How does subatomic matter organize itself?

A low-energy nuclear physics perspective

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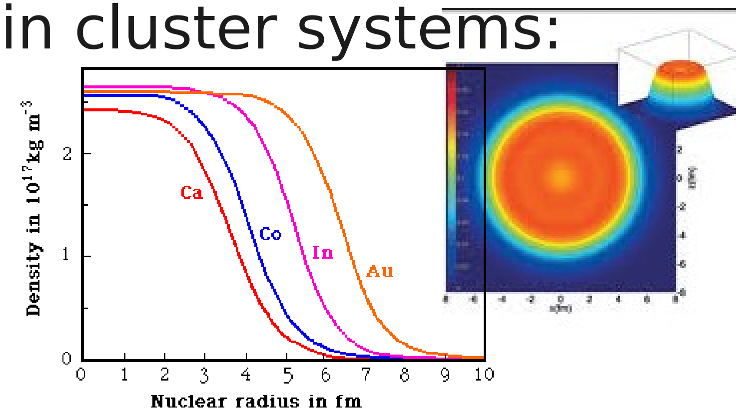
RESANET – webinar

Réactions, structure et Astrophysique Nucléaires: Expériences et Théories

October 24th 2022

Where can we find neutrons and protons? And in which form? Free? In clusters?

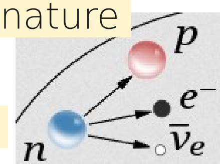
- Neutrons and protons in **Earth** are found in cluster systems: **nuclei**



  → The **interior** of all nuclei has **constant density** (10^{14} times denser than water) named **saturation density**

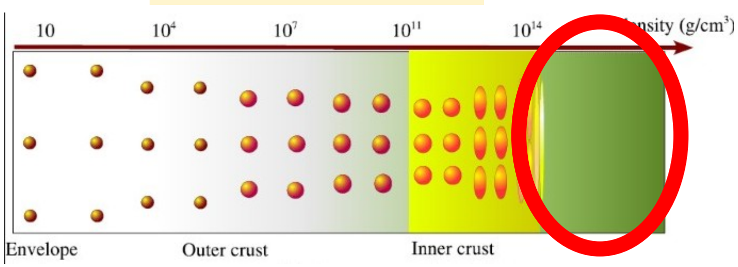
  → Saturation is originated from the **short range** nature of the **nuclear effective interaction**

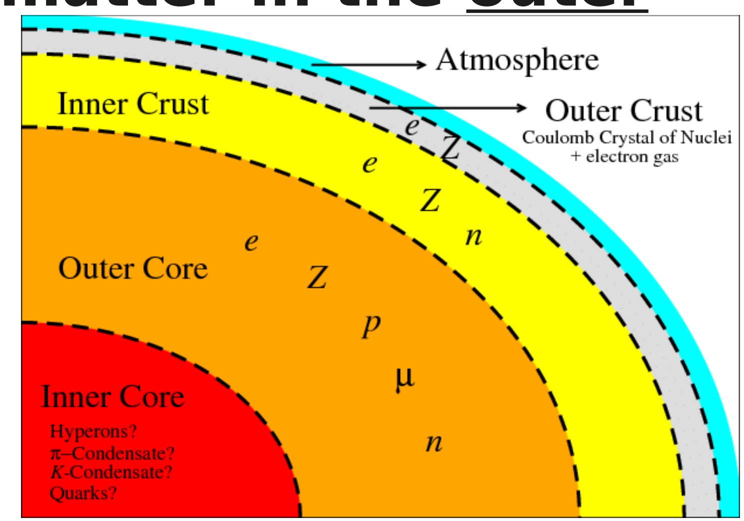
  → Neutron in 15 minutes must find a proton or …



- In **heavens**, neutrons and protons can be also found as an interacting and unbound Fermi liquid: **matter in the <u>outer core</u> of a neutron star**

  → Densities can reach several times nuclear saturation



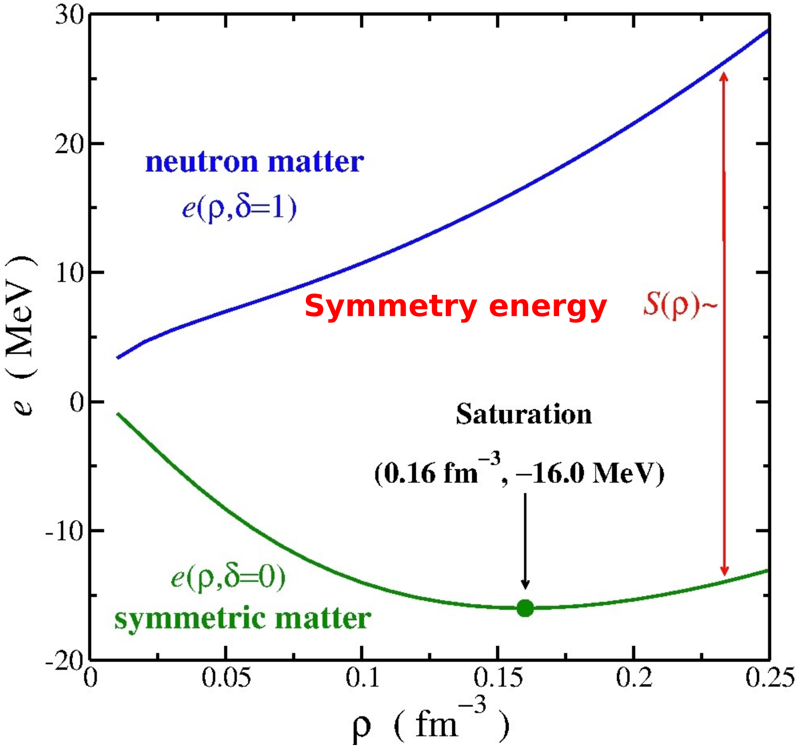


Nuclear Equation of State as an important **building block** of all **nuclear systems realized** in **nature.**

Nuclear Equation of State (EoS)

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* $V_{nn} = V_{pp} = V_{np}$):

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



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

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

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

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

Symmetric matter EoS at saturation:

Reproduction of exprimental binding energies and charge radii sets a tight constraint on the needed accuracy for e_0 and ρ_0

→ A **small change** in the **saturation density** will **impact** the **size** of the **nucleus. Charge radii** are determined to an average accuracy of 0.016 fm (Angeli 2013).

For example, if one aims at determining the $\mathbf{r_{ch}}$ **= 5.5012±0.0013 fm** in ^{208}**Pb** one must be **very precise** in the determination of $\boldsymbol{\rho_0}$:

$$\frac{\delta\rho_0}{\rho_0} = -3\frac{\delta R}{R} \rightarrow \frac{\delta\rho_0}{\rho_0} \lesssim 0.1\%$$

Note: typical average theoretical deviation of accurate EDFs ~ 0.02 fm → $\boldsymbol{\delta\rho_0/\rho_0}$ is determined up to about a **1% accuracy** (That is, third digit in ρ_0).

→ In a similar way, a **small change** in the **saturation energy** (about $e_0 \approx$ -16 MeV) will **impact** on the **nuclear masses.**

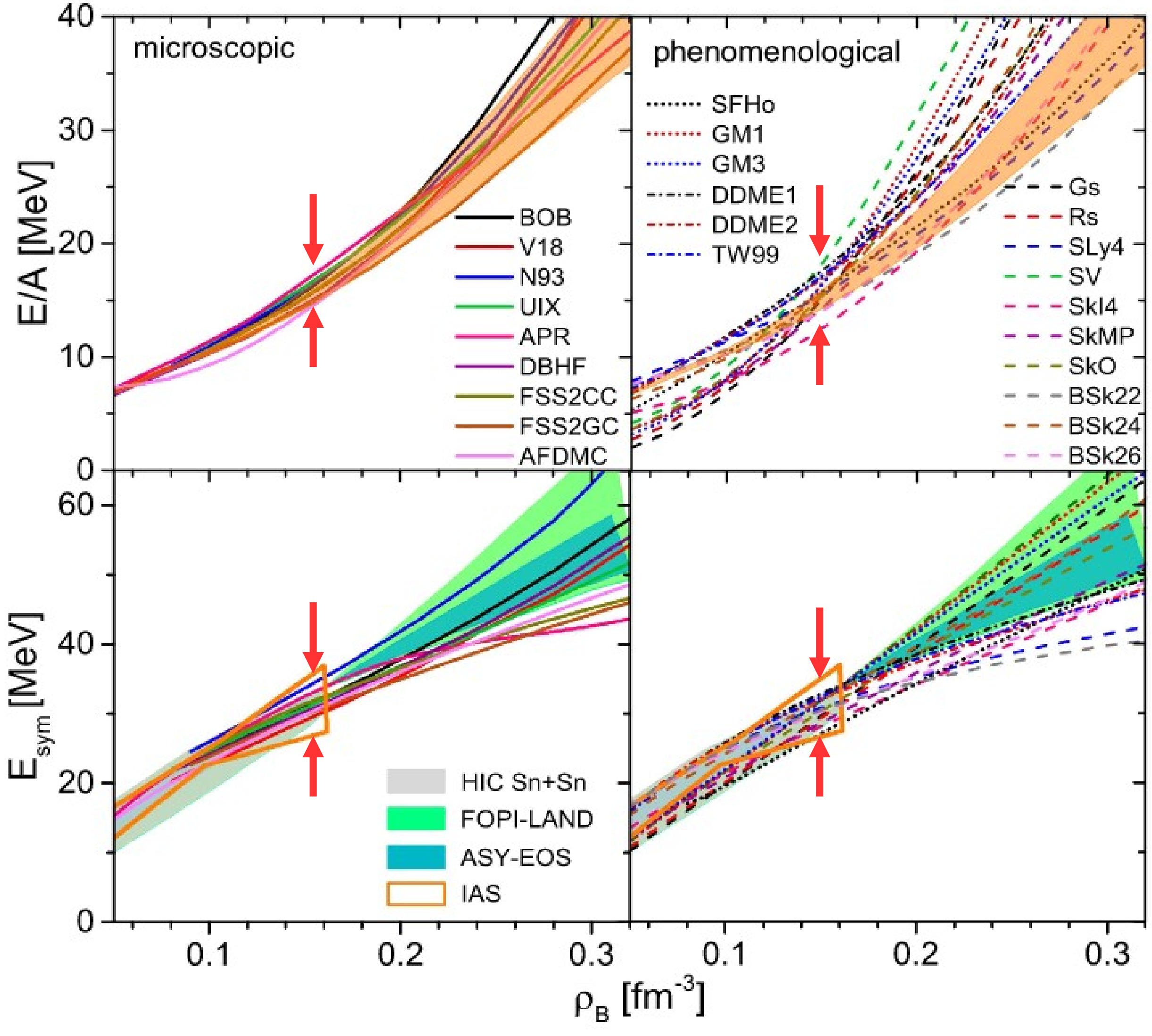
For example, if one aims at determining the **B = 1636.4296±0.0012 MeV** in ^{208}**Pb** one must be **very precise** in the determination of $\mathbf{e_0}$:

$$\frac{\delta B}{B} = \frac{\delta e_0}{e_0} \rightarrow \frac{\delta e_0}{e_0} \lesssim 10^{-6}$$

Note: typical average theoretical deviation of accurate EDFs ~ 1-2 MeV → $\boldsymbol{\delta e_0/e_0}$ is determined up to about a **0.1% accuracy** (That is, second decimal digit in e_0).

Neutron matter EoS

Micorscopic and phenomenological models constrainted by different data display similar discrepances on the EoS



Progress in Particle and Nuclear Physics 120 (2021) 103879

Light orange bands from χEFT from Drischler C., et al. Phys. Rev. Lett., 125 202702 (2020).

What can we learn from the Earth and the Heavens about the Nuclear Equation of State and, thus, how subatomic matter organize itself?

