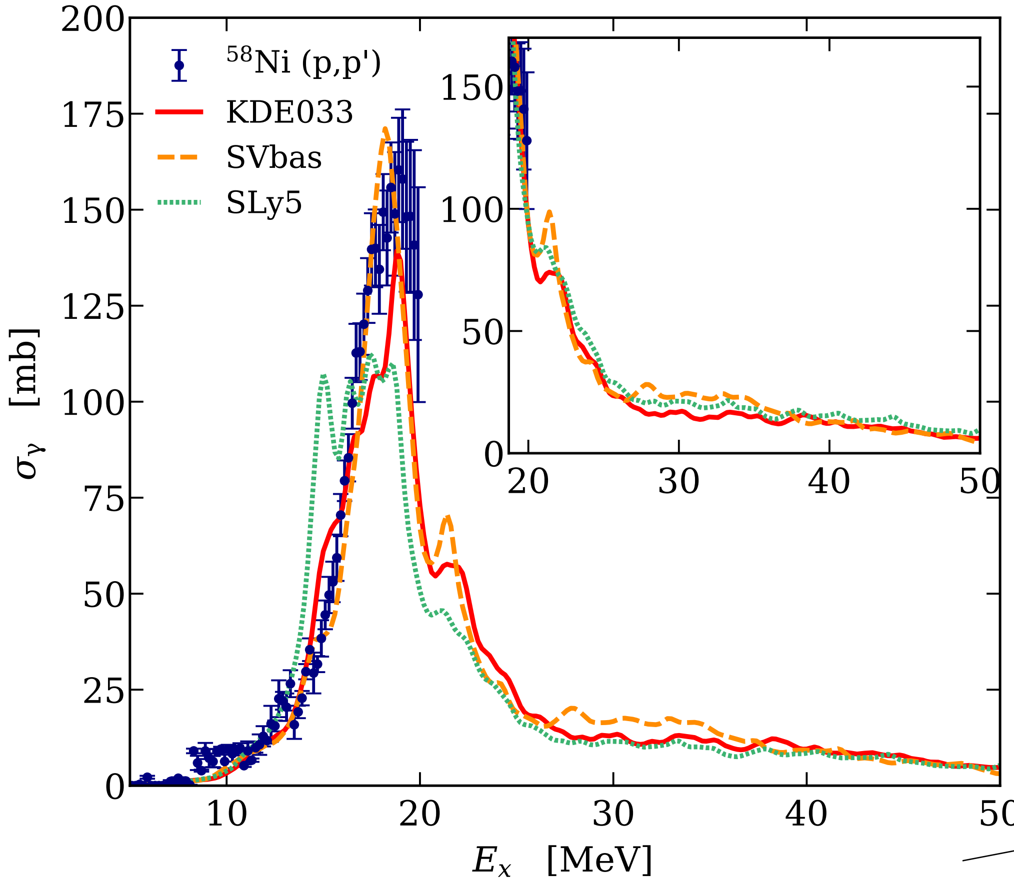
J. Da Providência, Nucl. Phys. 61, 87 (1965)
D. Gambacurta *et al.*, J. Phys. G 38, 035103 (2011)

IVGDR in different nuclei



Z.Z. Li *et al.*, Phys. Rev. C110, 064317 (2024). SAMi-T.

Photoabsorbtion of ^{58}Ni



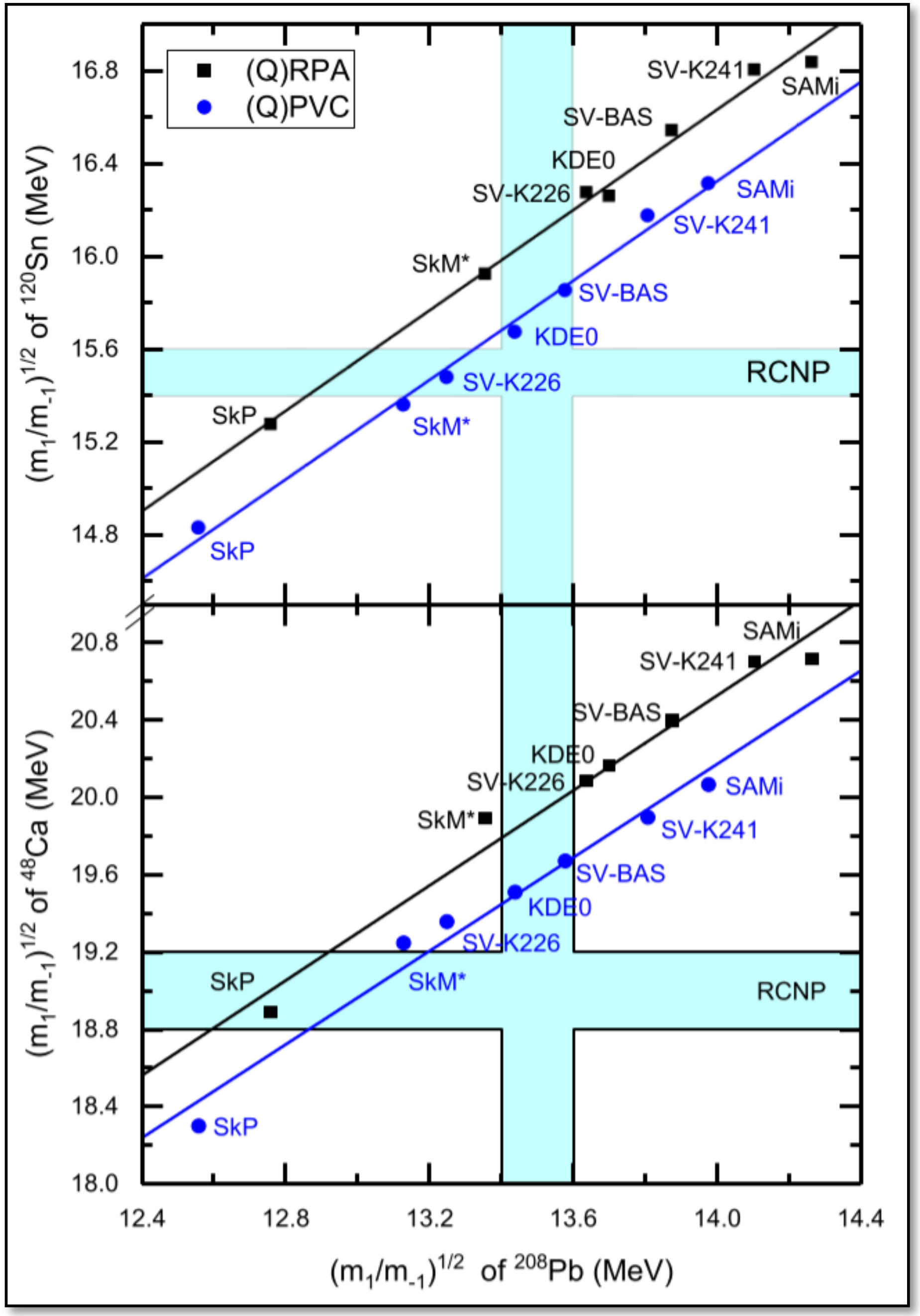
Comparison with recent data from (p,p') measured at RCNP, Osaka. Exp. data from I. Brandherm *et al.*

Theory reproduces very well the dipole polarizabilty and can be used to estimate the high-energy dipole tail.

