# Energy functionals constrained by ab initio nuclear matter calculations


## Francesco Marino


**Connections between cold atoms and nuclear matter: From low to high energies**

**ECT* (Trento)**


**Università di Milano and INFN**

# Introduction

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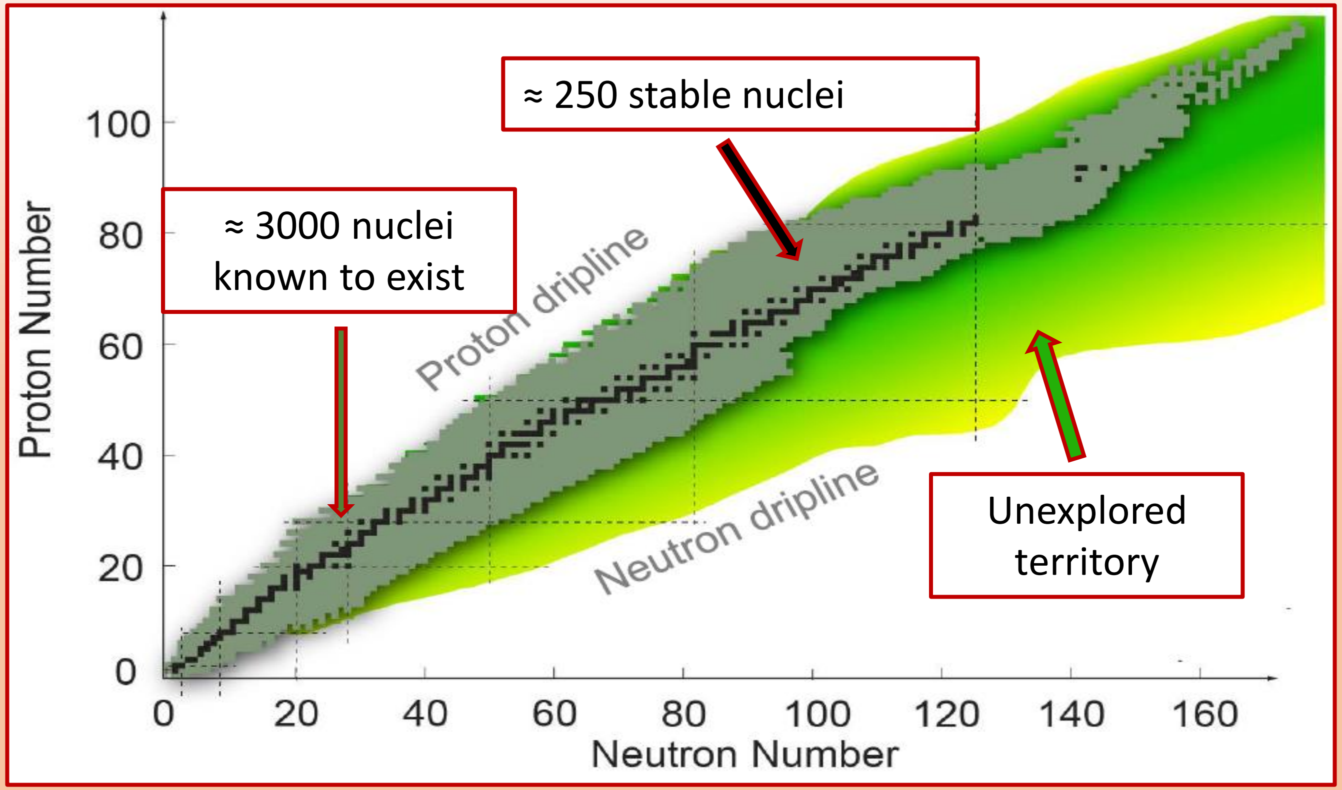
The **nucleus** is a complex interacting quantum many-body system



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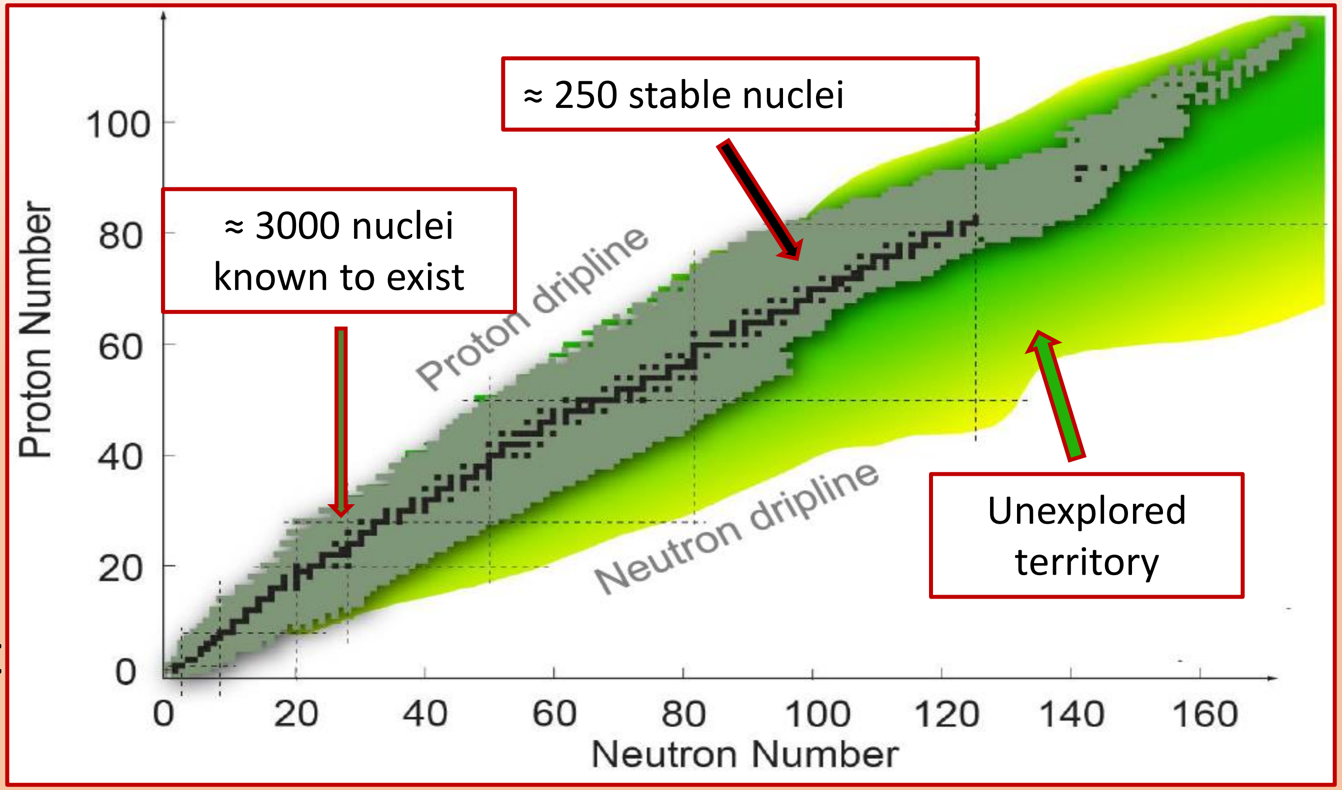


**Open questions**

- What are the **limits** of the nuclear chart (driplines)?
- Can we understand **nucleosynthesis**?
- Can we devise a **unified theoretical model**?