(some examples)

From Heaven:
Neutron Star Mass and Radius

Nuclear models that account for different nuclear properties on **Earth** predict a large **variety** of **Neutron Star Mass-Radius** relations → **Observation of a $2M_{sun}$ has constrained nuclear models.**

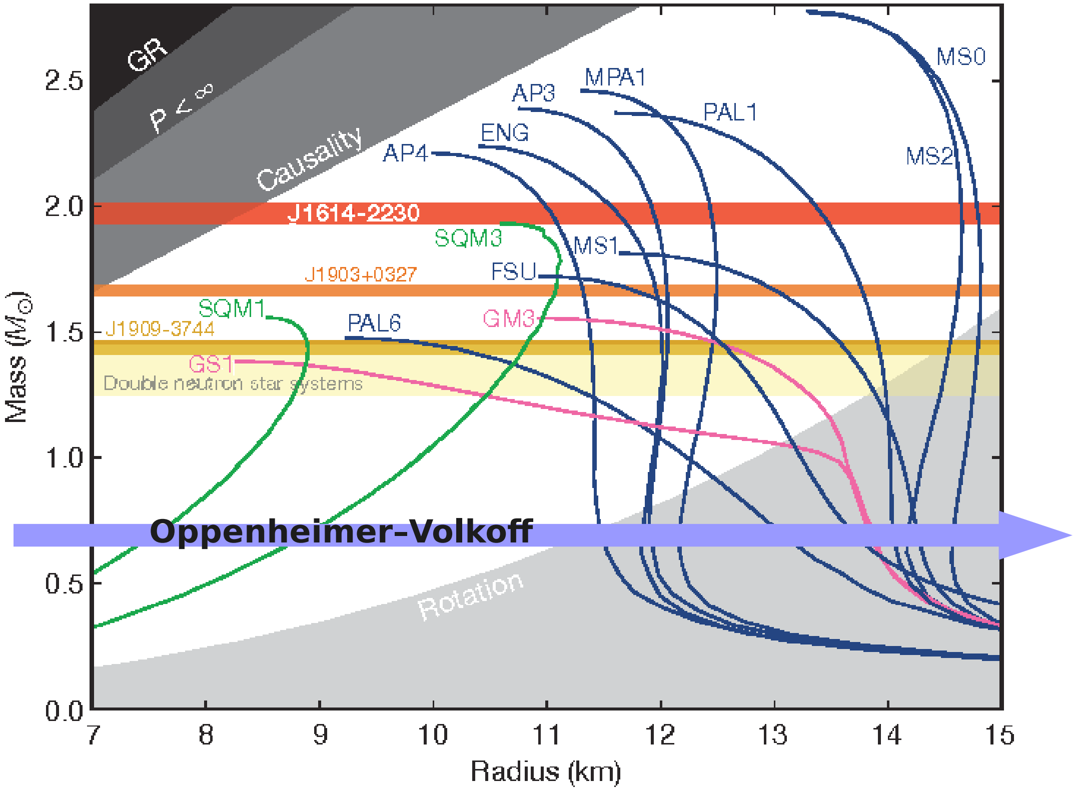
Tolman–Oppenheimer–Volkoff equation (sph. sym.):

$$\frac{dM(r)}{dr} = 4\pi r^2 \mathcal{E}(r);$$

$$\frac{dP}{dr} = -G\frac{\mathcal{E}(r)M(r)}{r^2}\left[1+\frac{P(r)}{\mathcal{E}(r)}\right]\left[1+\frac{4\pi r^3 P(r)}{M(r)}\right]\left[1-\frac{2GM(r)}{r}\right]^{-1}$$

$\mathcal{E}(r) \rightarrow$ degeneracy pressure from neutrons $\rightarrow M_{\max} = 0.7 M_{\rm sun}$

Nuclear Physics input is fundamental

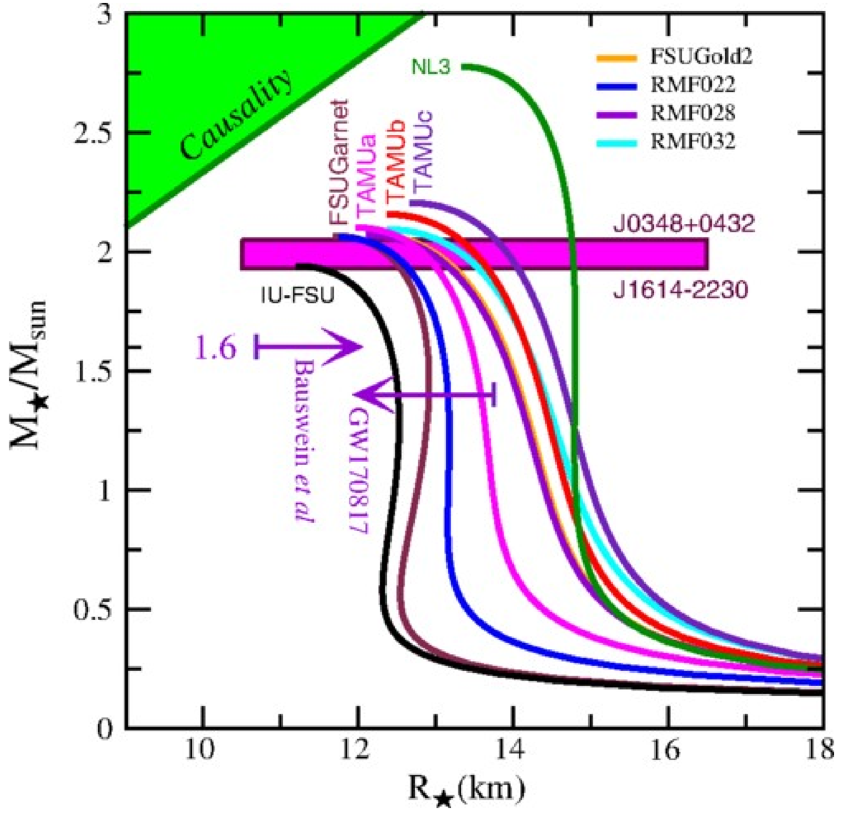


A two-solar-mass neutron star measured using Shapiro delay - P. B. Demorest, T. Pennucci, S. M. Ransom, M. S. E. Roberts & J. W. T. Hessels - Nature volume 467, 1081–1083(2010)

Crucial to reliably determine the mass and radius of neutron stars [see, e.g. Neutron Star Interior Composition Explorer (NICER)]

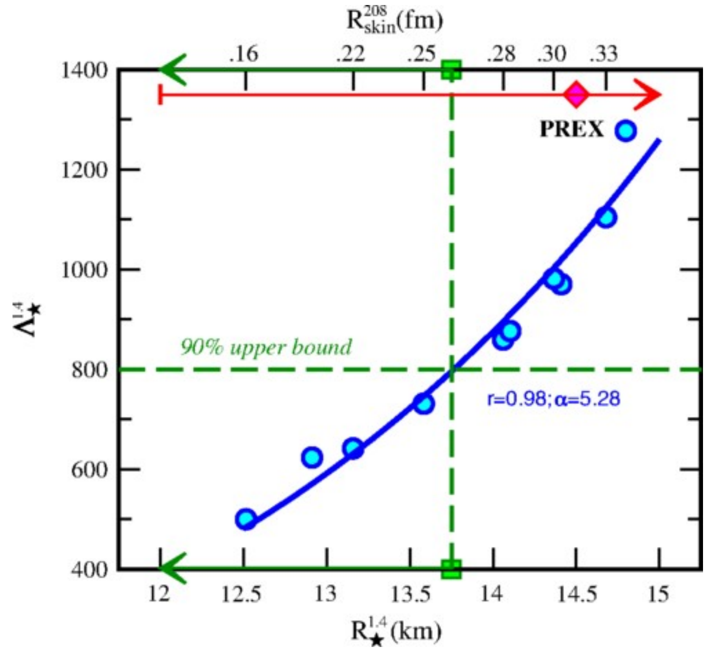
From Heaven: Gravitational wave signal from a binary neutron star merger

GW170817 from the binary neutron star merger → **constraint** neutron star **radius** and, thus, the **nuclear EoS**

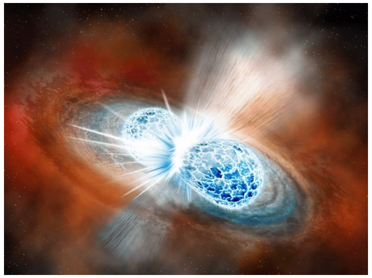


Neutron Skins and Neutron Stars in the Multimessenger Era

F. J. Fattoyev, J. Piekarewicz, and C. J. Horowitz Phys. Rev. Lett. 120, 172702 (2018)



Tidal deformability (Λ) is a quadrupole deformation inferred from **GW signal →** proportional to **restoring force.** Hence, sensitive to the **nuclear EoS**



Neutron-star merger (Courtesy: NASA)

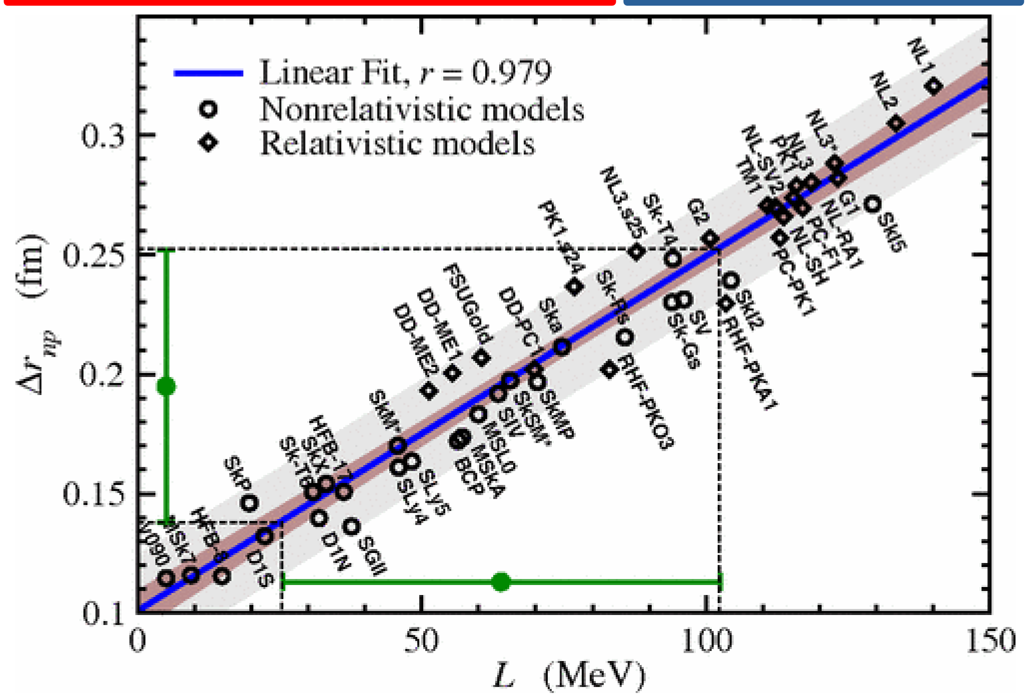
From Heaven & Earth: neutron skin and the Radius of a Neutron Star

Both, the **neutron skin thickness** ($\Delta r_{np}=r_n-r_p$) in neutron rich nuclei and the **radius** of a **neutron star** are related to the **neutron pressure** in infinite matter.
The former around ρ_0 (L) while the latter in a broad range of densities.