PHYSICAL REVIEW C **111**, 024312 (2025)

Electric dipole polarizability of ^{58}Ni

I. Brandherm,[1] F. Bonaiti,[2,3,4] P. von Neumann-Cosel,[1,*] S. Bacca,[2] G. Colò,[5,6] G. R. Jansen,[7,4] Z. Z. Li (李征征),[8,9,10] H. Matsubara,[11,12] Y. F. Niu (牛一斐),[9,10] P.-G. Reinhard,[13] A. Richter,[1] X. Roca-Maza,[14,15,5,6] and A. Tamii[11]



Using this model, we have been able, for the first time, to analyse **in a systematic manner** the consistency between ISGMR energies in different nuclei.

We have used many Skyrme EDFs.

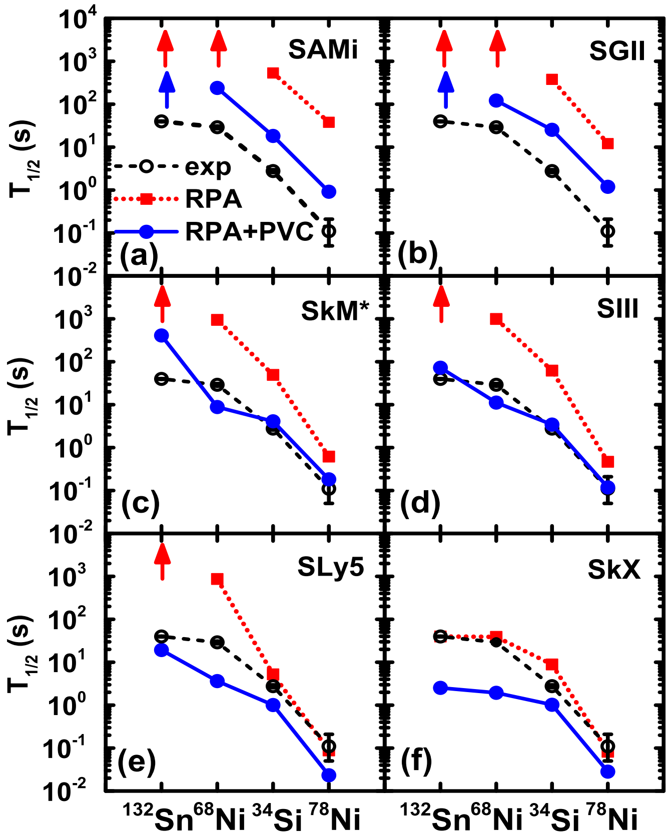
With the inclusion of QPVC effects, a big improvement is achieved.

Within QPVC, the ISGMR energy in ^{208}Pb is consistent with ^{120}Sn and points to <u>K around 225-230 MeV</u>.

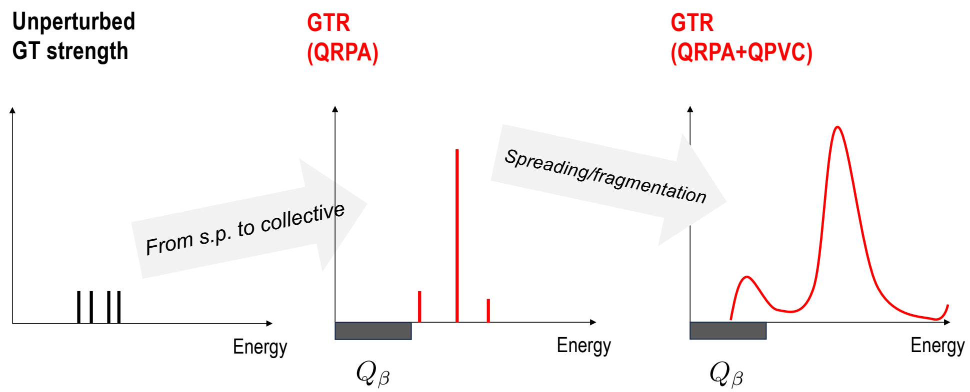
Z.Z. Li, Y.F. Niu, GC, Phys. Rev. Lett. 131, 082501 (2023)

QPVC and two-body currents for β-decay

Applying QPVC to β-decay



Y. F. Niu *et al.*, Phys. Rev. Lett. 114, 142501



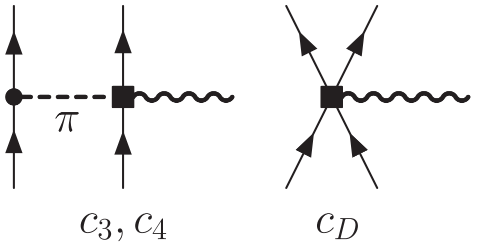
RPA may not leave strength in the Q_β window.

PVC redistributes the GT strength.

Two-body currents included.

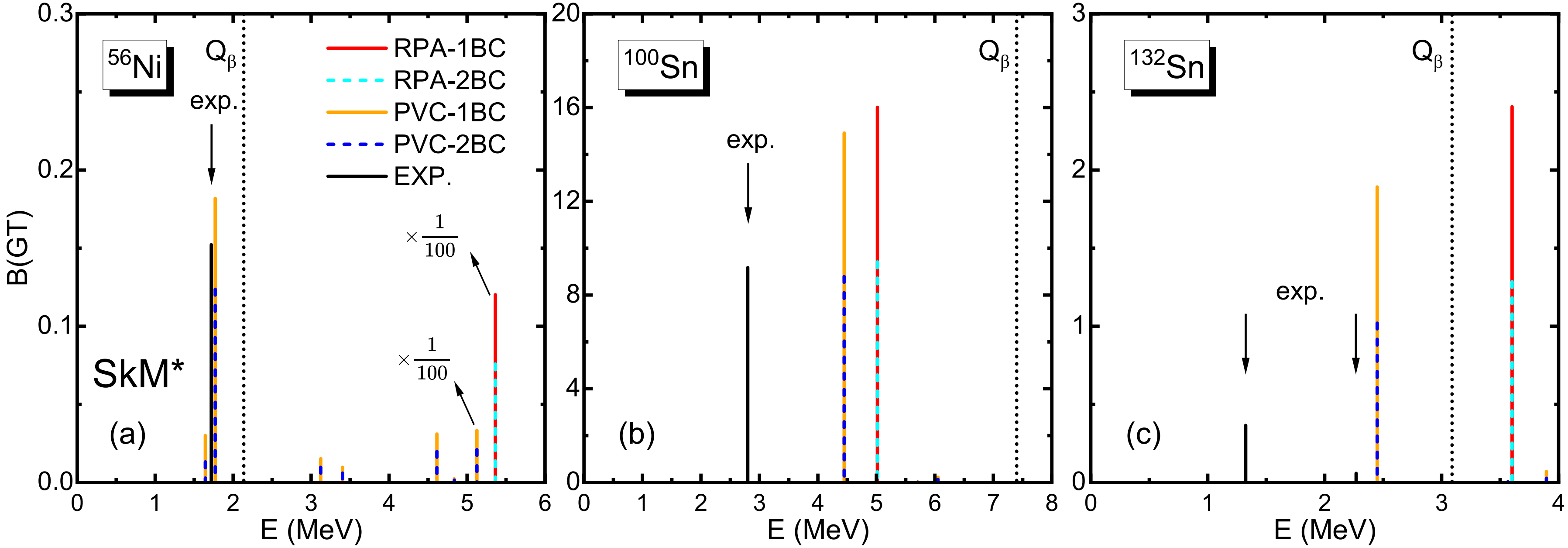
Not a consistent calculation.