  …

**Theory**

↕

**Experiment**

# *Ab initio*

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Front. Phys. **8**, 00379 (2020)

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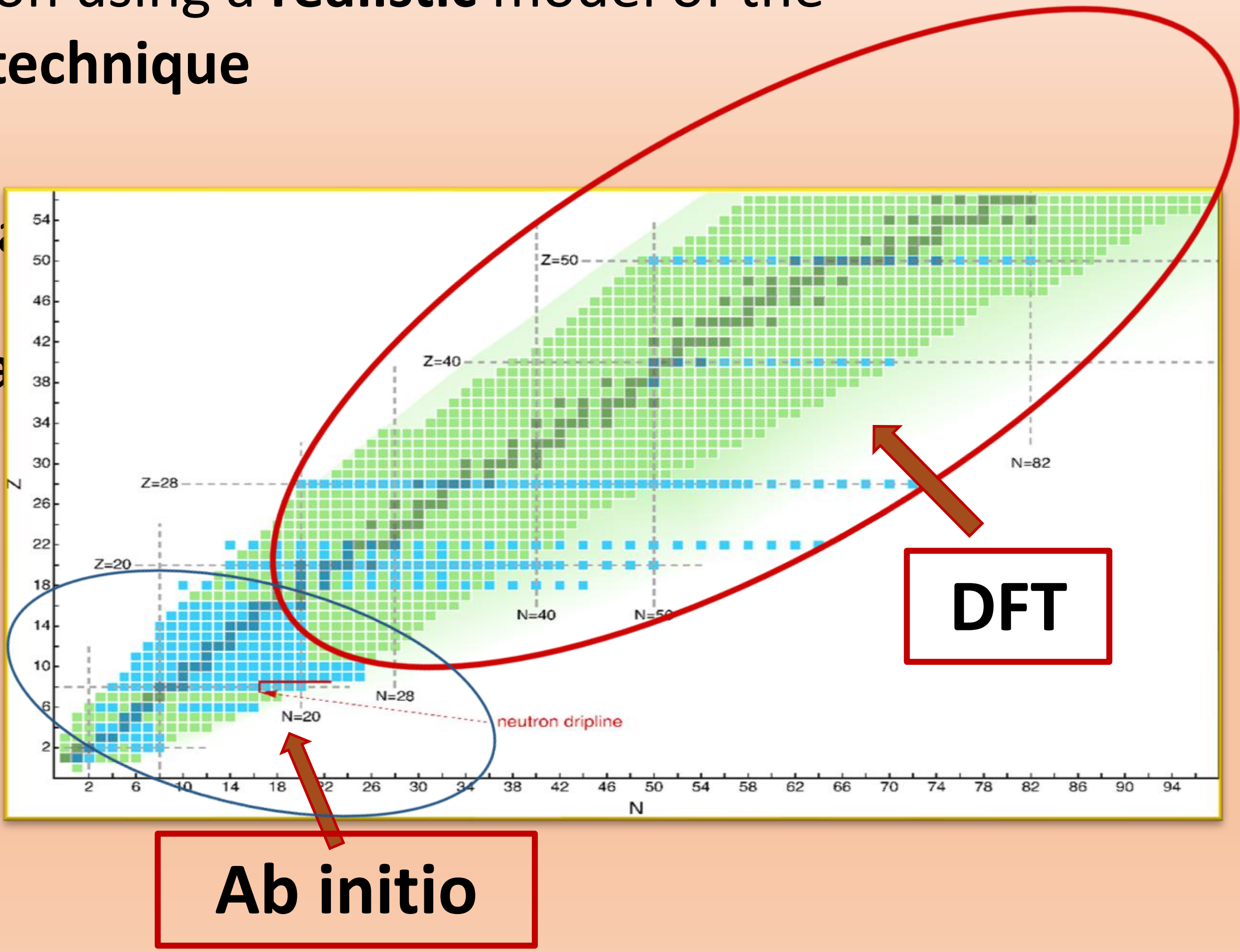


At the moment, *ab initio* theory is viable only for relatively **small systems**

But it is rapidly advancing.

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# Nuclear density functional theory 1

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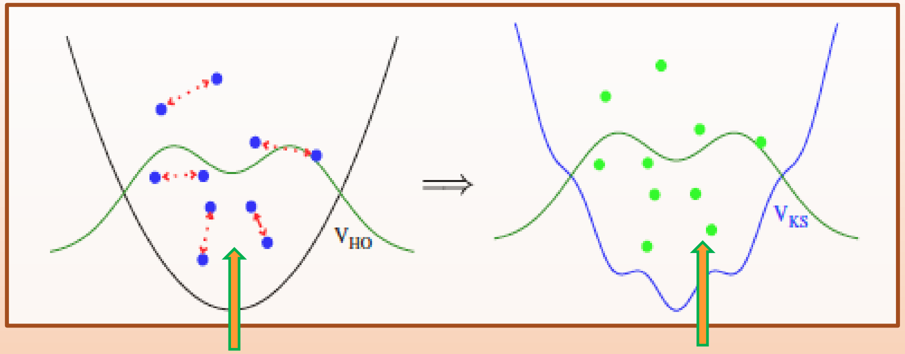


Interacting

Non-interacting

The key object in DFT is the **energy density functional** (EDF) $E[\rho]$

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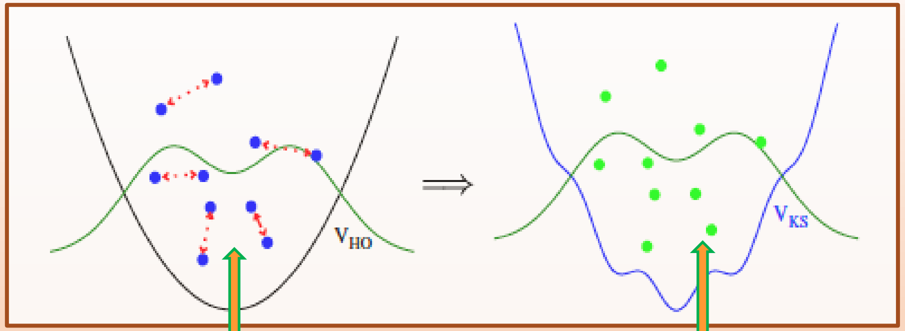