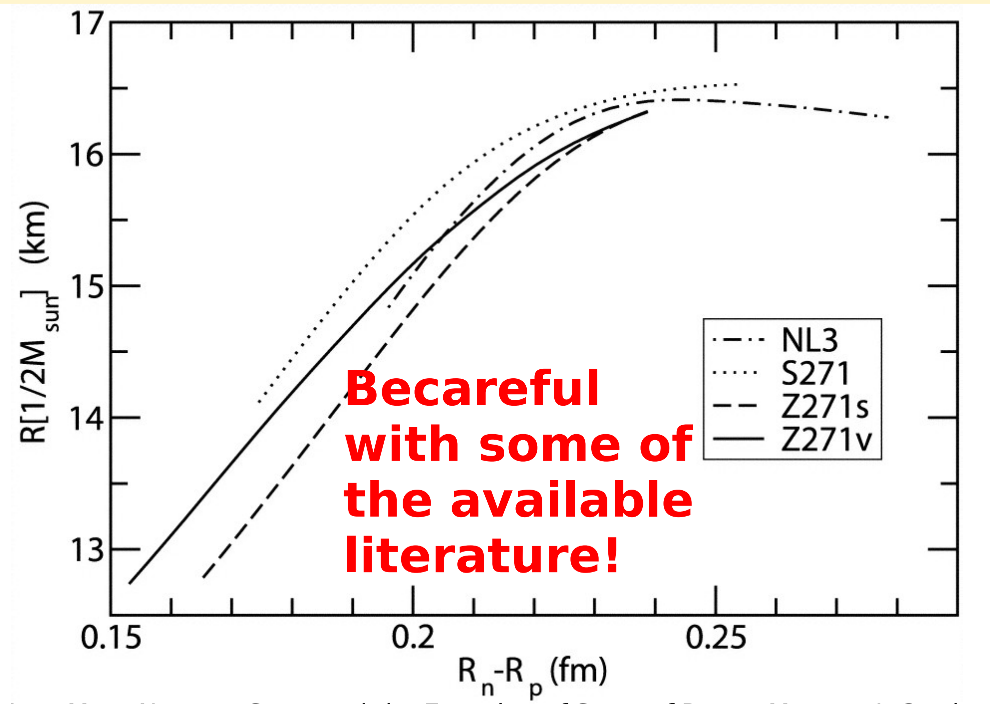
$$P(\rho_0,\delta)=\rho_0^2\frac{\partial e(\rho,\delta)}{\partial\rho}\Big|_{\rho=\rho_0}=\frac{1}{3}\rho_0\delta^2 L$$

$$\Delta r_{np}\approx\frac{1}{12}\frac{N-Z}{A}\frac{R}{J}L$$

→ Only for unrealistically **small neutron stars**, that is, for small central densities ($\rho_c\sim\rho_0$) a **linear** relation between **R** and **Δr_{np}** is physically meaningful.



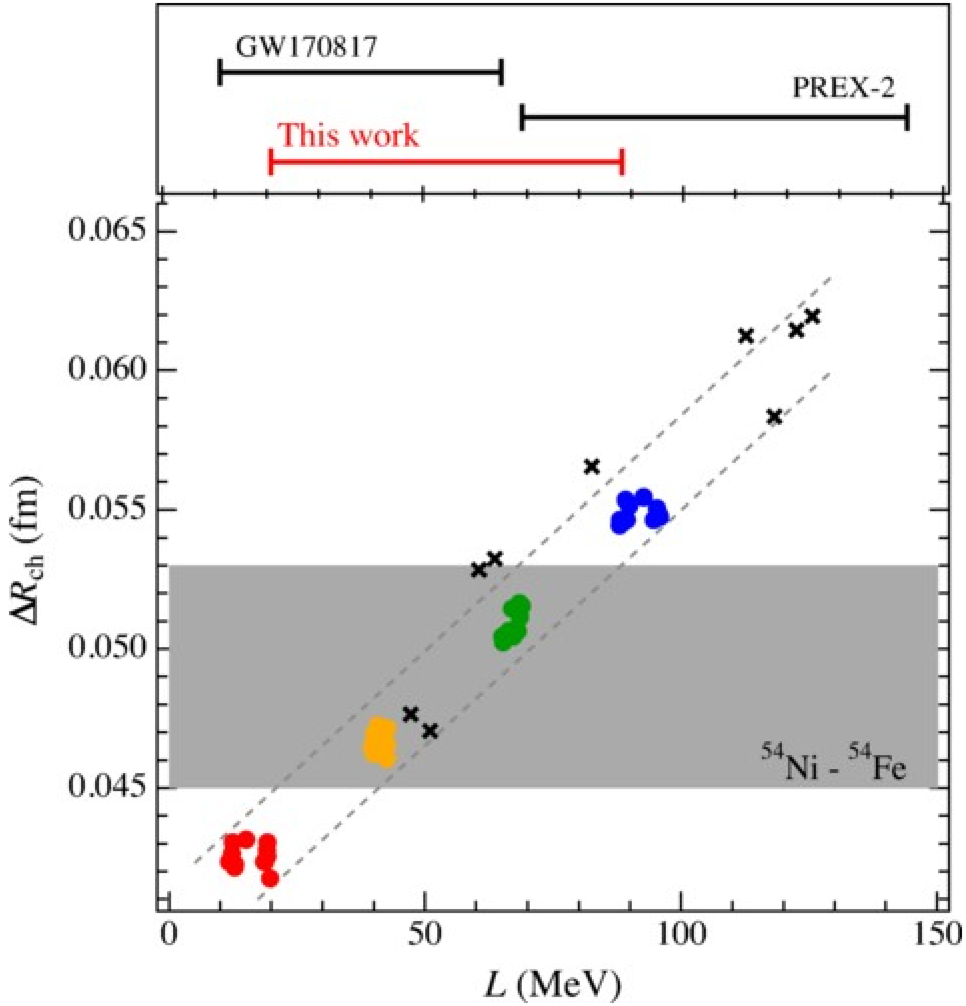
Neutron Skin of 208Pb, Nuclear Symmetry Energy, and the Parity Radius Experiment
X. Roca-Maza, M. Centelles, X. Viñas, and M. Warda Phys. Rev. Lett. 106, 252501 (2011)



Low-Mass Neutron Stars and the Equation of State of Dense Matter - J. Carriere, C. J. Horowitz, and J. Piekarewicz - The Astrophysical Journal, 593 (2003) 463

From Earth: Δr_{ch} in mirror mass nuclei

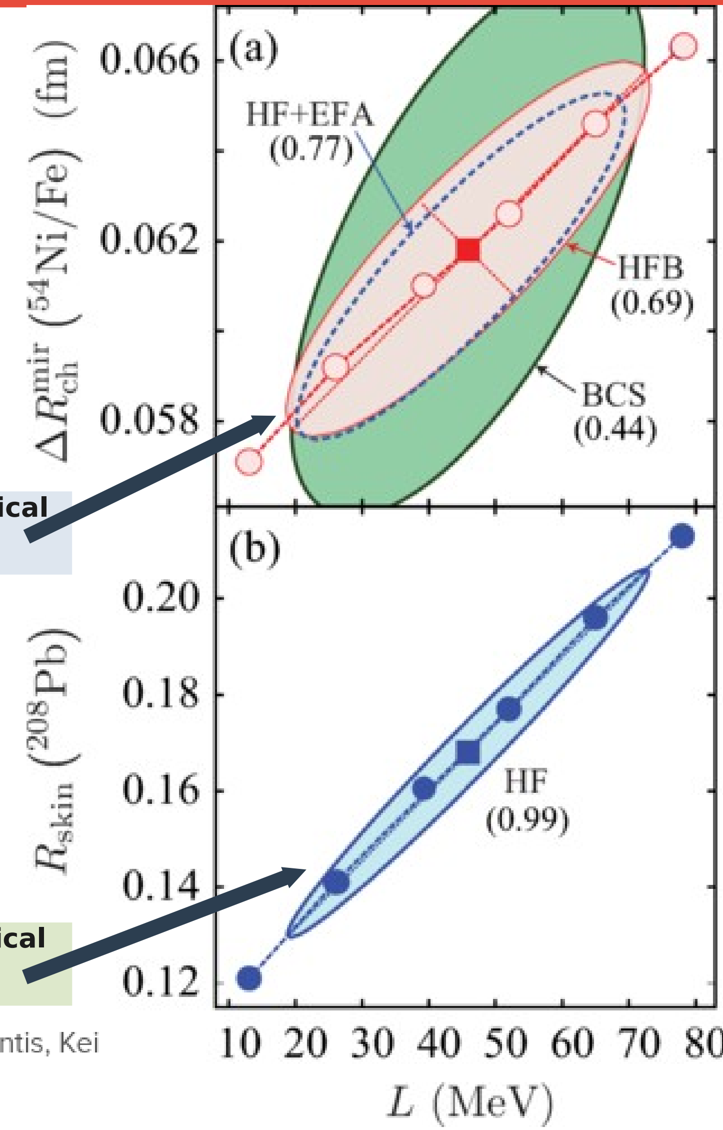
Isospin symmetry → $\Delta r_{ch} := r_{ch}(^{54}Ni) - r_{ch}(^{54}Fe) = \Delta r_{np}(^{54}Fe)$



Skyy V. Pineda, Kristian König, Dominic M. Rossi, B. Alex Brown, Anthony Incorvati, Jeremy Lantis, Kei Minamisono, Wilfried Nörtershäuser, Jorge Piekarewicz, Robert Powel, and Felix Sommer
Phys. Rev. Lett. **127**, 182503 – Published 29 October 2021

Large theoretical uncertainties

Small theoretical uncertainties



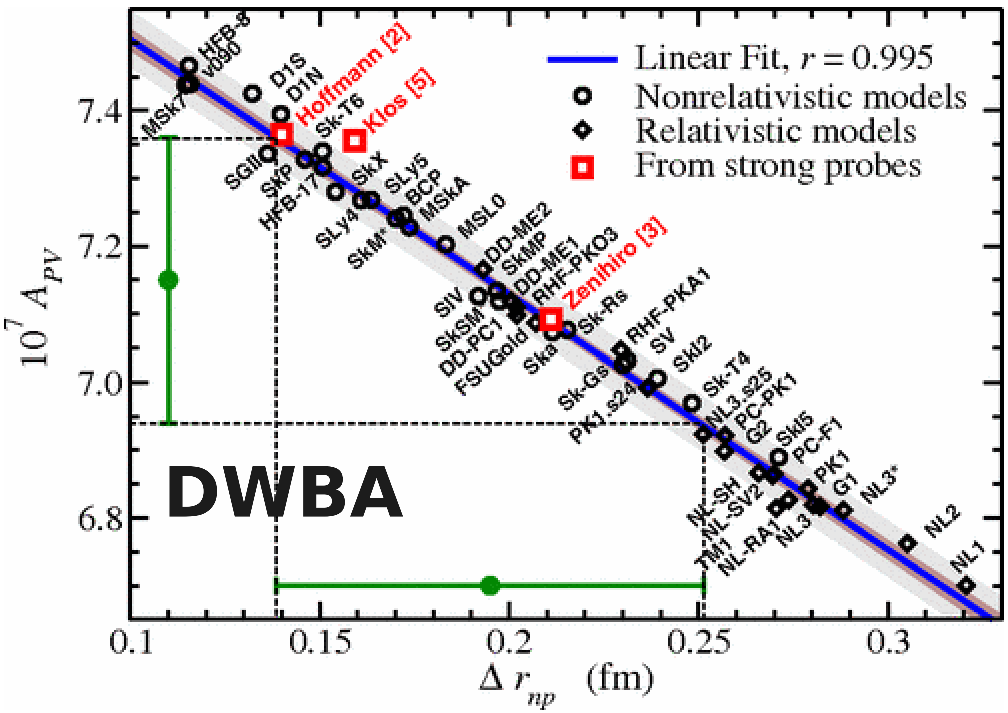
Paul-Gerhard Reinhard and Witold Nazarewicz
Phys. Rev. C **105**, L021301 – Published 3 February 2022