$$c_3, c_4, c_D = -4.78, 3.96, 0$$

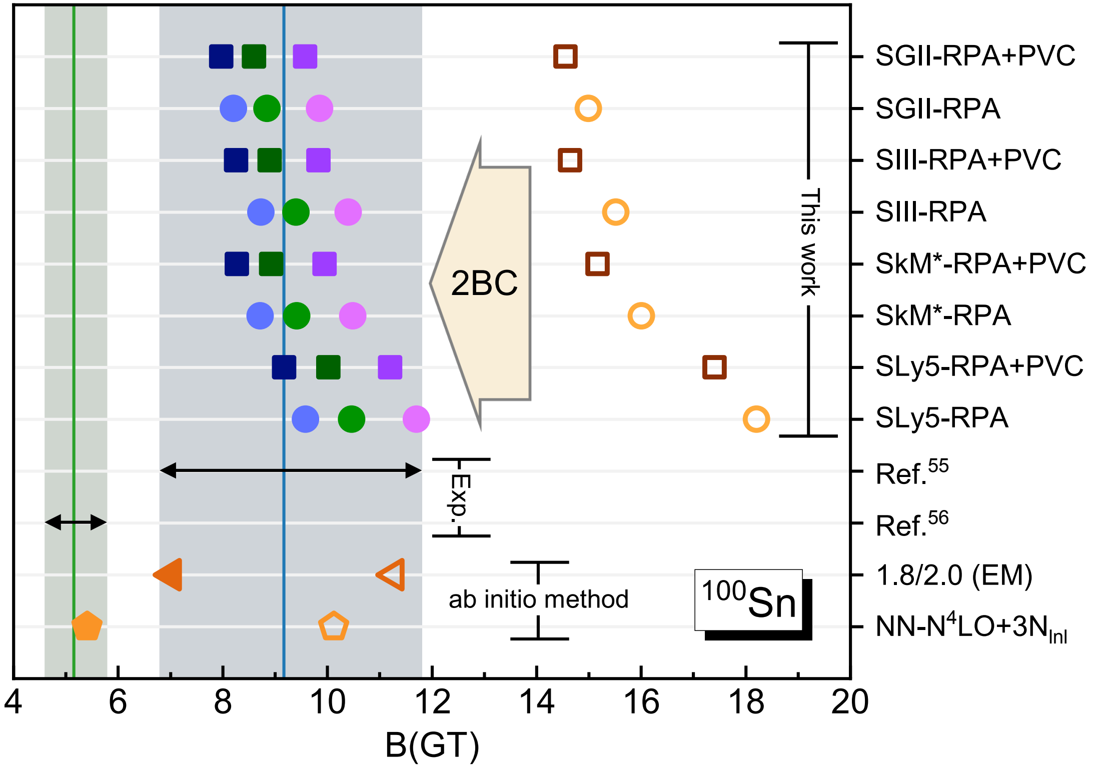


J. Menéndez *et al.*, PRL 107, 062501 (2011)

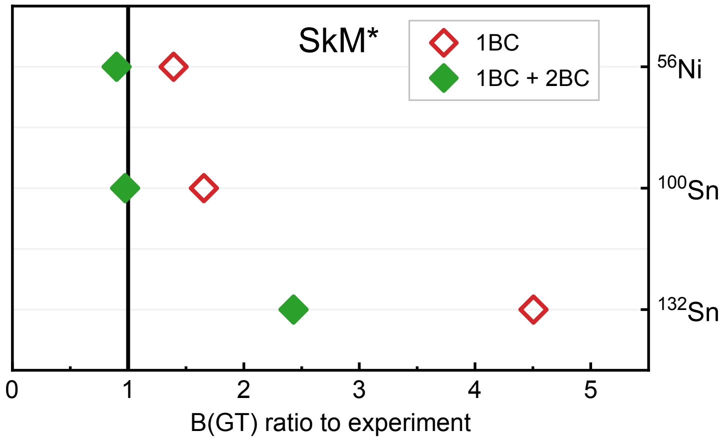
T.-S. Park *et al.*, PRC 67, 055206 (2003)



B. L. Wang *et al.* (to be published)



see P. Gysbers *et al.*, Nat. Phys. 15, 428 (2019)



We need to start from QPVC because in simple QRPA **the B(GT) in the decay window would vanish (!) for ^{56}Ni and ^{132}Sn**

B. L. Wang *et al.* (to be published)

Bayesian inference of nuclear matter parameters

Observables used for the inference

Ground-state properties			
	$B.E.$ [MeV]	$R_{\rm ch}$ [fm]	$\Delta E_{\rm SO}$ [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		
	$E^{\rm IS}_{\rm GMR}$ [MeV]	$E^{\rm IS}_{\rm GQR}$ [MeV]
^{208}Pb	13.5 ± 0.5*	10.9 ± 0.5*
^{90}Zr	17.7 ± 0.5*	-

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

"hfbcs-qrpa[1]" code to compute observables from parameters

$B.E.$: Binding Energy

R_{ch} : Charge radius

ΔE_{SO} : Spin-orbit splitting

E^{IS}_{GMR} : IsoScalar Giant monopole resonance excitation energy (constrained)

E^{IS}_{GQR} : IsoScalar Giant quadrupole resonance excitation energy (centroid)