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$$E = \int d\boldsymbol{x} \left[ \frac{\hbar^2}{2m}\tau + \sum_{\gamma} c_\gamma(\beta)\rho_0^{\gamma+1} + \sum_{t=0,1} C_t^{\tau}\rho_t\tau_t + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\nabla J}\rho_t\nabla\cdot\boldsymbol{J}_t \right]$$

Kinetic — Density-dependent — Effective mass — Gradient — Spin-orbit

$\rho$: number density
$\tau$: kinetic energy density
**J**: spin-orbit density
$\beta = \rho_1/\rho_0$: isospin asymmetry

$t = 0$: isoscalar channel $\quad \rho_0 = \rho_n + \rho_p$

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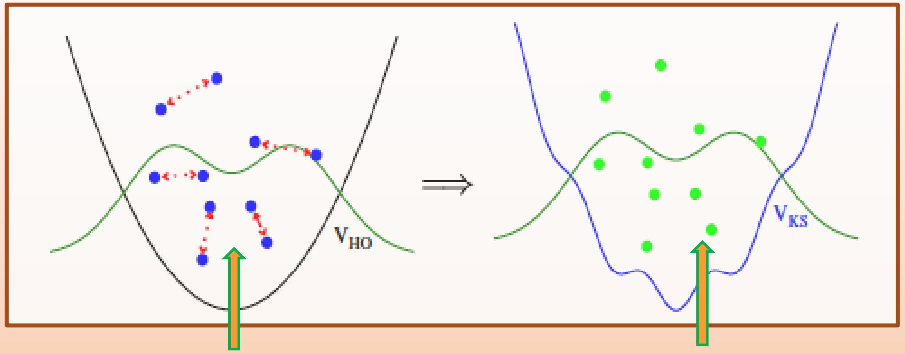


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The **ground state** is determined by $\delta E = 0$ which yields the **self-consistent** single-particle equations: $h[\rho]\phi_j(\boldsymbol{x}) = \epsilon_j\, \phi_j(\boldsymbol{x})$

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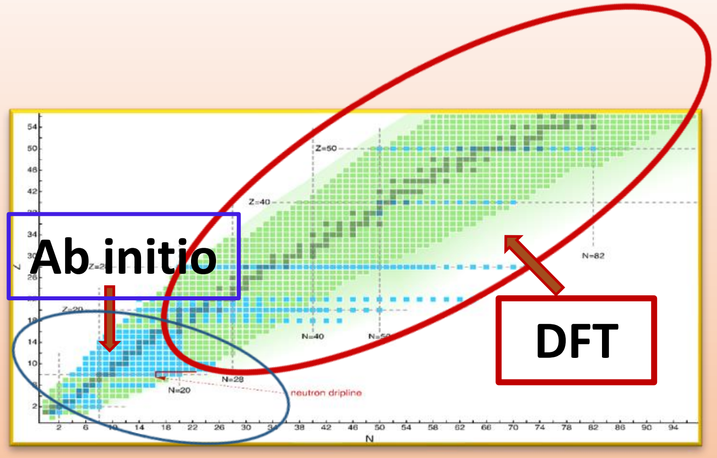
- Applications: ground state, collective excitations, neutron stars…
- A good **overall accuracy** is achieved




Adv. Phys.-X **5,** 1740061 (2020)

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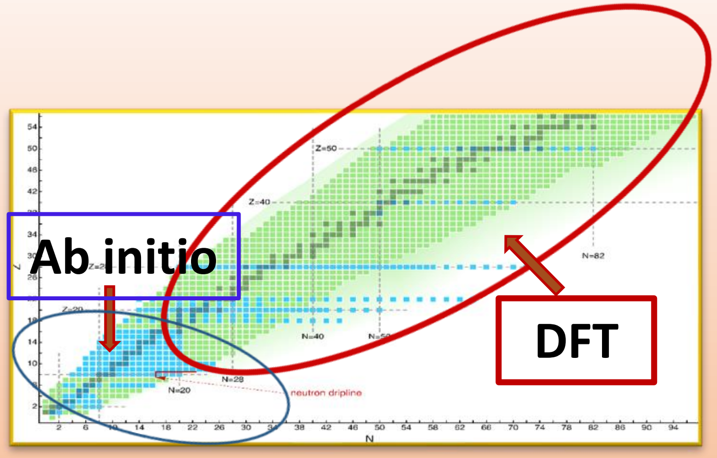


DFT is in principle an **exact** theory, but the EDF is known only **approximately.**

Current nuclear EDFs have an **empirical** character:
A functional form is chosen based on symmetries and heuristic arguments and the parameters (about 10-15) are **fitted on experimental data**