From Earth: Parity violating electron scattering and the neutron skin

Polarized electron-Nucleus scattering:

→ In good approximation, **the weak interaction** probes the **neutron distribution** in nuclei while **Coulomb interaction** probes the **proton distribution**

→ **Different experimental efforts @ Jlab (USA) & MAMI (Germany)**



Neutron Skin of 208Pb, Nuclear Symmetry Energy, and the Parity Radius Experiment
X. Roca-Maza, M. Centelles, X. Viñas, and M. Warda Phys. Rev. Lett. 106, 252501 (2011)

→ **Electrons** interact by **exchanging** a **γ** (couples to **p**) or a **Z_0** boson (couples to **n**)

→ **Ultra-relativistic electrons**,depending on their helicity (±), will interact with the nucleus seeing a slightly different potential: **Coulomb** ± **Weak**

$$A_{pv} = \frac{d\sigma_+/d\Omega - d\sigma_-/d\Omega}{d\sigma_+/d\Omega + d\sigma_-/d\Omega} \sim \frac{\text{Weak}}{\text{Coulomb}}$$

→ Main **unknown** is **ρ_n**

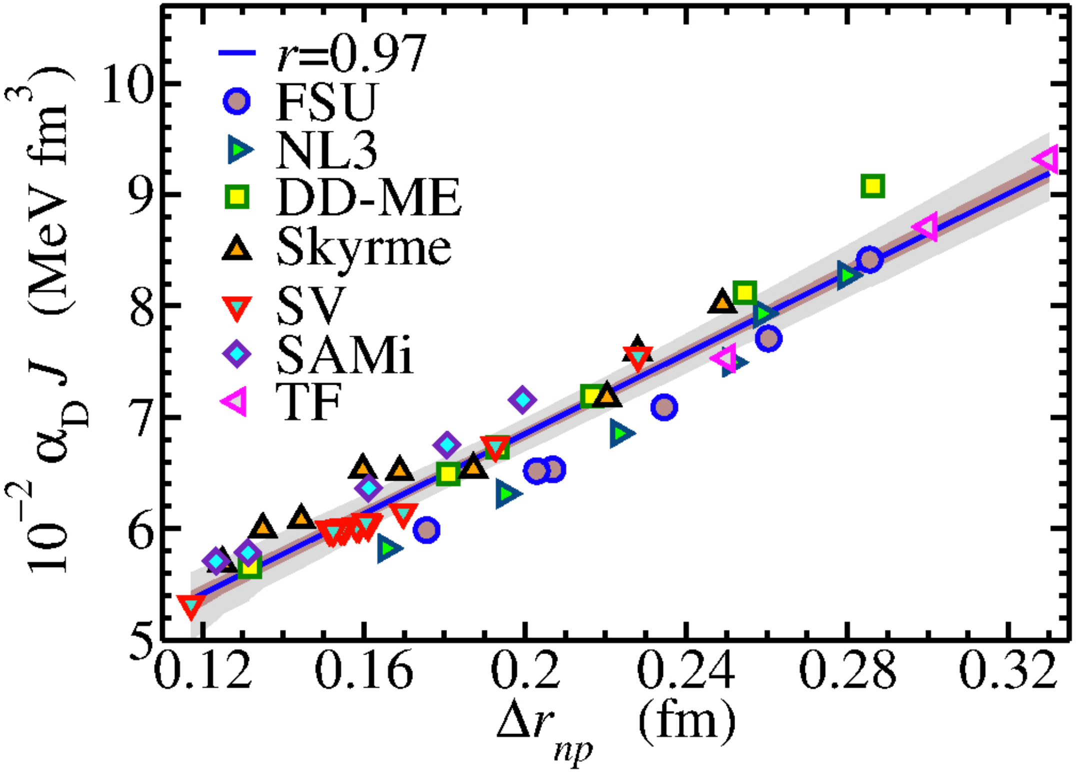
→ In **PWBA** for small momentum transfer **q**:

$$A_{pv} = \frac{G_F q^2}{4\sqrt{2}\pi\alpha}\left(1 - \frac{q^2 r_p^2}{3F_p(q)}\right)\Delta r_{np}$$

From Earth: dipole polarizability and neutron skin

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

From a macroscopic point of view **α ~ (electric dipole moment)/(external electric field)**



→ Using the **dielectric theorem**: the polarizability can be computed from the expectation value of the Hamiltonian in the constrained ground state H′=H+λD

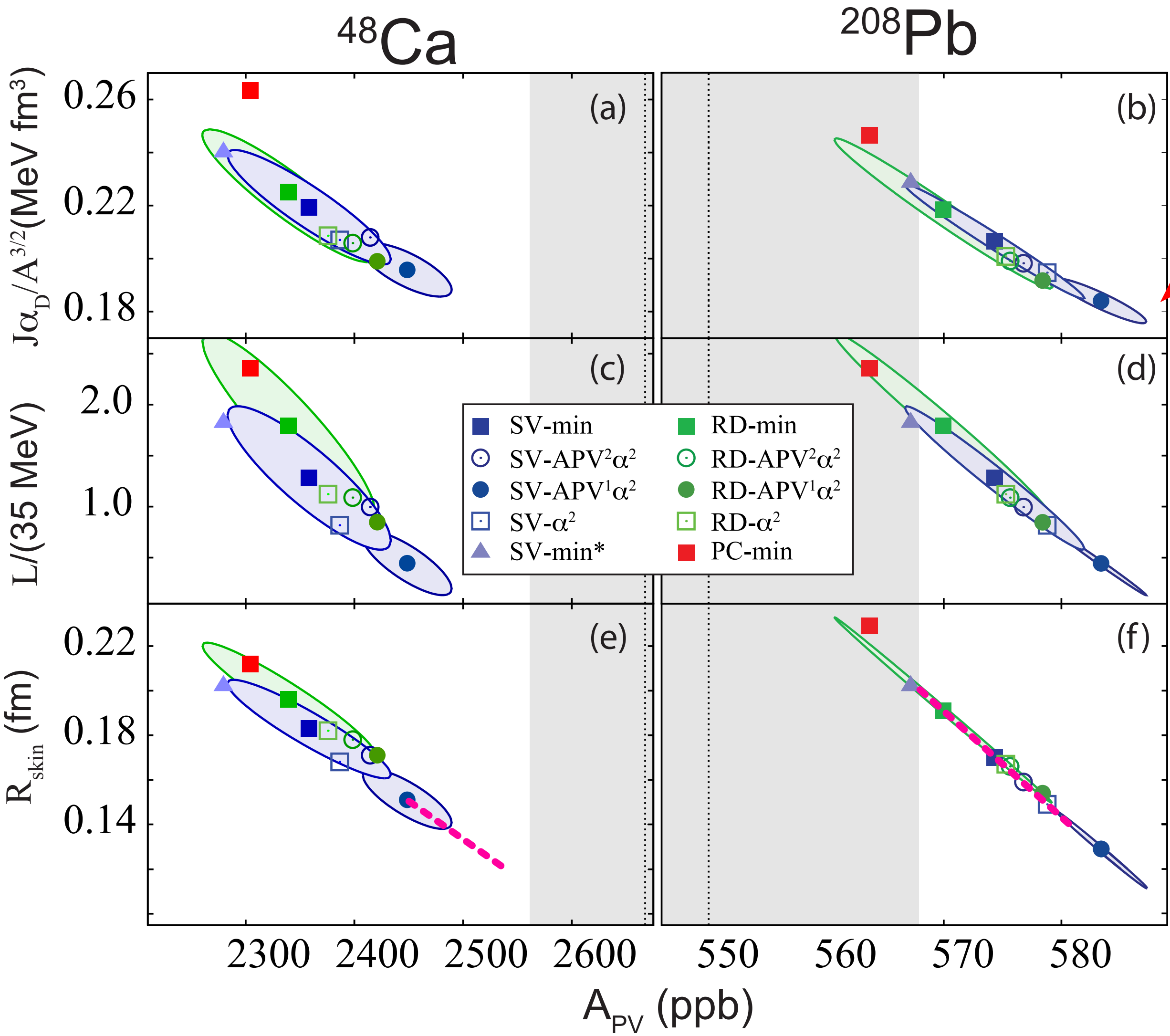
→ For guidance assuming the **Droplet model** for H, one would find:

$$\alpha_D \approx \frac{\pi e^2}{54}\frac{\langle r^2\rangle}{J}A\left(1+\frac{5}{2}\frac{\Delta r_{np}-\Delta r_{np}^{\rm surf}-\Delta r_{np}^{\rm Coul}}{\langle r^2\rangle^{1/2}(I-I_{\rm Coul})}\right)$$

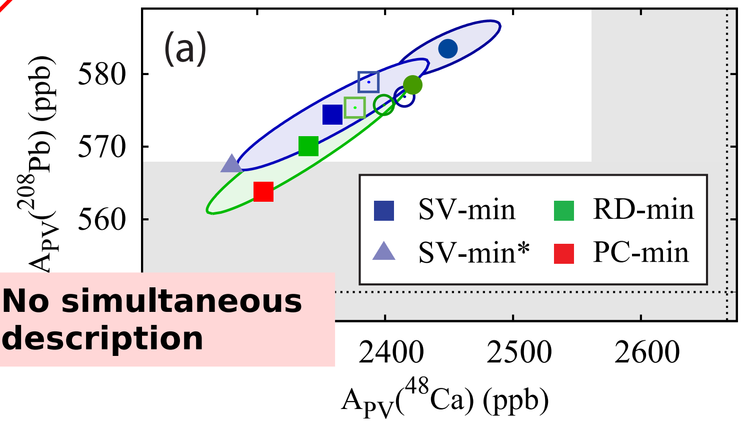
Electric dipole polarizability in 208Pb: Insights from the droplet model - X. Roca-Maza, M. Brenna, G. Colò, M. Centelles, X. Viñas, B. K. Agrawal, N. Paar, D. Vretenar, and J. Piekarewicz

Phys. Rev. C 88, 024316 (2013)

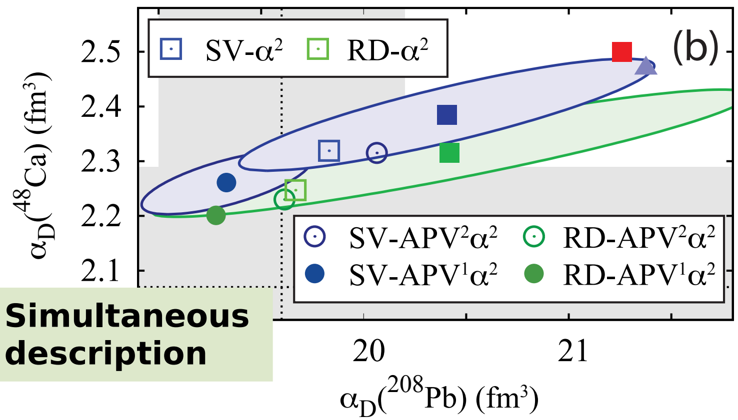
From Earth:
A_{PV} versus α_D ↔ experiment versus theory



Theoretical (**EDFs** and **ab initio**) and experimental 1σ errors overlap in ^{208}Pb but not in ^{48}Ca