α_D: Nuclear polarizability

$m(1)$: EWSR of IVGDR

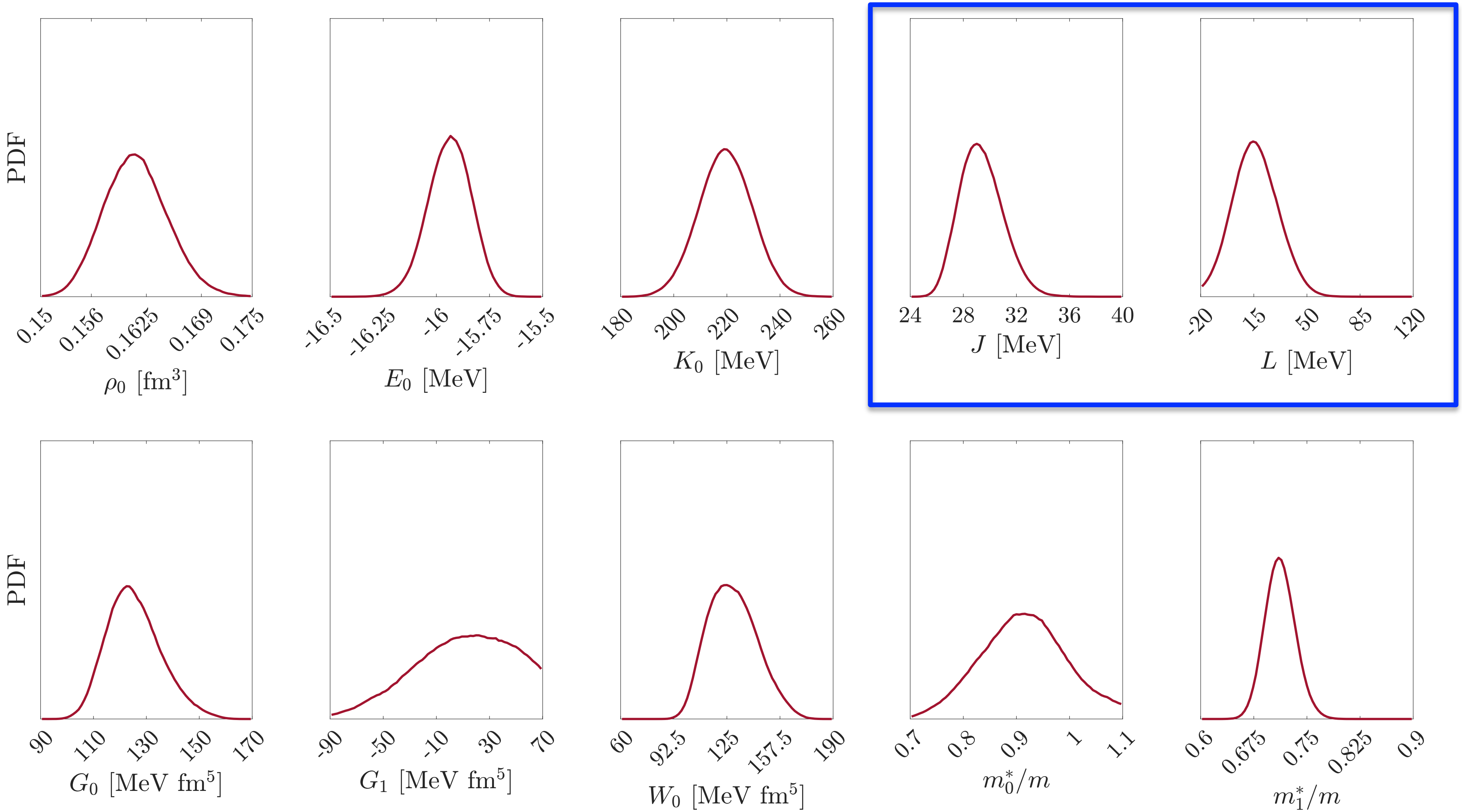
A_{PV}: Parity violating asymmetry

* Theoretical error

[1]G. Colò, X. Roca-Maza, arXiv:2102.06562v1 [nucl-th]

Standard Skyrme EDF.

Results: marginalized posterior distributions



P. Klausner *et al.*, PRC 111, 014311 (2025)

- We have indications that a larger pool of nuclei is needed to better fix J and L (open-shell and possibly deformed).

- The posterior distributions have been used as priors for an inference based on data taken from observations of neutron stars (P. Klausner *et al*., arXiv:2505.16929).

Neutron Star crust informed by nuclear structure data

Pietro Klausner,[1,2,3,*] Marco Antonelli,[1,†] and Francesca Gulminelli[1,‡]

[1] *Université de Caen Normandie, CNRS/in2p3, LPC Caen (UMR6534), 14050 Caen, France*
[2] *Dipartimento di Fisica "Aldo Pontremoli", Università degli Studi di Milano, 20133 Milano, Italy*
[3] *INFN, Sezione di Milano, 20133 Milano, Italy*

- PDFs and correlation matrices from different models can and should be confronted.

Inferred values of the parameters / predictions

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

Ground-state properties			
	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		–
Isovector properties			
	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

All observables are within experimental errors. The BE of ^{56}Ni and so splitting of ^{208}Pb are within 1 and 2σ while only the A_{PV} of ^{208}Pb lies at more than 2σ.

Ab initio-based DFT

- D. Gambacurta, L. Li, G. Colò, U. Lombardo, N. Van Giai, and W. Zuo, Phys. Rev. C 84, 024301 (2011).

- G. Salvioni, J. Dobaczewski, C. Barbieri, G. Carlsson, A. Idini, and A. Pastore, J. Phys. G 47, 085107 (2020).

- L. Zurek, E. A. Coello Pérez, S. K. Bogner, R. J. Furnstahl, and A. Schwenk, Phys. Rev. C 103, 014325 (2021).

In these works (plus others not quoted here) the idea is that *ab initio* can be used to constrain, or inform, specific terms of the EDF.

Instead, we would like to use *ab initio* calculations of **model systems** like it has been done, or advocated, for electronic systems.

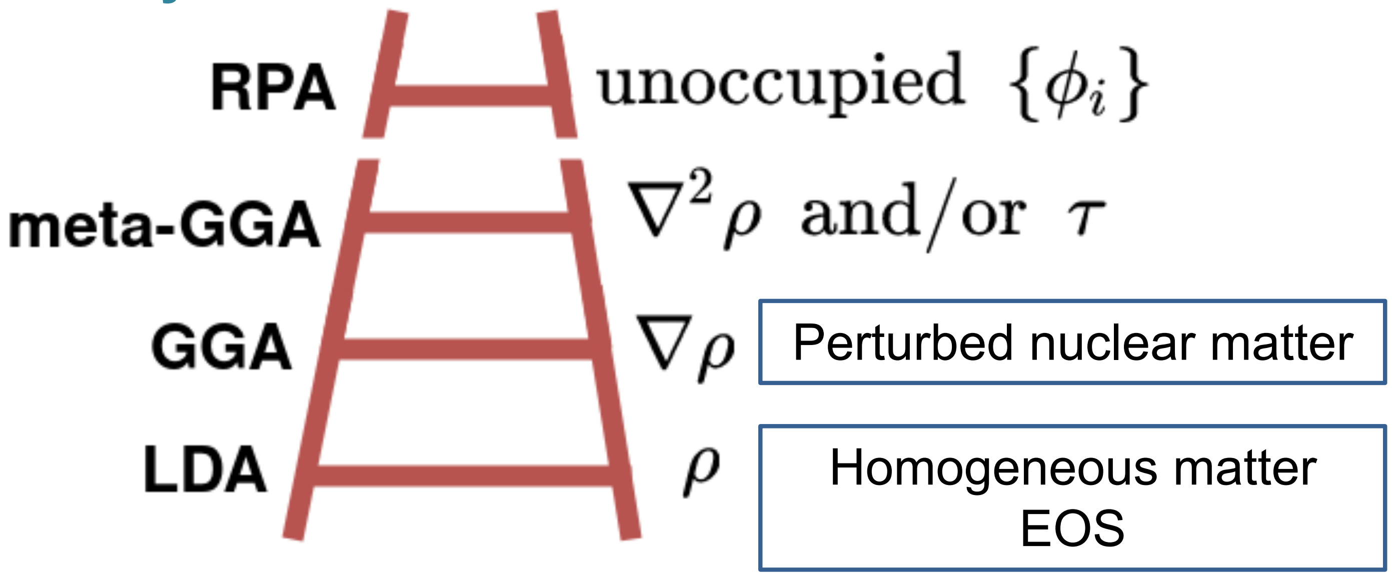
A systematic hierarchy of approximations

Our recently proposed strategy is **systematic** and based on the **Jacob's ladder** of electronic DFT.

J. Perdew, K. Schmidt, AIP Conf. Proc. 577, 1 (2001).

Heaven of chemical accuracy

Earth of Hartree



- **Follow a step-by-step approach**
- **Use *ab initio* simulations of model systems as a constraint**

The Equation of State (EoS)

$$\rho = \rho_n + \rho_p$$

$$\beta = \frac{\rho_n - \rho_p}{\rho}$$

QMC with simple AV4'+UX$_c$

SCGF with NNLO$_{sat,}$ ΔNNLO$_{GO}$

We parametrise the potential part of the EoS.

1. v is quadratic in β
2. v is a polynomial in k_F

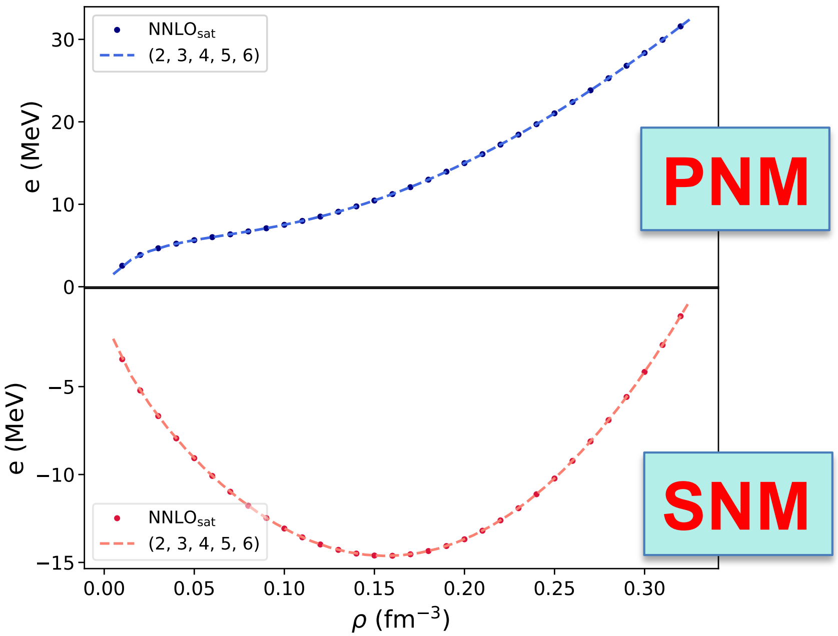
$$v(\rho, \beta) = \sum_{\gamma} \left(c_{\gamma,0} + \beta^2 c_{\gamma,1}\right) \rho^{\gamma} \qquad \gamma = \frac{n}{3}$$

3. The optimal set of powers is chosen by model selection.

More powers that in empirical EDFs.