Nuclei close to the **stability valley** are well reproduced

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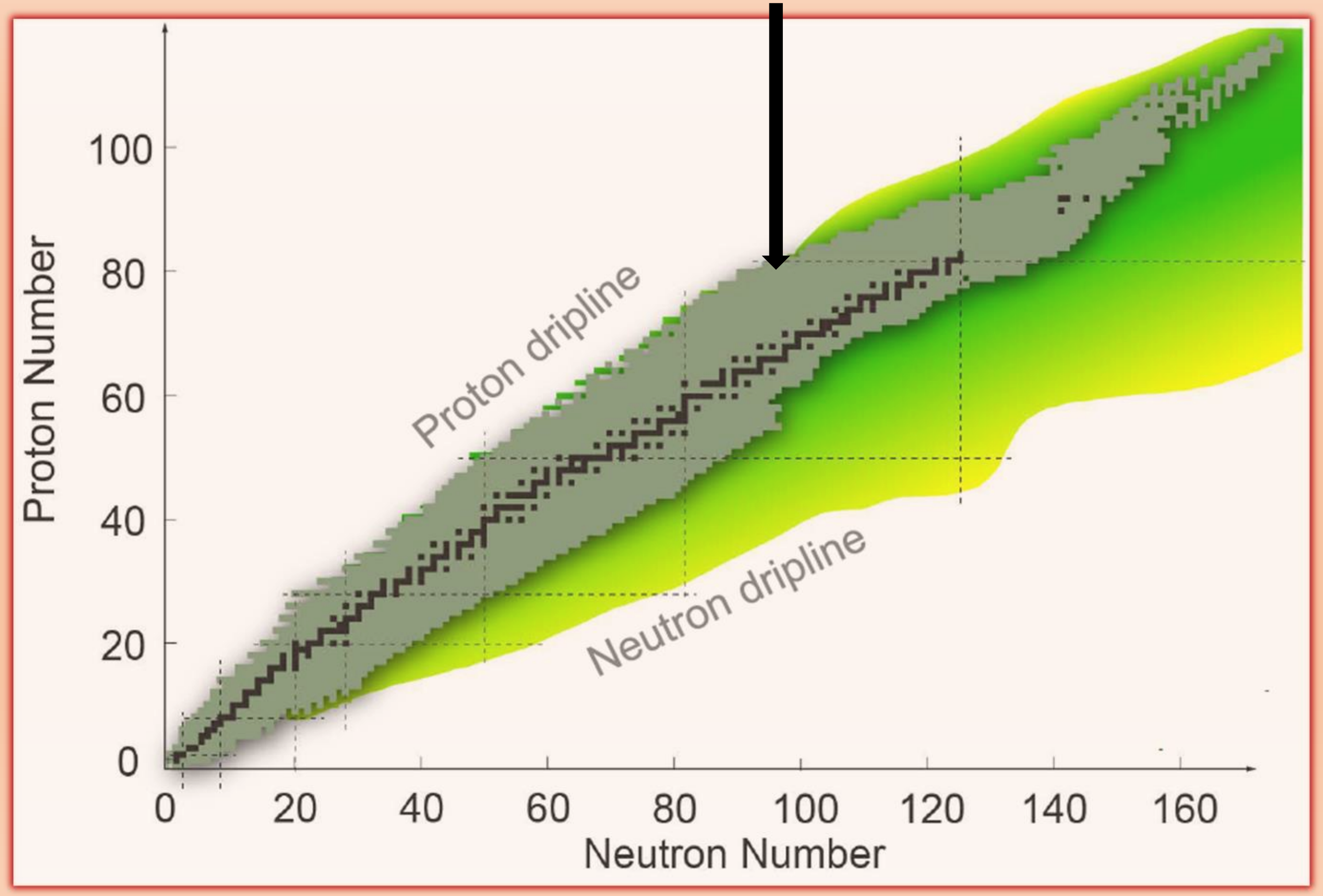

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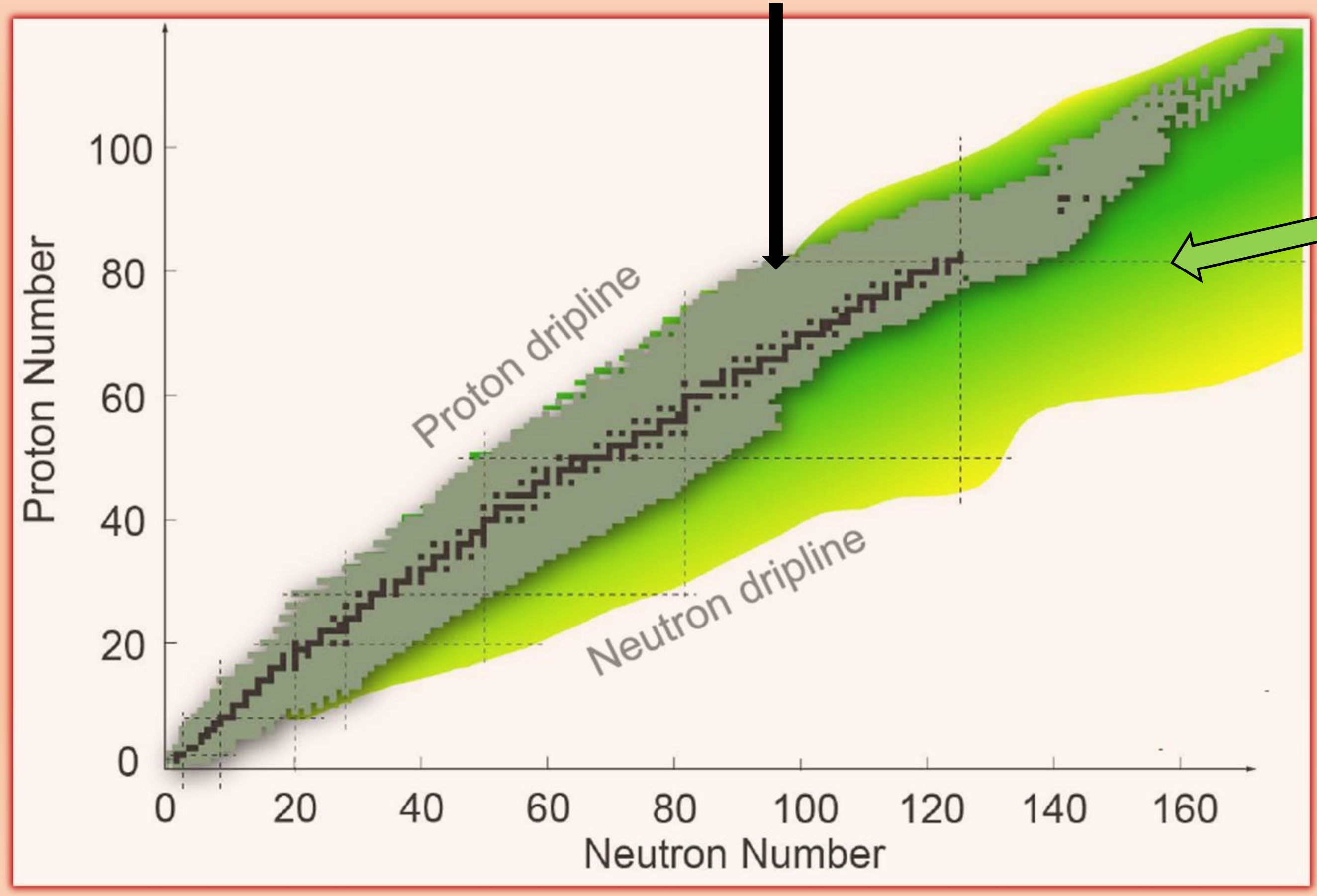