No simultaneous description



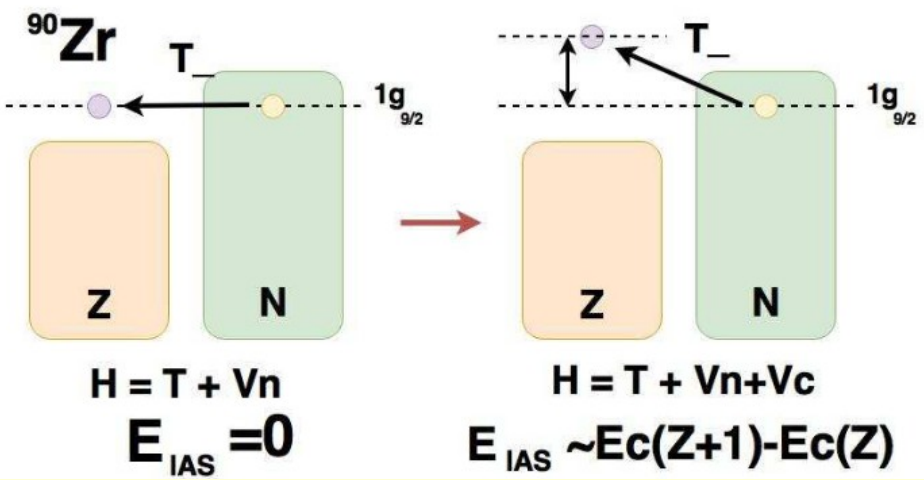
Simultaneous description

Paul-Gerhard Reinhard, Xavier Roca-Maza, and Witold Nazarewicz arXiv:2206.03134 (2022)

Magenta dashed lines from Δr_{np} in G. Hagen et al. Nature Physics 12, 186–190 (2016) and H. Bu et al. Nature Physics (2022)

From Earth: Isobaric Analog State

$$F = T_\pm = \sum_i^A t_\pm(i)$$



→ non-energy weighted sum rule:

$$m_0^- - m_0^+ = \langle 0|T_+T_-|0\rangle - \langle 0|T_-T_+|0\rangle$$
$$= \langle 0|[T_+,T_-]|0\rangle = \langle 0|2T_z|0\rangle$$
$$= N - Z$$

→ energy weighted sum rule:

$$m_1 = \sum_\nu (E_\nu - E_0)|\langle \nu|F|0\rangle|^2 = \langle 0|T_+[\mathcal{H},T_-]|0\rangle$$

[H,T₋] different from zero only if **H** contains terms that **breaks isospin invariance**

→ Hence, the **centroid energy** m_1/m_0 (neglecting isospin mixing, i.e., $\langle 0|T_-T_+|0\rangle \approx 0$):

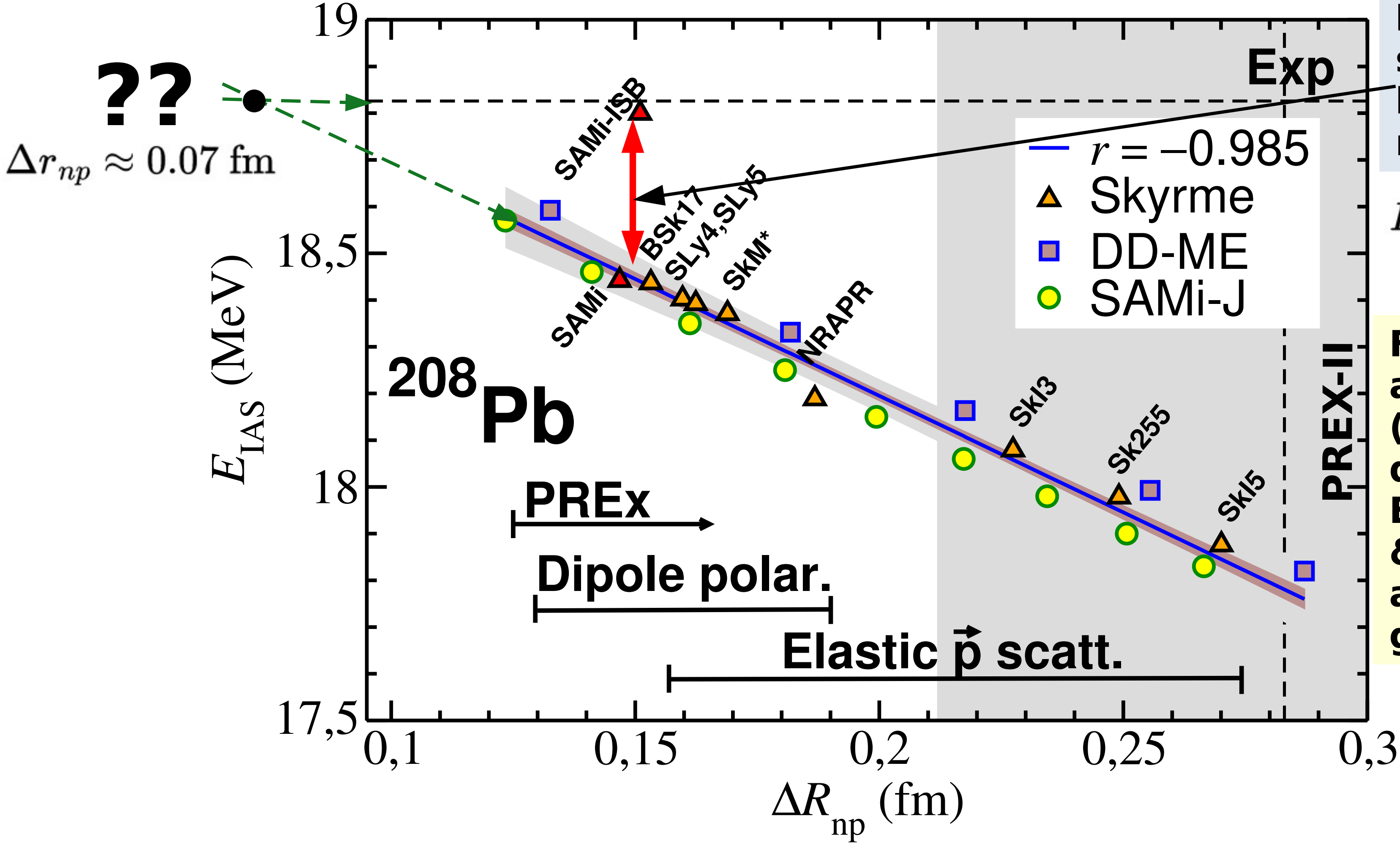
$$E_{\rm IAS} = \frac{\langle 0|T_+[\mathcal{H},T_-]|0\rangle}{\langle 0|T_+T_-|0\rangle} = \frac{1}{N-Z}\langle 0|T_+[\mathcal{H},T_-]|0\rangle$$

→ Assuming a simple model: **indepenent particle** model with only **Coulomb breaking isospin symmetry** (neglect exchange effects)

$$E_{\rm IAS}^{\rm C,direct} = \frac{1}{N-Z}\int \left[\rho_n(\vec r) - \rho_p(\vec r)\right] U_{\rm C}^{\rm direct}(\vec r)d\vec r$$

$$E_{\rm IAS} \approx E_{\rm IAS}^{\rm C,direct}$$
$$\approx \frac{6}{5}\frac{Ze^2}{R_p}\left(1 - \frac{1}{2}\frac{N}{N-Z}\frac{R_n - R_p}{R_p}\right)$$
$$\approx \frac{6}{5}\frac{Ze^2}{r_0A^{1/3}}\left(1 - \sqrt{\frac{5}{12}}\frac{N}{N-Z}\frac{\Delta R_{\rm np}}{r_0A^{1/3}}\right)$$

From Earth:
Isobaric Analog State, ISB and Δr_{np}



Isospin symmetry breaking in the nuclear force

$$E_{\mathrm{IAS}} \sim \langle T_+[\mathcal{H}, T_-]\rangle$$

Further studies are needed (uncertainty quantification; Extended EDFs & ab initio guidance)

X. Roca-Maza, G. Colò, and H. Sagawa
Phys. Rev. Lett. **120**, 202501 – Published 18 May 2018

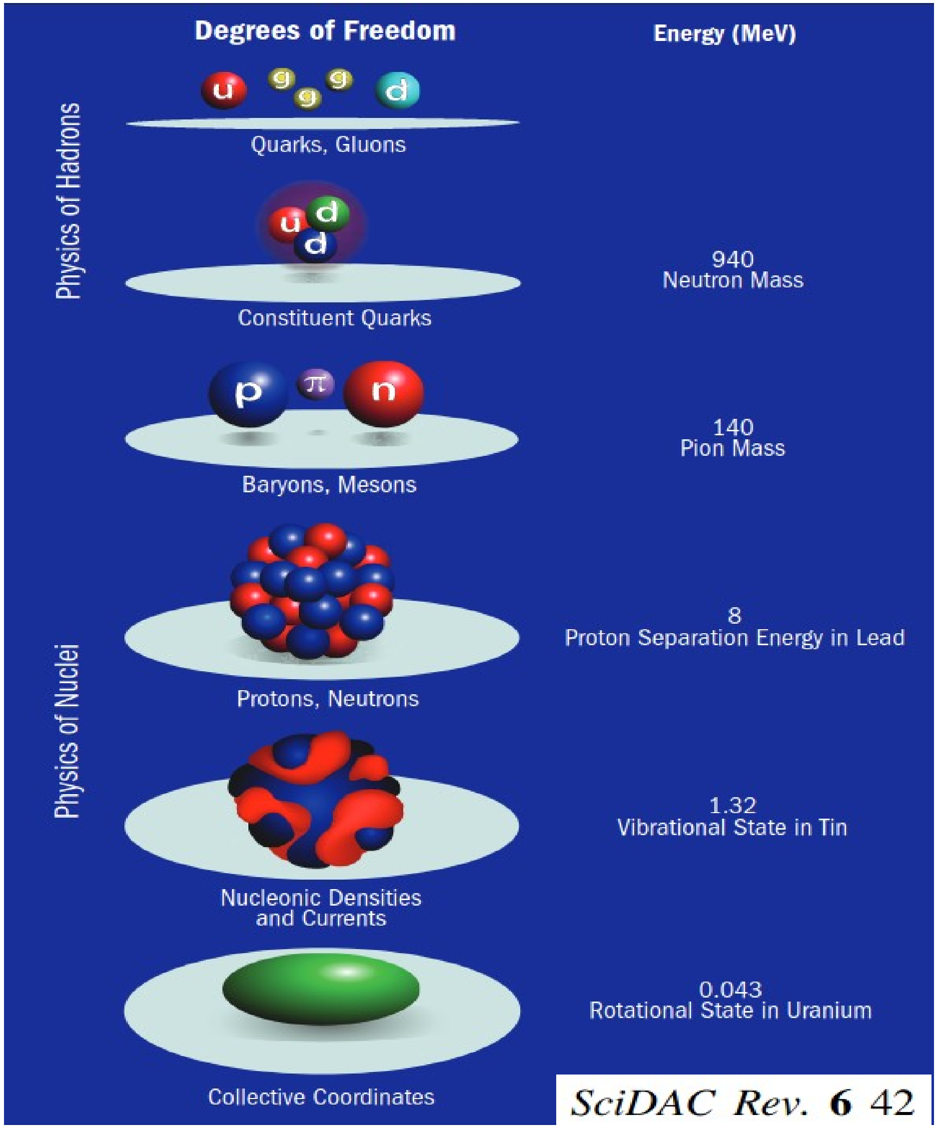
How are we dealing with the nuclear many-body problem?