Local Density Approximation (LDA)

We find the best series of terms like $\rho^{n/3}$



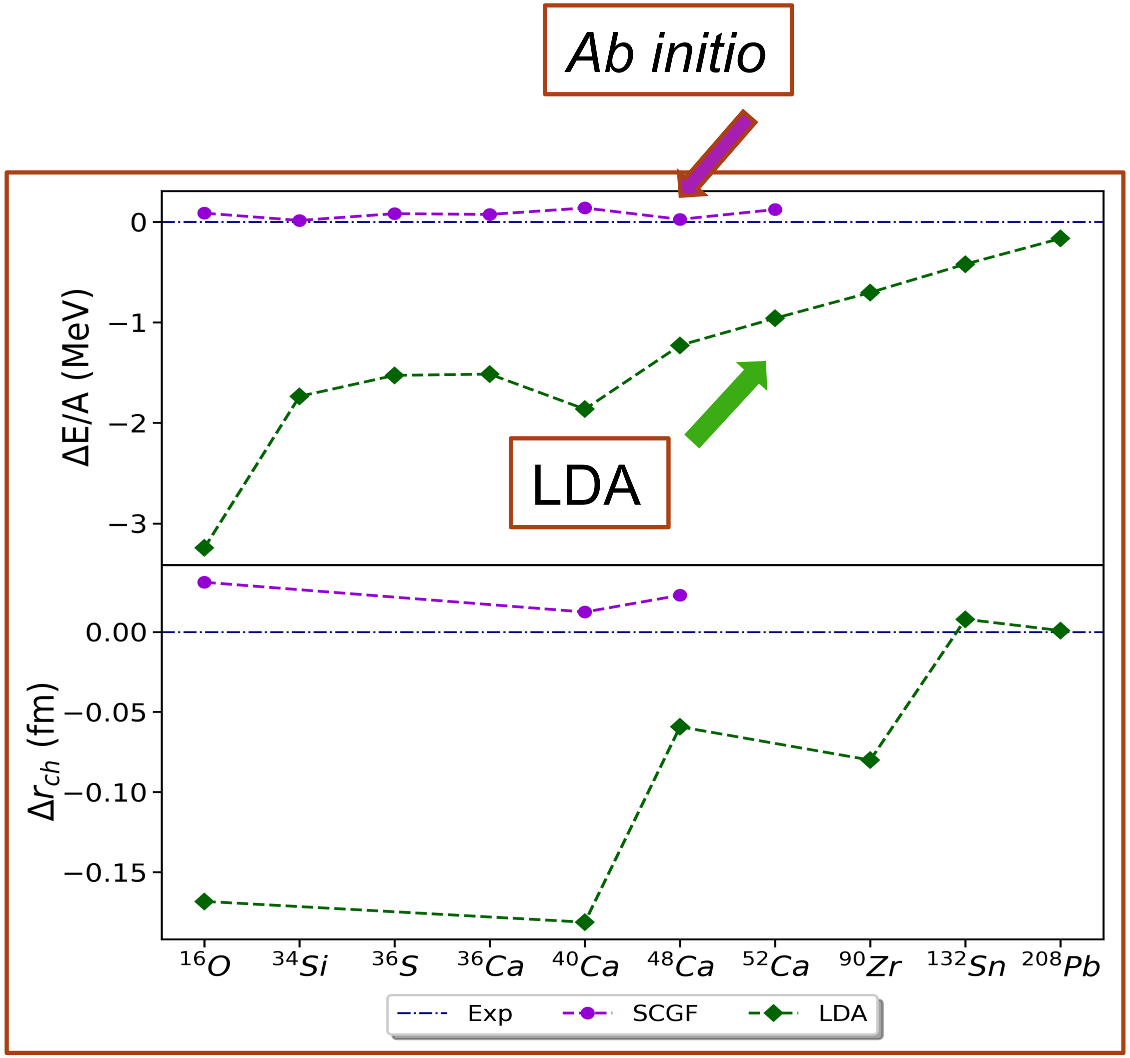
Within LDA, the energy functional is the same as in uniform matter.

We apply it to finite systems as if their local density were uniform.

$$e = \frac{E}{A} = \frac{\mathcal{E}}{\rho}$$

$$E_{\rm pot} = \int d^3r\ \rho(\vec{r})e[\rho]$$

Results: $NNLO_{sat}$



Difference with respect to experiment for

E/A (upper panel)

r_{ch} (lower panel)

Encouraging results in heavy nuclei (^{132}Sn, ^{208}Pb)

Something still missing

F. Marino *et al.*, PRC 104, 024315 (2021)

Perturbed nuclear matter

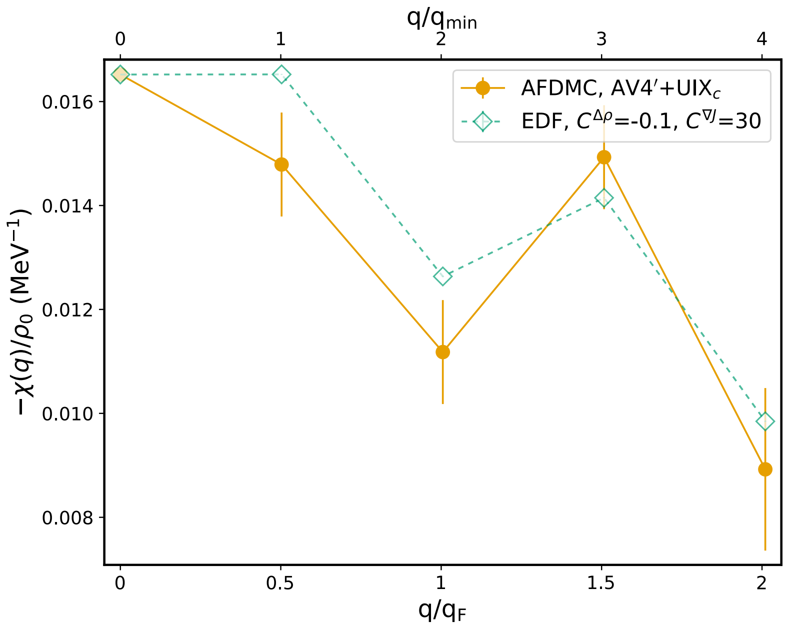
Add a **weak external potential** of the type: $v_{\rm ext} = 2v_q cos(\vec{q}\cdot\vec{r})$