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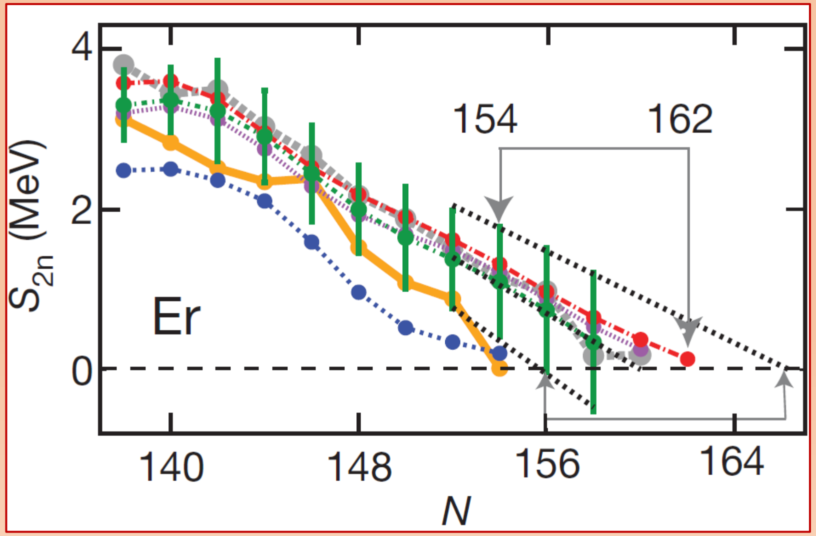


No clear consensus on the position of the **neutron dripline**

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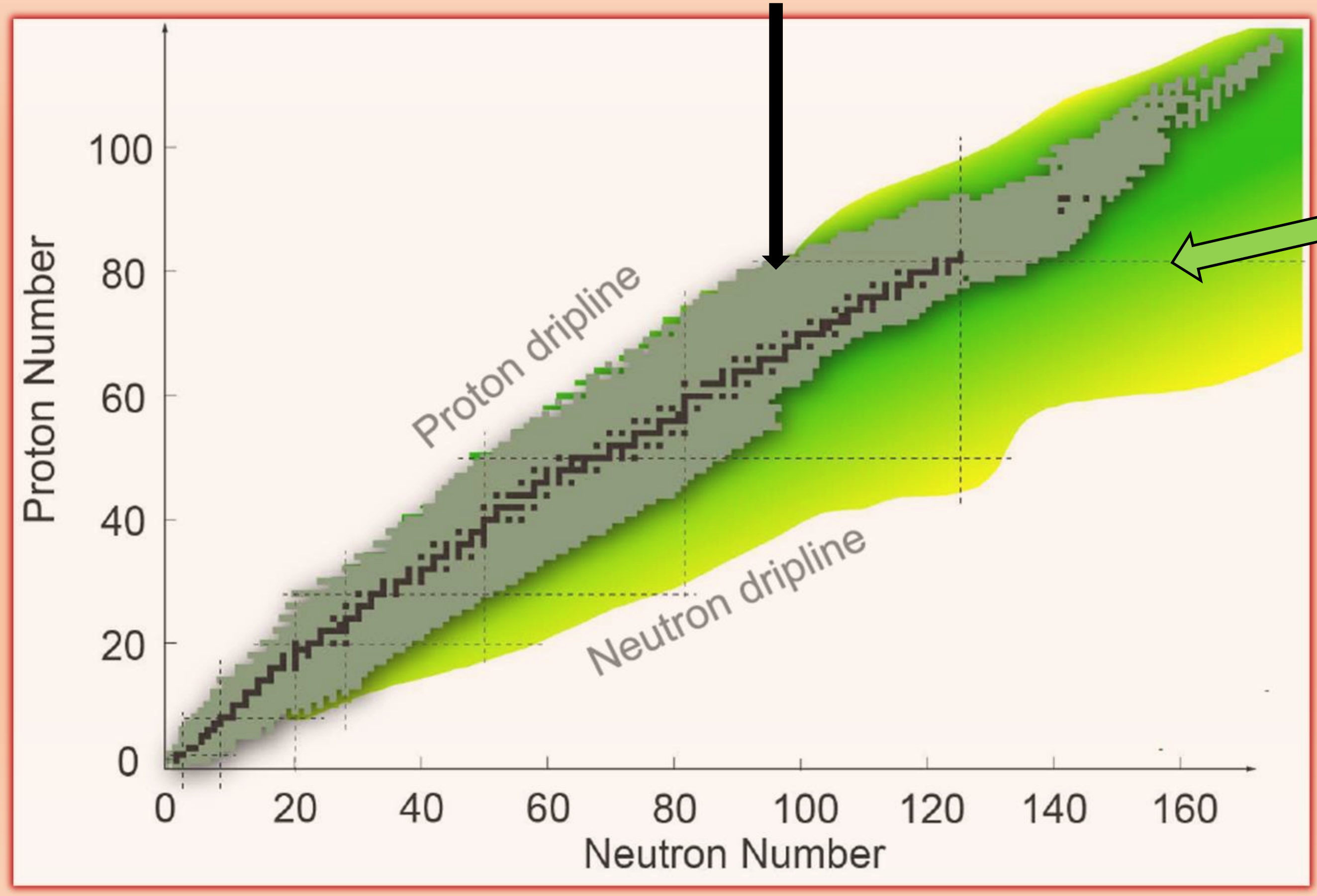
How can we **improve** the EDF accuracy in regions where there are few or no experimental data?

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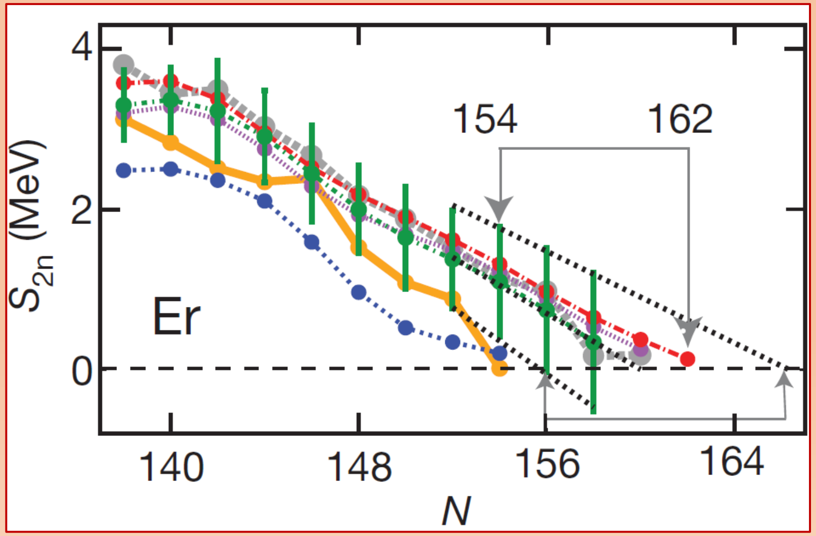


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***Ab initio*** → **Density functional theory**

Attempts at non-empirical EDFs:

Constraining the EDF by perturbing finite nuclei [J. Phys. G **47**, 085107 (2020)]
DFT and effective field theory [Eur. Phys. J. A **56**, 85 (2020)]
Density matrix expansion [Phys. Rev. C **103**, 014325 (2021)]

See **D. Lacroix** and **A. Boulet** for EDFs inspired by the **unitary gas**

Phys. Rev. C **97**, 014301 (2018)
arXiv:2201.07626 (2022)

# Our systematic strategy

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AIP Conf. Proc. **577**, 1 (2001)

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Two key principles

1. Follow a **step by step** approach

2. Use ***ab initio*** simulations of model systems as a **constraint** to the EDF

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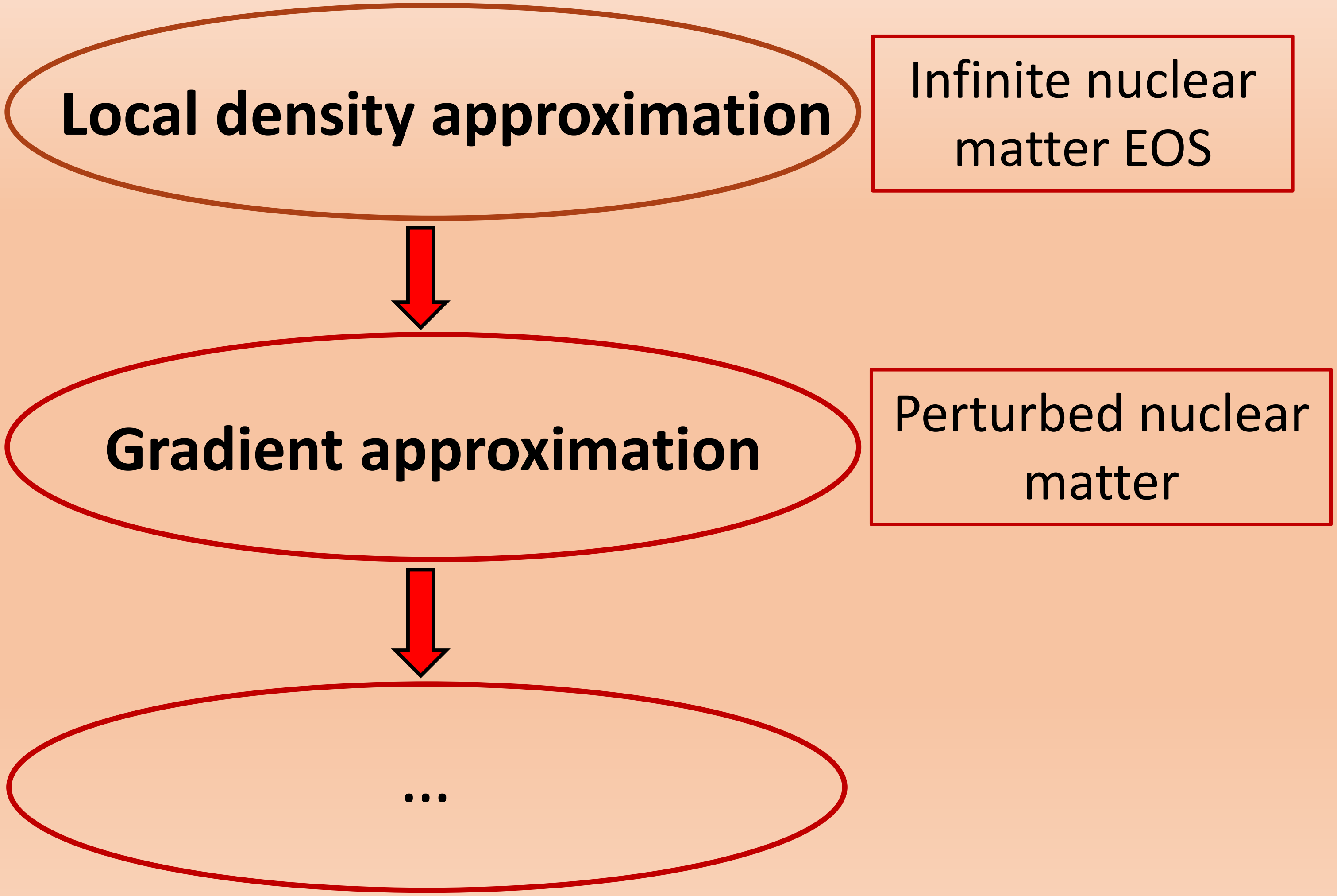


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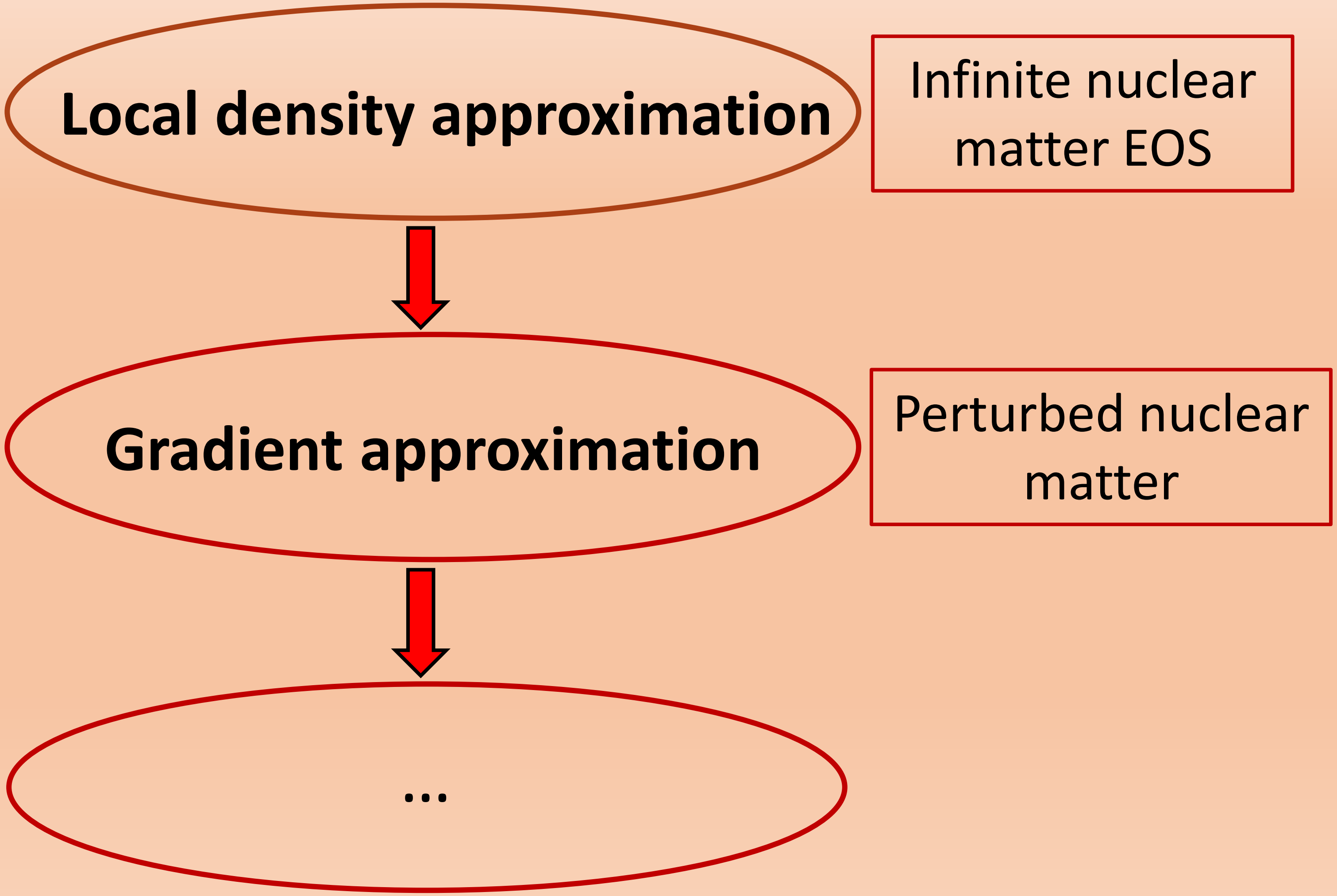