→ Ab inito methods

→ Density Functional Theory

→ …

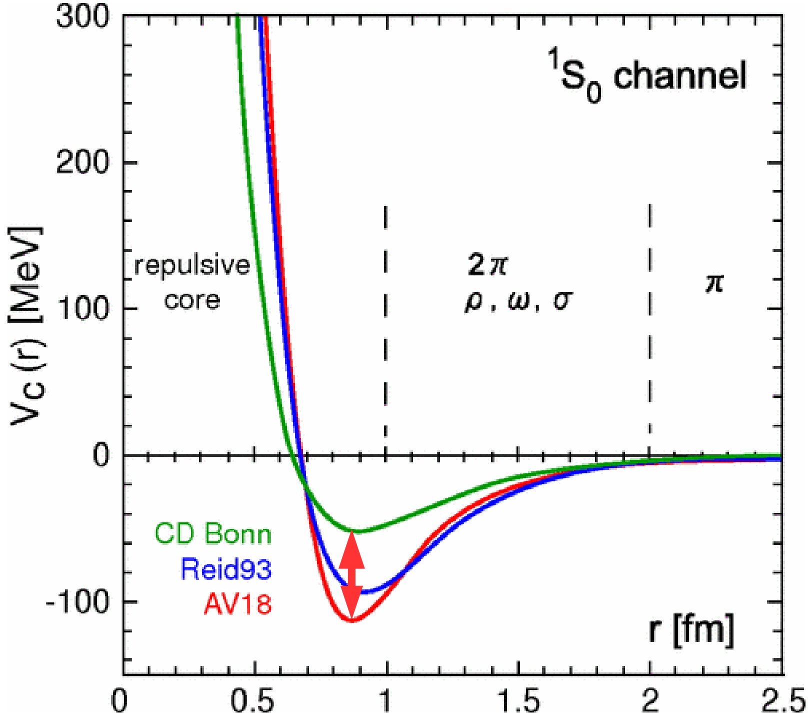
(brief discussion)



Nuclear Many-Body Problem:
Nuclear interaction

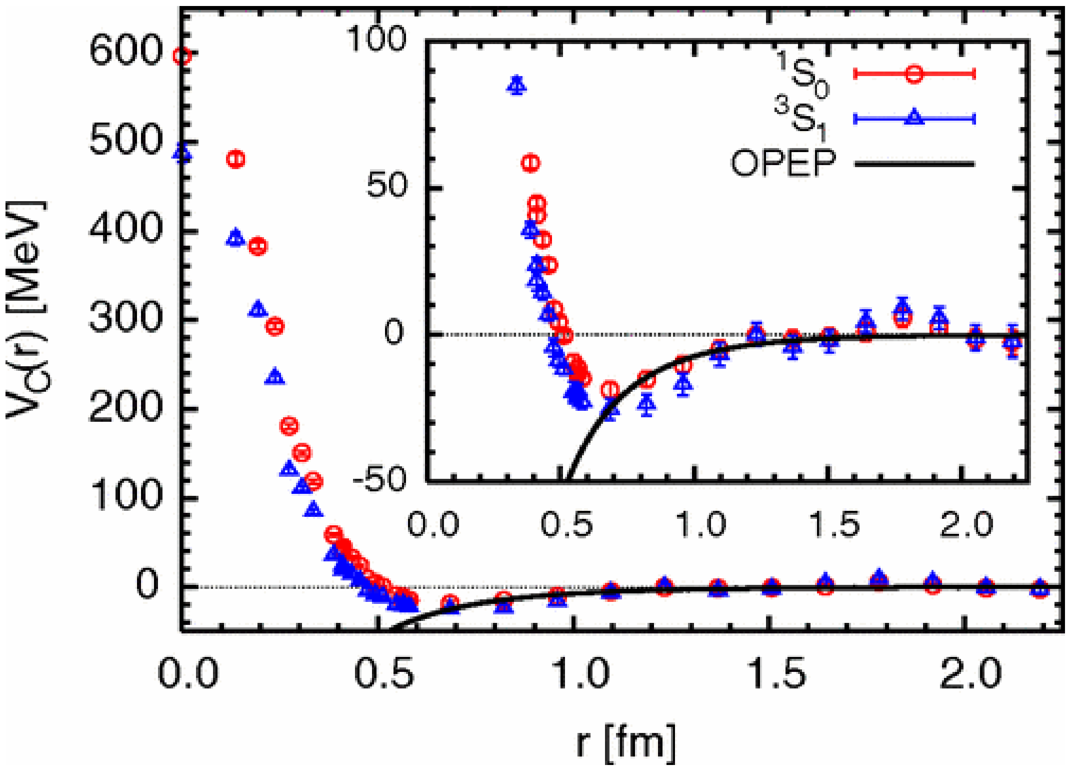
Underlying interaction: the “so called” **residual strong interaction** = **nuclear force** has **not** been **derived yet** (with the precision needed) from first principles as **QCD** is **non-perturbative** at the **low-energies** (~ below $m_\pi \approx 140$ MeV) relevant for the description of nuclei.

Phenomenological



Nuclear Force from Lattice QCD - N. Ishii, S. Aoki, and T. Hatsuda
Phys. Rev. Lett. 99, 022001 (2007)

Lattice QCD ($m_\pi/m_\rho \sim 0.6$)



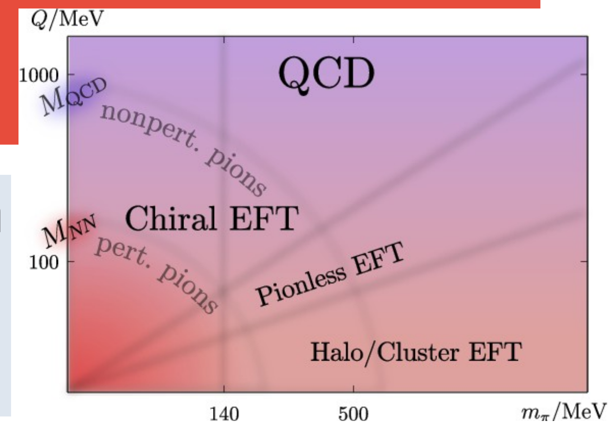
$\Delta V(r_{min}) \approx 60$ MeV !! →
different saturation energy

Similar to CD-Bonn $V(r_{min}) \approx -40$ MeV but postion of the **minimum diff. → diff. saturation density** ($m_\pi/m_\rho \sim 0.6$ scaled to physical value $140/775 \approx 0.18$)

Chiral effective field theory

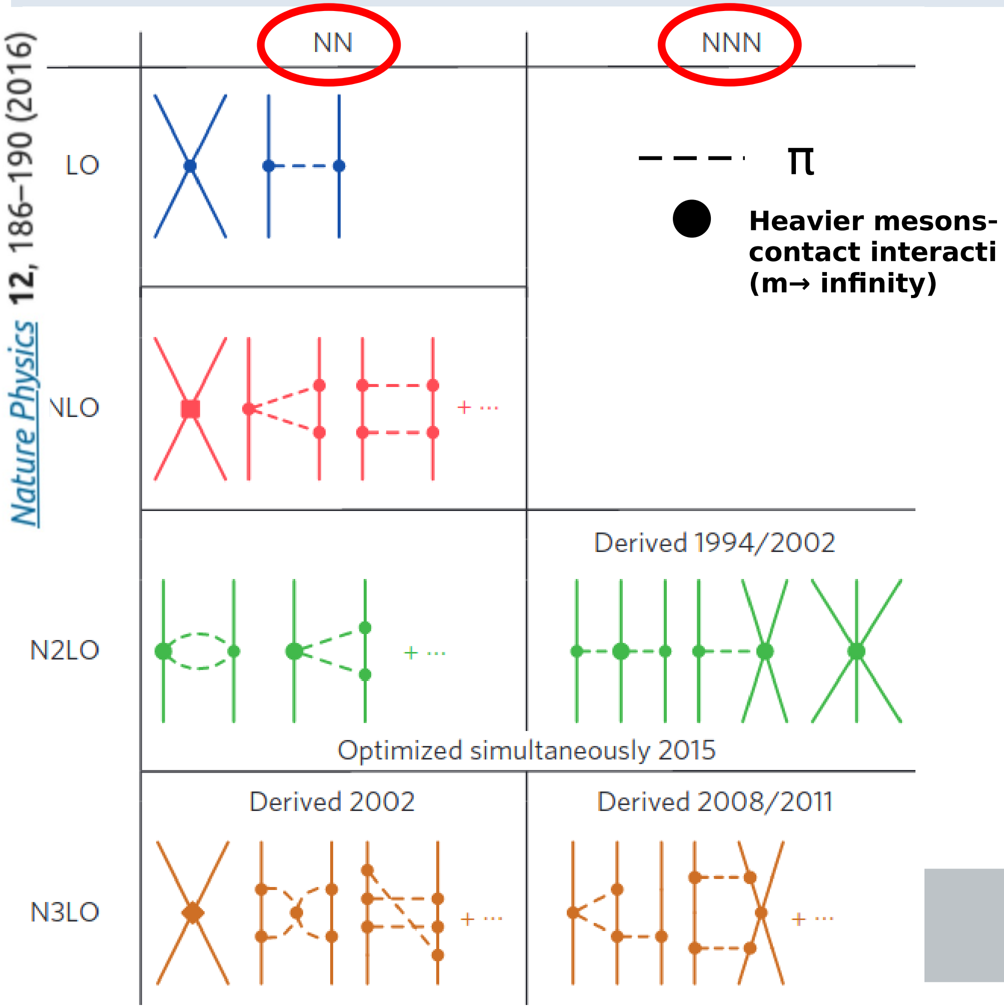
Building the interaction from QCD

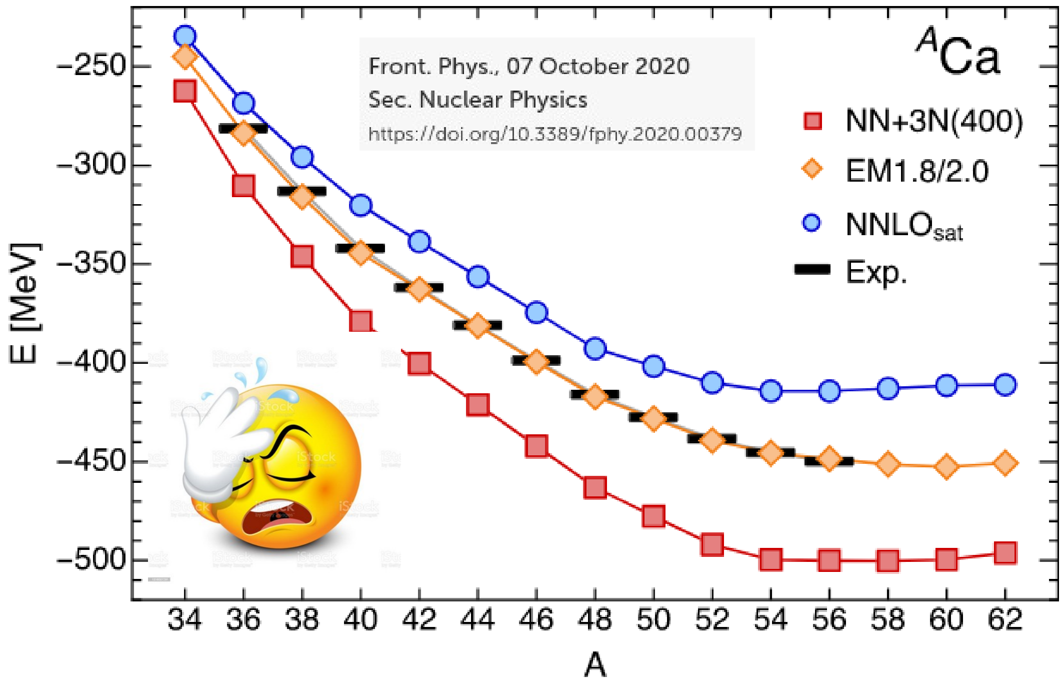
H.-W. Hammer, Sebastian König, and U. van Kolck
Rev. Mod. Phys. **92**, 025004 – Published 23 June 2020



Chiral EFT for nuclei: pions + nucleons with breaking scale Λ~500 MeV

[there exist also other possibilities such as pionless Chiral EFT or pions+Delta+nucleons]





Determination of the **EFT** parameters is **not unique** → different Hamiltonians that agree with experimental data on NN scattering and 3N data **do not agree** on the prediction of many body data (e.g. Ca isotopes Z=20)

Many-body methods:

Nuclei are made from few to hundreds of nucleons!