In linear response:

$$\delta\rho(\vec{r}) = 2\chi(q) v_q cos(\vec{q}\cdot\vec{r})$$

$$\delta e = \frac{\chi(q)}{\rho_0} v_q^2$$

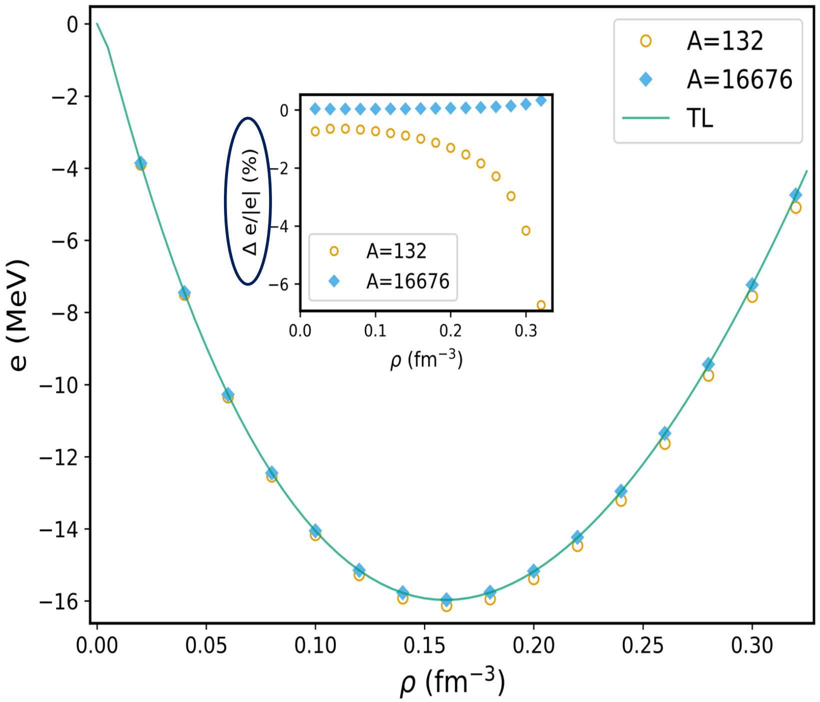
One should check that one is in this **lowest-order** PT regime.
Then, one can try to **optimise the parameters so that EDF matches these results.**



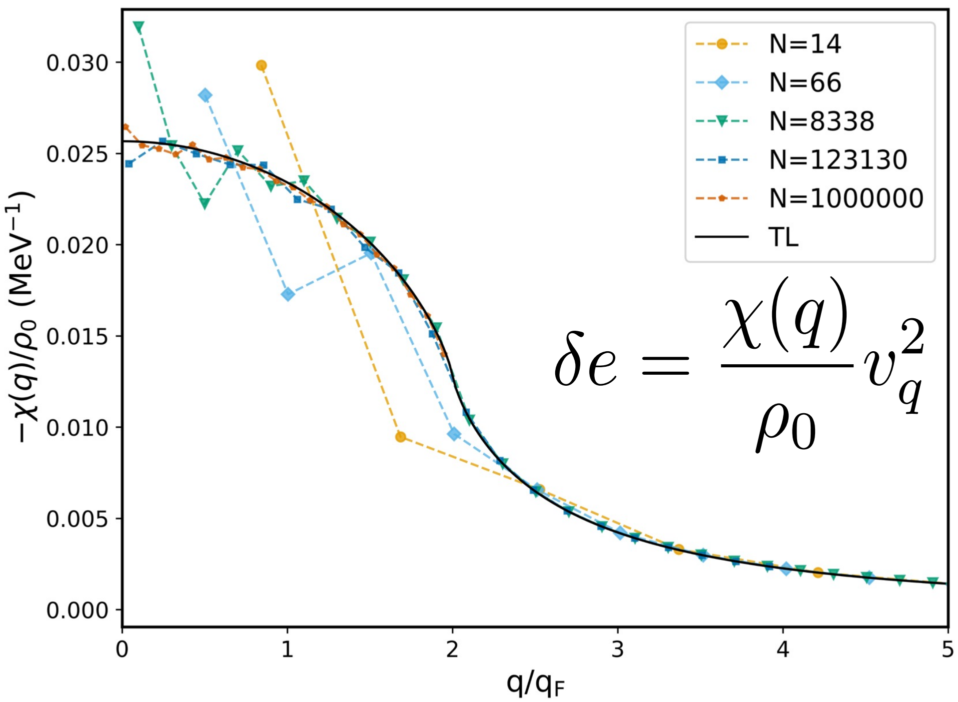
Uncertainties on AFDMC points are of the same order of the variations of the response function with *q*.

Finite size effects

SNM EOS



Fermi gas response



Finite size effects are **weak** on the EOS but **strong** on $\chi(q)$

- C. Barbieri, **P. Klausner**, E. Vigezzi (Milano)
- D. Gambacurta (LNS)
- F. Pederiva (Trento)
- M. Antonelli, F. Gulminelli (LPC Caen, France)
- **F. Marino** (JGU Mainz, Germany)
- **A. Porro** (TU Darmstadt, Germany)
- X. Roca-Maza (Milano, now at U. Barcelona, Spain)
- A. Lovato (ANL, USA, now at U. Valencia, Spain)
- **Z.Z. Li** (PKU, China)
- L. Cao, **B.L. Wang** (Beijing Normal University, China)
- Y. Niu, **W.L. Lv** (Lanzhou University, China)

Conclusions

- **Grounding DFT in *ab initio*** is highly desirable but it has not been achieved yet.

- In our attempt, we are stuck by **finite size effects** in the nuclear response.

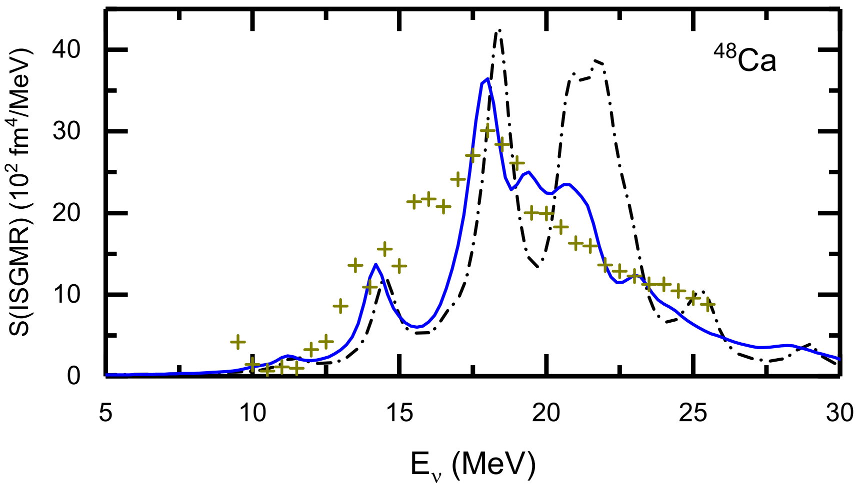
- Other interesting avenues: comparison of NM parameters and associated correlations from *ab initio*, from different EDFs...

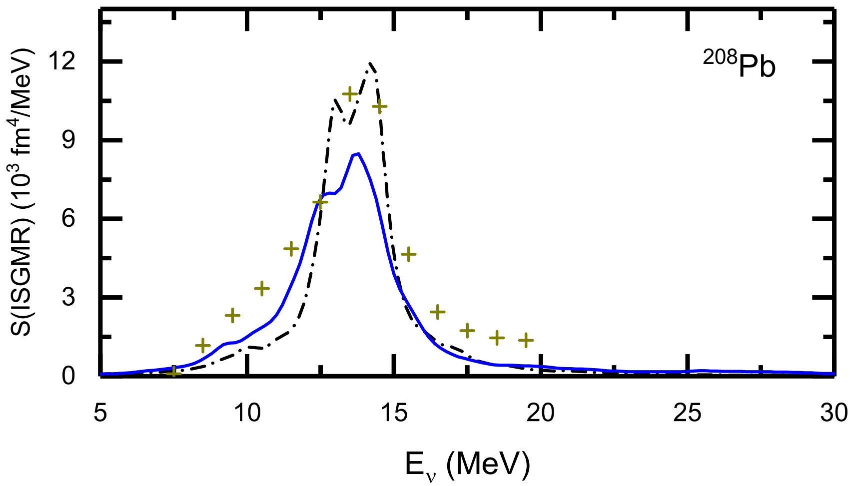
- More generally: we have some expertise coming from DFT applied to high-lying excited states that can be useful when discussing *ab initio* approaches.