**Warning**: the nuclear interaction is **not unique** and much more complicated than the Coulomb interaction

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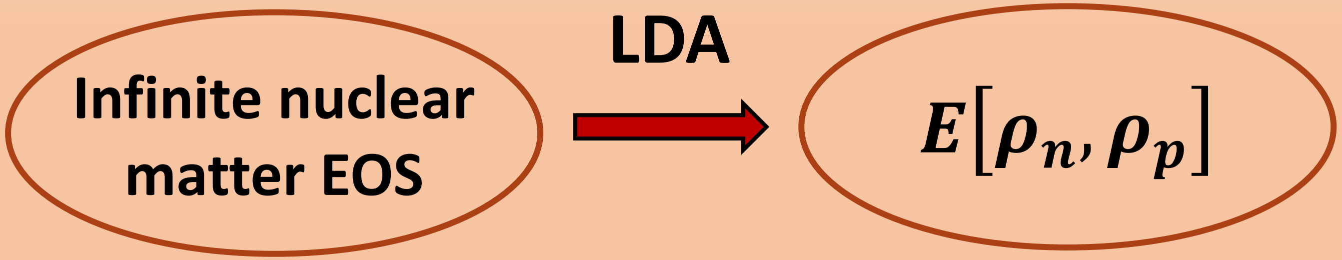
The **equation of state** (EOS) $e(\rho, \beta)$ can be converted into an EDF



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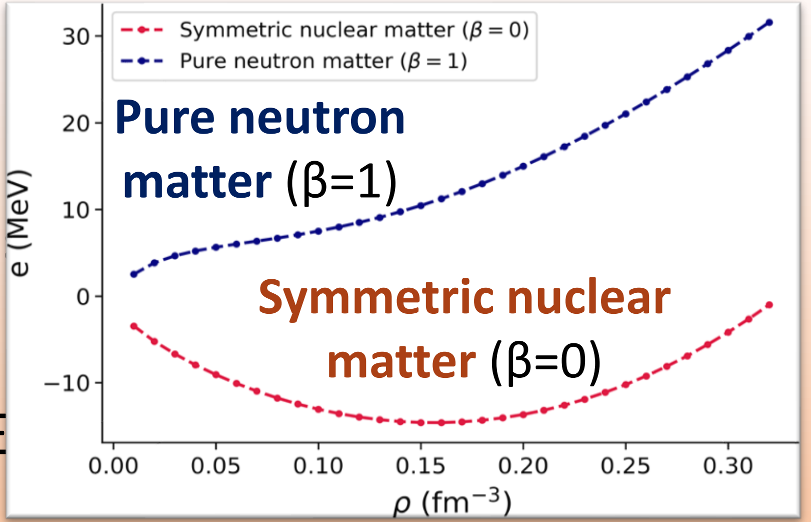


**Infinite nuclear matter EOS** → **LDA** → $E[\rho_n, \rho_p]$

$e$: energy per particle

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

Infinite matter *ab initio*

$$e(\rho, \beta) = t(\rho, \beta) + v(\rho, \beta)$$

Kinetic energy per nucleon

Potential energy per nucleon

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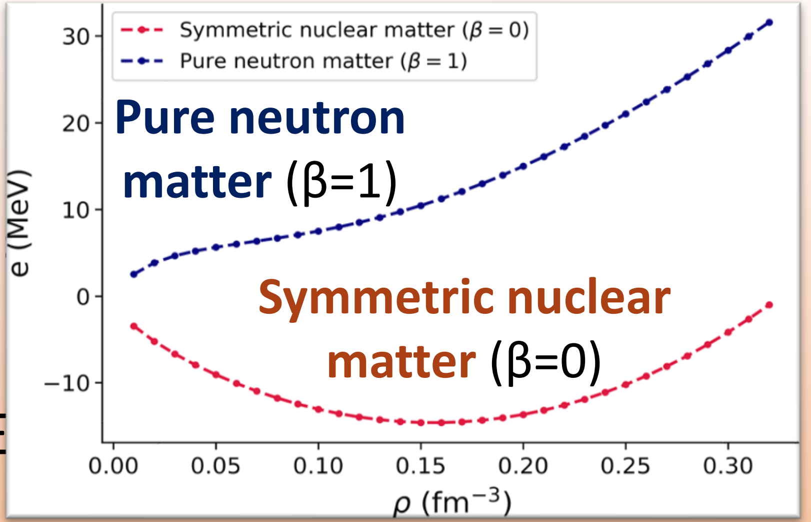


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EDF for **finite nuclei**

$$E_{pot}[\rho_n, \rho_p] = \int d\boldsymbol{r}\, \rho(\boldsymbol{r}) v(\rho, \beta)$$