Once the **Hamiltonian** has been built, a **many-body method** is needed to **calculate nuclei**

Main many-body approaches seem to agree well if the same Hamiltonian is assumed:

→ No core shell model (**NCSM**)

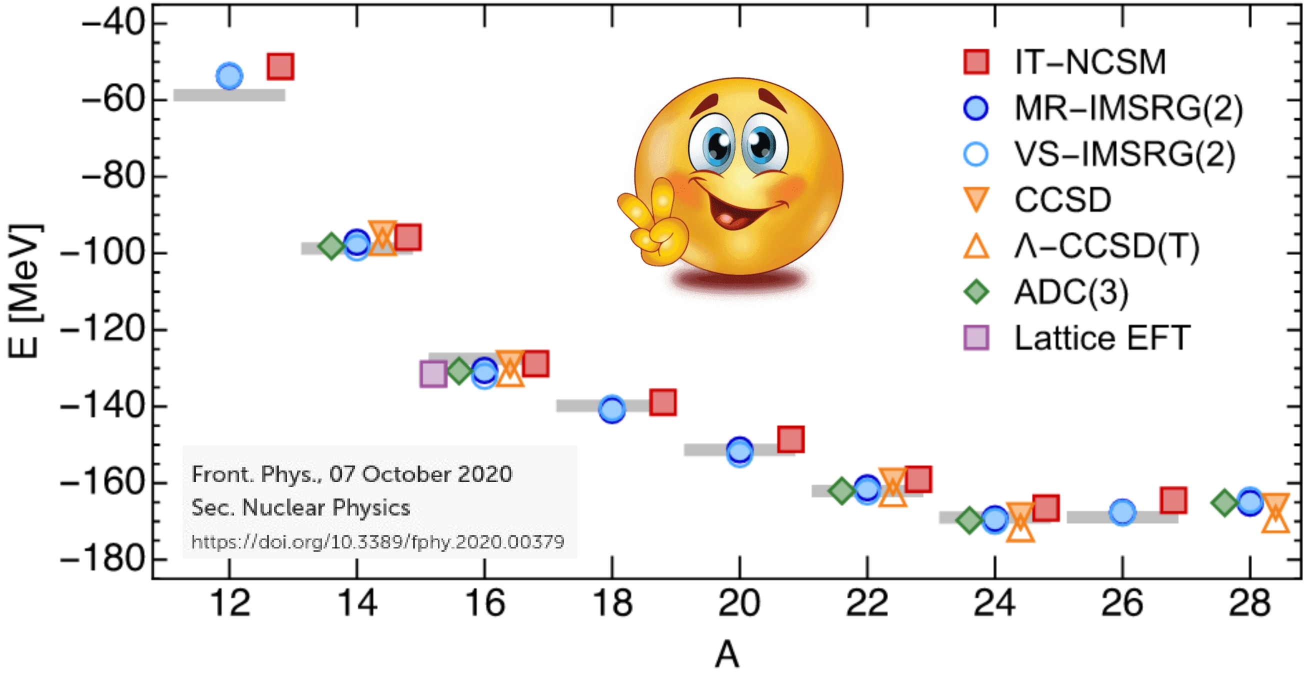
→ In medium similarity renormalization group (**IMSRG**)

→ Coupled cluster (**CC**)

→ Algebraic Diagrammatic Construction (**ADC** for Self-Consistent Green's Functions)

→ Quantum Monte Carlo (**QMC**)

→ Many-body perturbation theory (**MBPT**)



Ground-state energies of the **oxygen (Z=8)** isotopes for **various many-body approaches**, using the **same chiral NN+3N(400) Hamiltonian**. Gray bars indicate experimental data.

DENSITY FUNCTIONAL THEORY
Hohenberg-Kohn theorems
P.Hohenberg, W. Kohn, Phys. Rev. 136, B864 (1964)

→ Assuming a system of **interacting fermions** in a confining **external potential**, there exist a **universal** functional **F[ρ]** of the fermion density **ρ**:

$$E[\rho] = \langle \Psi | T + V + V_{\text{ext}} | \Psi \rangle = F[\rho] + \int V_{\text{ext}}(r)\rho(r)d\vec{r}$$

→ and it can be shown that

$$\min_{\Psi} \langle \Psi | T + V + V_{\text{ext}} | \Psi \rangle = \min_{\rho} E[\rho]$$

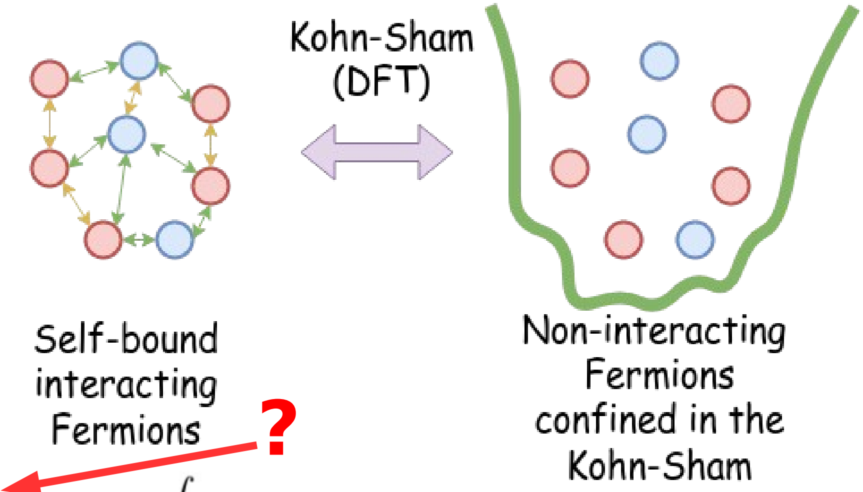
so **E[ρ]** has a **minimum** for the **exact ground-state density** where it assumes the **exact energy** as a value.

Kohn-Sham realization
$F[\rho] \rightarrow T_{\text{non-int.}}[\rho] + V_{KS}[\rho]$

In nuclei no need of external confining potential

For **any interacting system**, there exists a **<u>local</u> single-particle potential $V_{ks}(r)$**, such that the **exact ground-state** density of the **interacting system** equals the **ground-state density** of the **auxiliary non-interacting system**:

$$\rho_{\text{exact}}(\vec{r}) = \rho_{\text{KS}}(\vec{r}) = \sum_{i=1}^{A} |\phi(\vec{r})|^2$$



$$F[\rho] = \int d^3r \; f(\mathbf{r}, \rho, \nabla\rho, \ldots).$$

where φ are single-particle orbitals and the total wave-function correspond to a Slater determinant. The **E[ρ] is unique**

$$E[\rho] = T[\rho] + \int V_{\text{KS}}(\vec{r})\rho(\vec{r})d\vec{r}$$

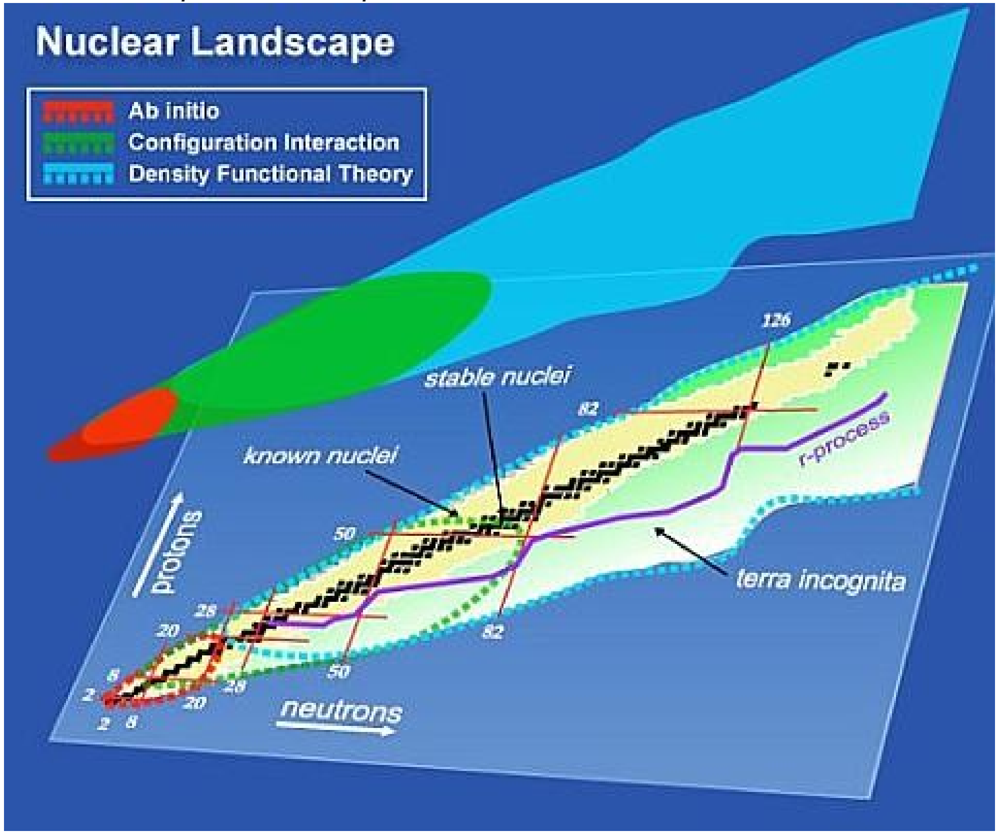
where **T[ρ]** is the **kinetic energy of the non-interacting system** and for which the variational equation

$$0 = \frac{\delta E[\rho]}{\delta \rho} = \frac{\delta T[\rho]}{\delta \rho} + V_{\text{KS}}$$

yields to the **exact ground state density and energy**

Advantadges and disadvantages of DFT

UNEDF http://unedf.mps.ohio-state.edu/



→ **ADVANTAGES OF DFT:**

- **exact theory** that can be applied to the **whole nuclear chart**
- **many-body** problem mapped onto a **one-body** problem without the need of explicitly involving inter-nucleon interactions!!! (computational cost and interpretation of observables in terms of single-particle properties)
- **HK generalised in (almost all) possible ways**: time dependence, degenerate ground-state, magnetic systems, finite T, relativistic case ...
- **any one body observable is within the DFT framework** (this includes also some sum rules related to nuclear excitations)

→ **DISADVANTAGES OF DFT:**

- various **proofs of HK theorems** do **not** give any clue on **how to build the functional**.
- **no** direct **connection** with **realistic NN or NNN interaction** if current approaches to EDF are not improved (some attempts already exist)
- **no systematic** way of **improvement** (evaluate syst. Errors) so far.

Avenues to improve EDFs? (@Milano)

→ We are working in two main directions:

A) **Inverse Kohn-Sham (IKS) problem**: determine the V_{KS} and then E[ρ,…] from experimental and/or ab initio density distributions. With different **Bachelor and Master Thesis** students

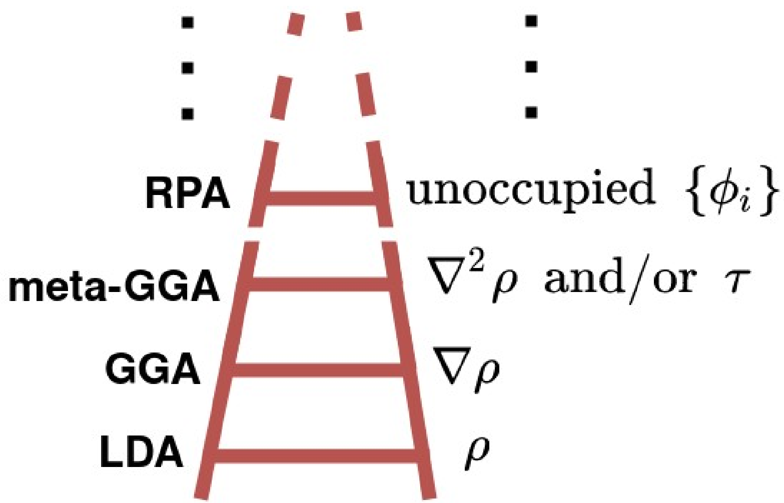
First step in the nuclear inverse Kohn-Sham problem: From densities to potentials

G. Accorto, P. Brandolini, F. Marino, A. Porro, A. Scalesi, G. Colò, X. Roca-Maza, and E. Vigezzi
Phys. Rev. C **101**, 024315 – Published 28 February 2020

Complete solution to the inverse Kohn-Sham problem: From the density to the energy

A. Liardi, F. Marino, G. Colò, X. Roca-Maza, and E. Vigezzi
Phys. Rev. C **105**, 034309 – Published 7 March 2022

B) **Mimic** strategy (**Jacob's Ladder**) in **many-electron systems** to systematically improve nuclear EDFs without using *phenomenological* parameters (as long as possible). With one **PhD** (Francesco Marino) and hopefully one postdoc in the future.