Thank you for listening

Backup slides

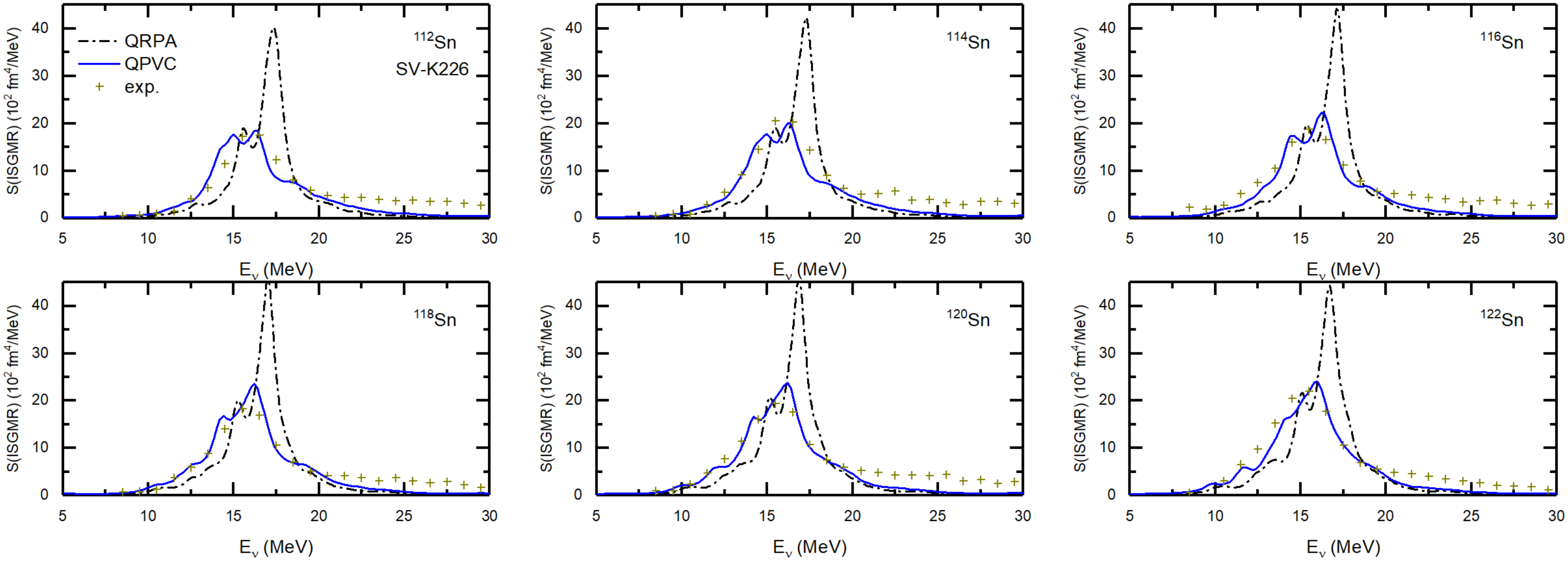
ISGMR in ^{48}Ca and ^{208}Pb





- Exp. data from T. Li *et al*., Phys. Rev. Lett. 99, 162503 (2007) and S.D. Olorunfunmi, Phys. Rev. C 105, 054319 (2022).
- In these two cases there is no pairing.

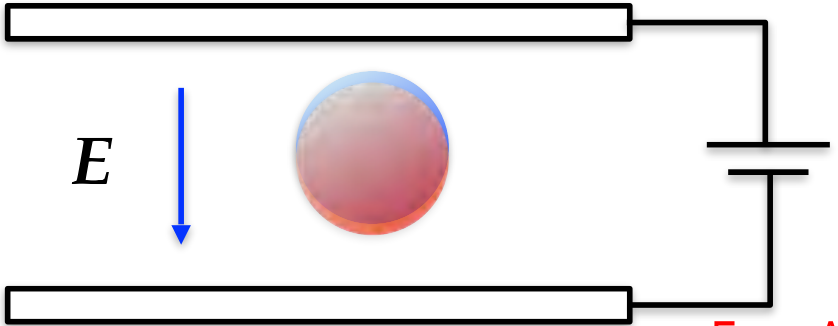
ISGMR in Sn isotopes



- Exp. data from D. Patel *et al*., Phys. Lett. B726, 178 (2013)
- QPVC reproduces the experimental data quite well.
- The best description is obtained with the Skyrme EDF SV-K226.

Klüpfel, Reinhard, *et al*., PRC 79, 034310 (2009)

The dipole polarizability



From A. Tamii

If the nucleus were under the action of a static electric field

$$p = \alpha_D E$$

The **polarizability** can be deduced from the so-called **inverse energy-weighted sum rule** associated with dipole field

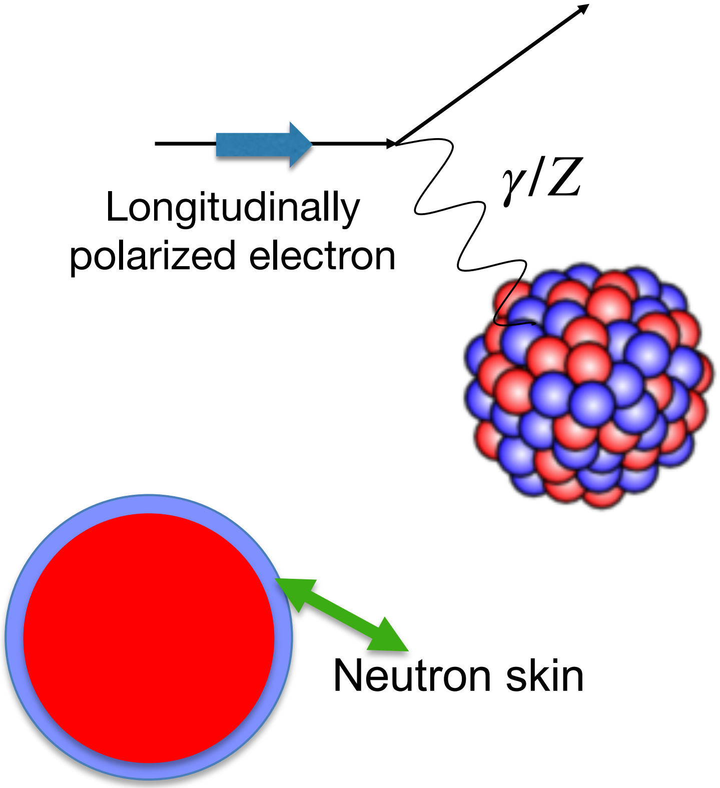
$$\alpha_D = \frac{8\pi e^2}{9} \int dE \, \frac{dB(E1)}{dE} \equiv \frac{8\pi e^2}{9} m_{-1}$$