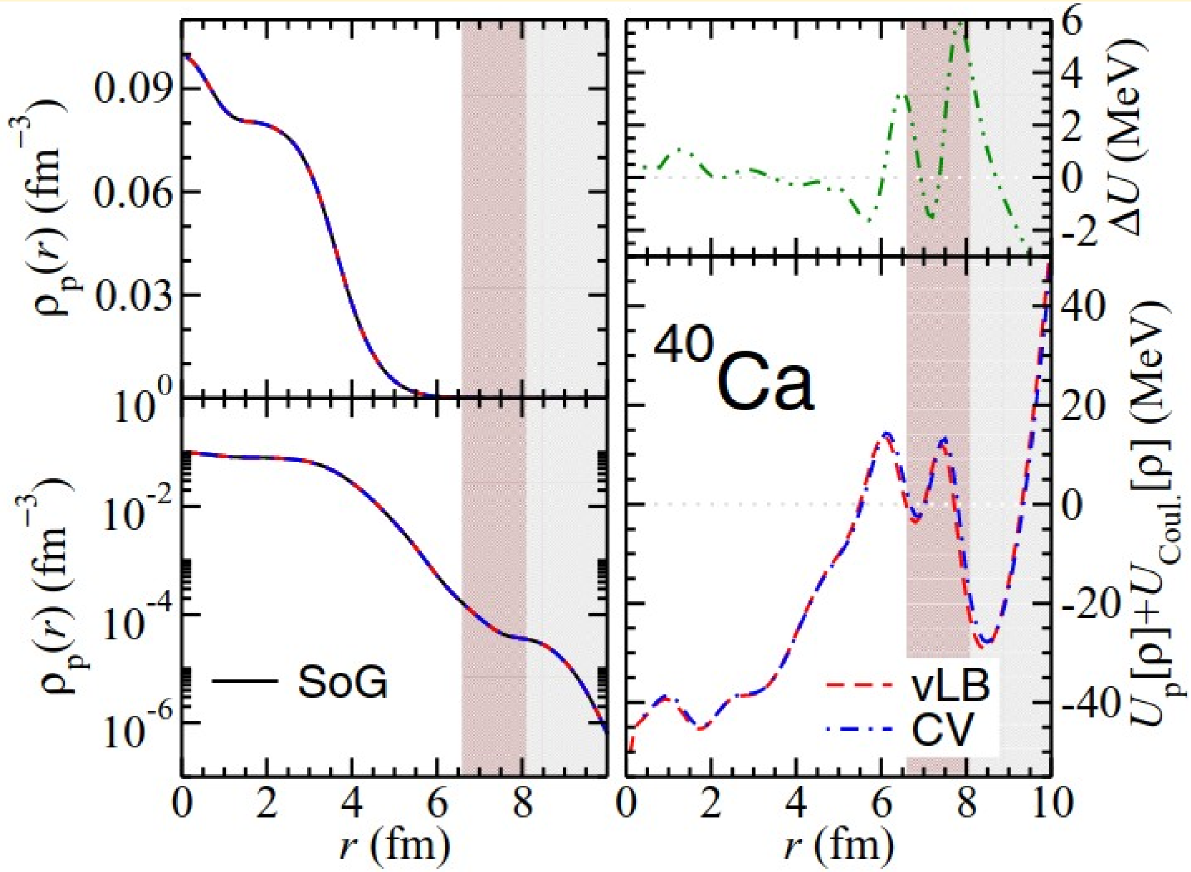


Nuclear energy density functionals grounded in *ab initio* calculations

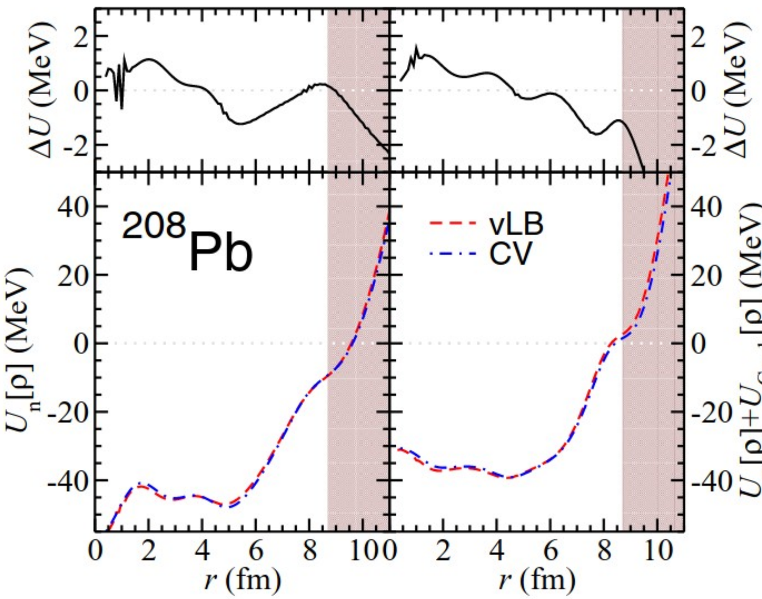
F. Marino, C. Barbieri, A. Carbone, G. Colò, A. Lovato, F. Pederiva, X. Roca-Maza, and E. Vigezzi
Phys. Rev. C **104**, 024315 – Published 9 August 2021

Inverse Kohn Sham potential form experimental densities (examples)

CV: Minimization of the **non-interacting kinetic energy** with the **constraint** that the auciliar orbitals are **orthonormal** and that the density must coincide with the **target density** (vLB is an alternative method for inversion)



Experimental densities parametrized as sum of gaussians[1] (GoS)



[1] H. D. Vries, C. D. Jager, and C. D. Vries, At. Data Nucl. Data Tables 36, 495 (1987)

Ab initio EDF: first two steps

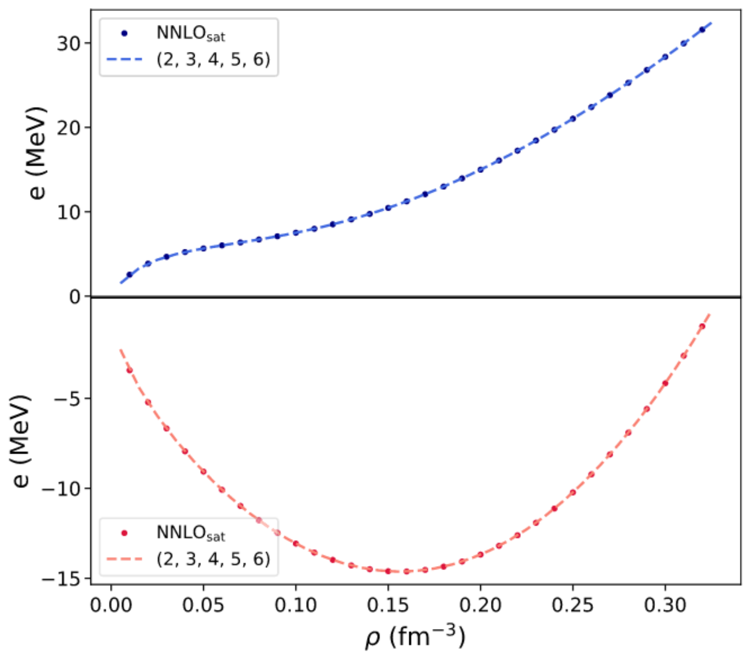
1) mapping the EoS → LDA
2) linear response (χ) → GGA

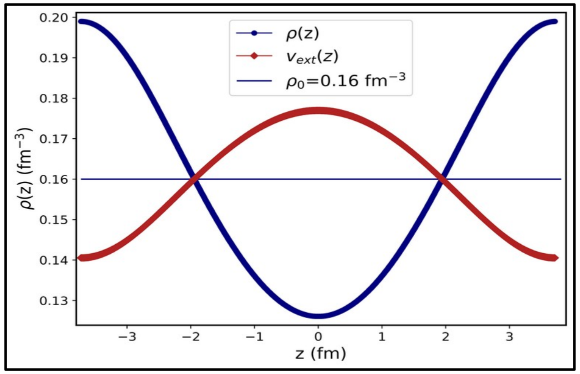
1) Checking optimal density dependencies in EDFs (exponents and coefficients) that **reproduce ab initio EoS.**

2) Solve the **Schrodinger** equation of a **finite** number of **particles** under the **action of an external potential** (v cos(qr)) **in a box** with **periodic boundary conditions** in **ab anitio** and **EDF**.

$$v(\rho,\beta) = \sum_{\gamma=1/3\ldots6/3} c_\gamma(\beta)\rho^\gamma = \sum_{\gamma=1/3\ldots6/3} [c_{\gamma,0} + c_{\gamma,1}\beta^2]\rho^\gamma$$

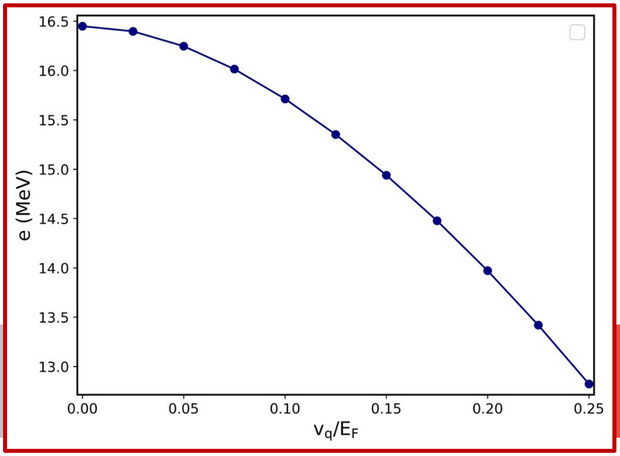
$$\rho(\mathbf{x}) = \rho_0 + 2v_{\mathbf{q}}\chi_{\mathbf{q}}\cos(\mathbf{q}\cdot\mathbf{x})$$





Fix gradient terms of the **EDF** from **ab initio** results of energy variation (v,q).

$$\frac{E[v]}{N} - \frac{E_0}{N} = \frac{v_q^2}{\rho_0}\chi(q)$$



Main collaborators:

→ **Students:**

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→ Gianluca **Colò** & Enrico **Vigezzi** (University of Milan)

→ Hiroyuki **Sagawa** (University of Aizu & RIKEN)

→ Shihang **Shen** (Forschungszentrum Jülich)

→ Xavier **Vinyes** & Mario **Centelles** (University of Barcelona)

→ Jorge **Piekarewicz** (Florida State University)

→ Nils **Paar** (University of Zagreb)

→ P.-G. **Reinhard** (University of Erlangen-Nürnberg)

→ Misha **Gorchtein** & Oleksandr **Koshchii** (Johannes Gutenberg-Universität)

→ Chuck **Horowitz** (Indiana University)

→ Haozhao **Liang** (University of Tokyo)

→ Witold **Nazarewicz** (FRIB and Michigan State University)