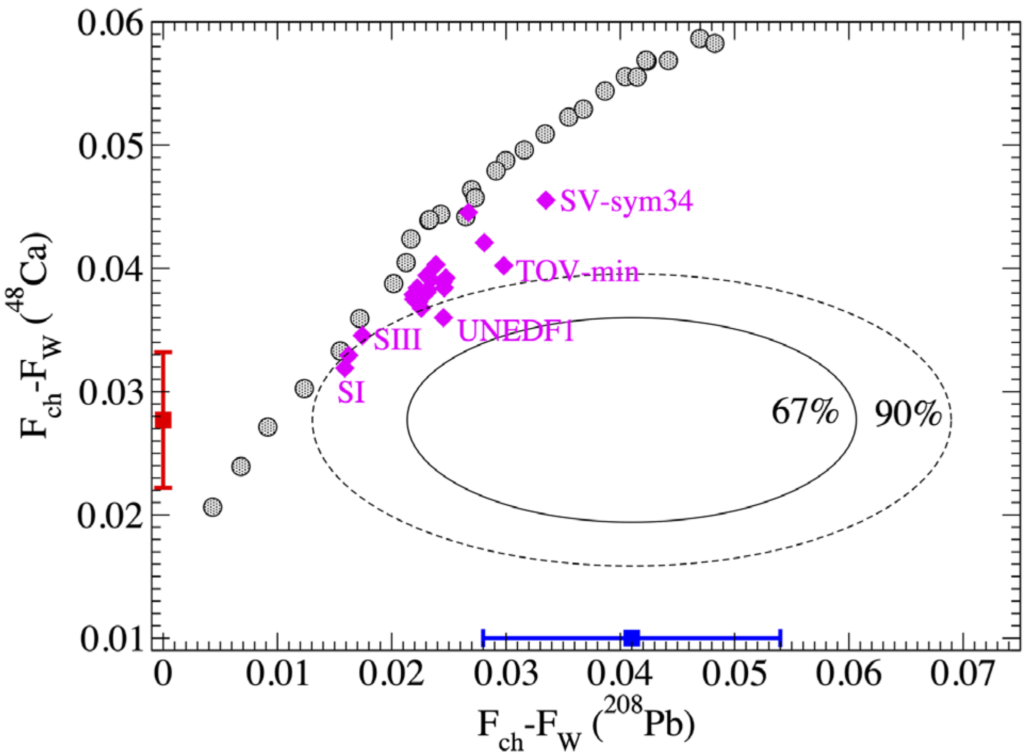
A. Migdal, Quadrupole and dipole γ-radiation of nuclei, J. Phys. Acad. Sci. USSR 8(1-6), 331-336 (1944)

$$\alpha_D = \frac{\pi e^2}{54} \frac{A\langle r^2 \rangle}{J}$$

Parity-violating asymmetry (and weak FF)

Parity-violating asymmetry measured in electron scattering is a probe of the **neutron distribution** (in principle, a model-independent probe).





D. Adhikari *et al.*, Phys. Rev. Lett. 129, 042501 (2022)

PHYSICAL REVIEW C **110**, 054322 (2024)

Editors' Suggestion

Diagrammatic *ab initio* methods for infinite nuclear matter with modern chiral interactions

F. Marino[1,*] W. G. Jiang[1,2] and S. J. Novario[3]

[1] *Institut für Kernphysik and PRISMA+ Cluster of Excellence, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany*

[2] *Mainz Institute for Theoretical Physics, Johannes Gutenberg-Universität, 55128 Mainz, Germany*

[3] *Department of Physics, Washington University in Saint Louis, Saint Louis, Missouri 63130, USA*

(Received 24 July 2024; revised 10 October 2024; accepted 22 October 2024; published 22 November 2024)

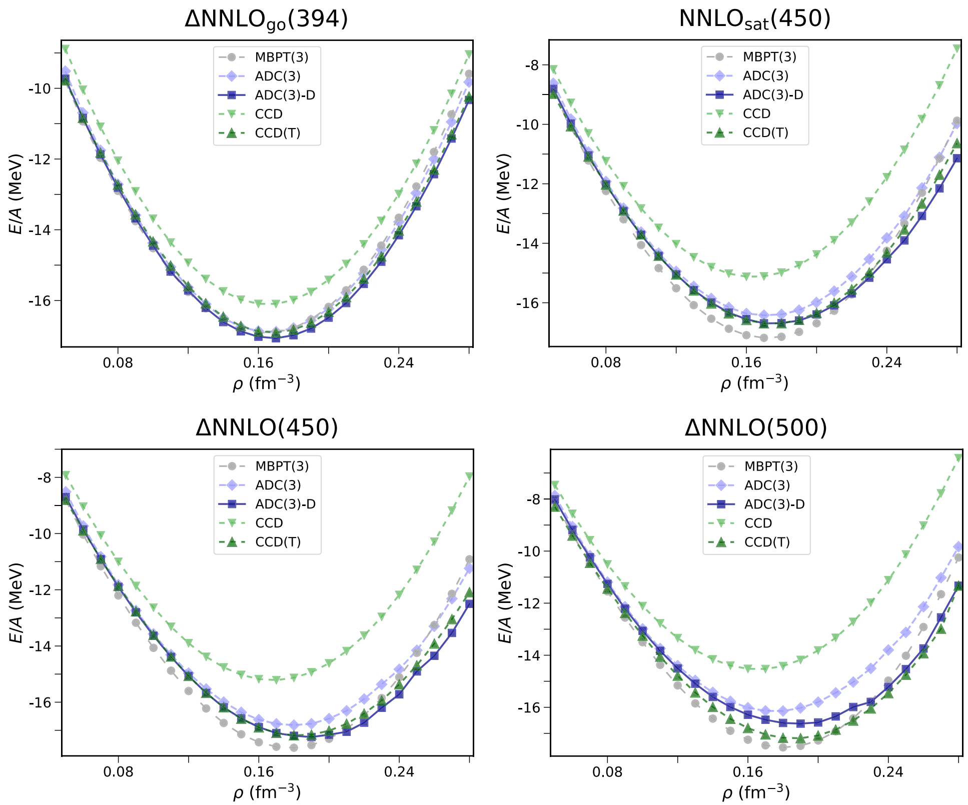
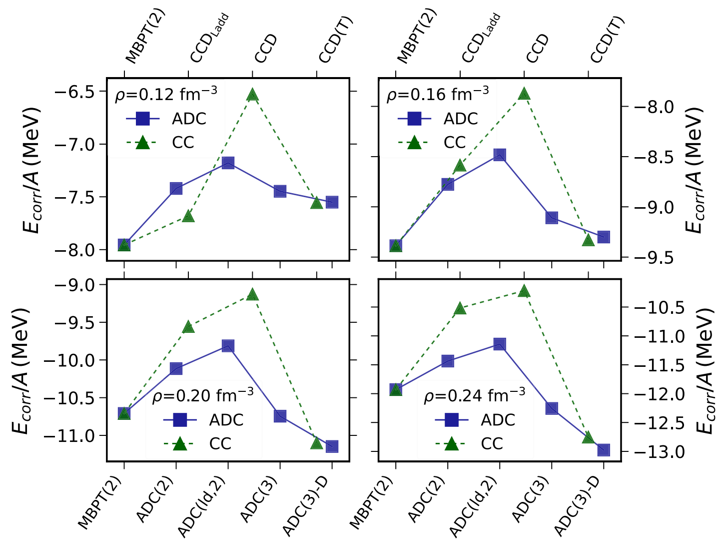


FIG. 6. SNM equations of state obtained with four different chiral interactions. Each panel reports the outcomes of five many-body techniques (see legend). $A = 132$ nucleons subject to PBCs are employed to simulate SNM.



Including appropriate classes of Feynman diagrams, the different MB methods are very close (at a given level of approximation)