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Four-component system

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Front. Phys. **8**, 387 (2020)
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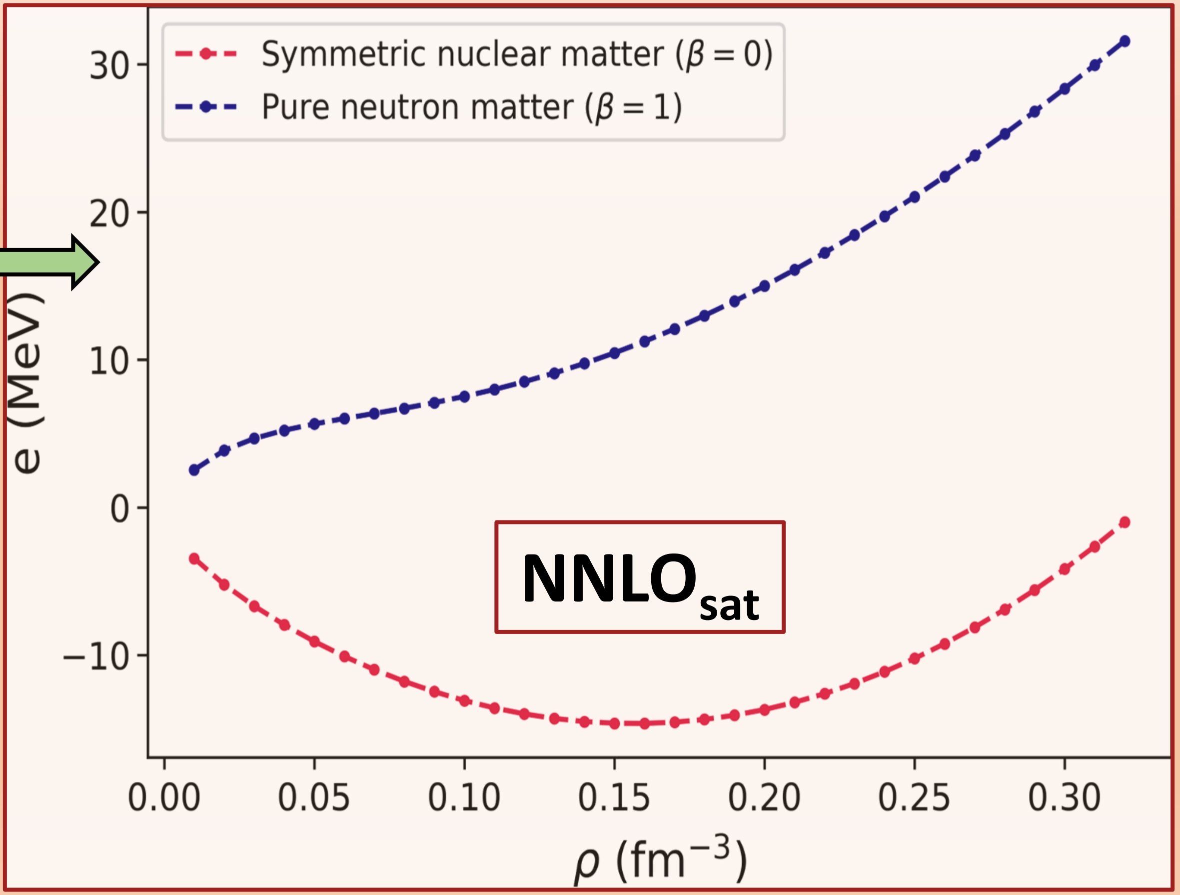


Phys. Rev. C **104**, 024315 (2021)

Note: symmetric matter is essential for nuclei!

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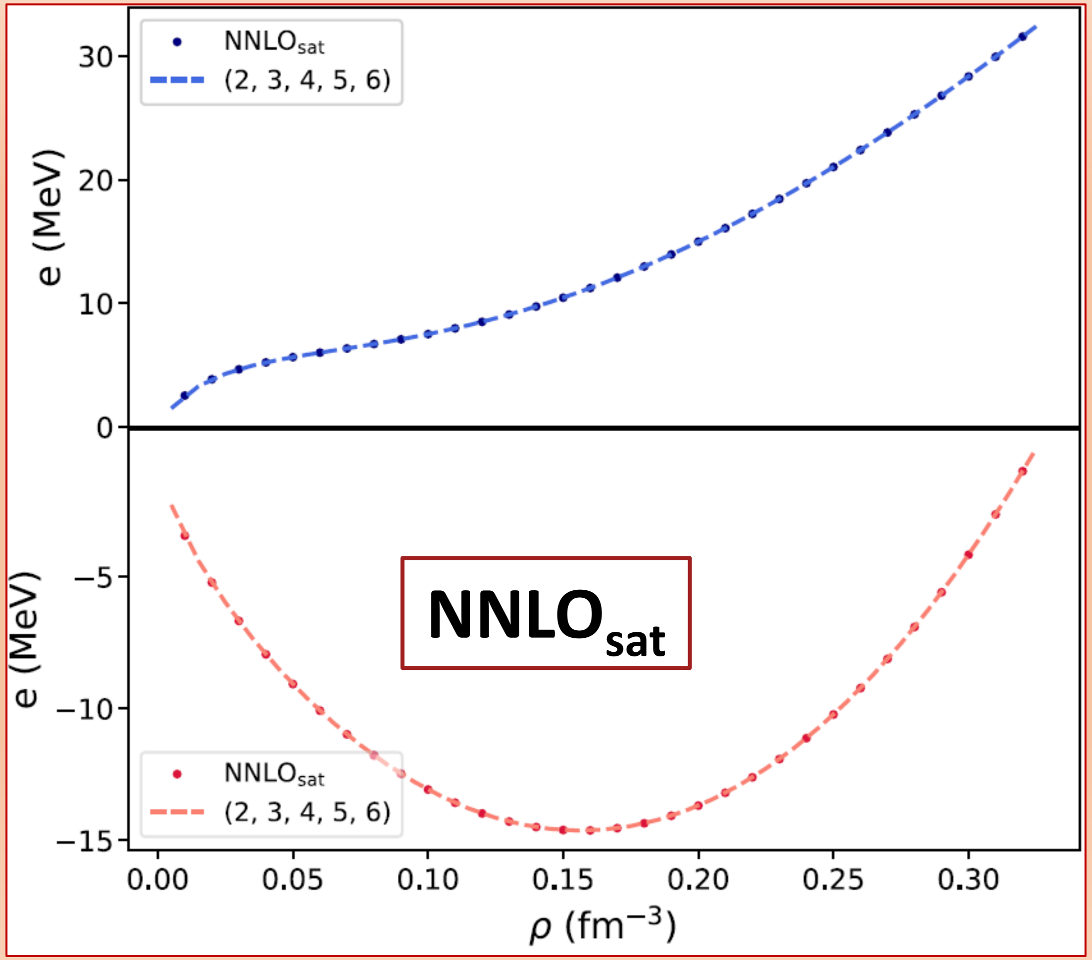

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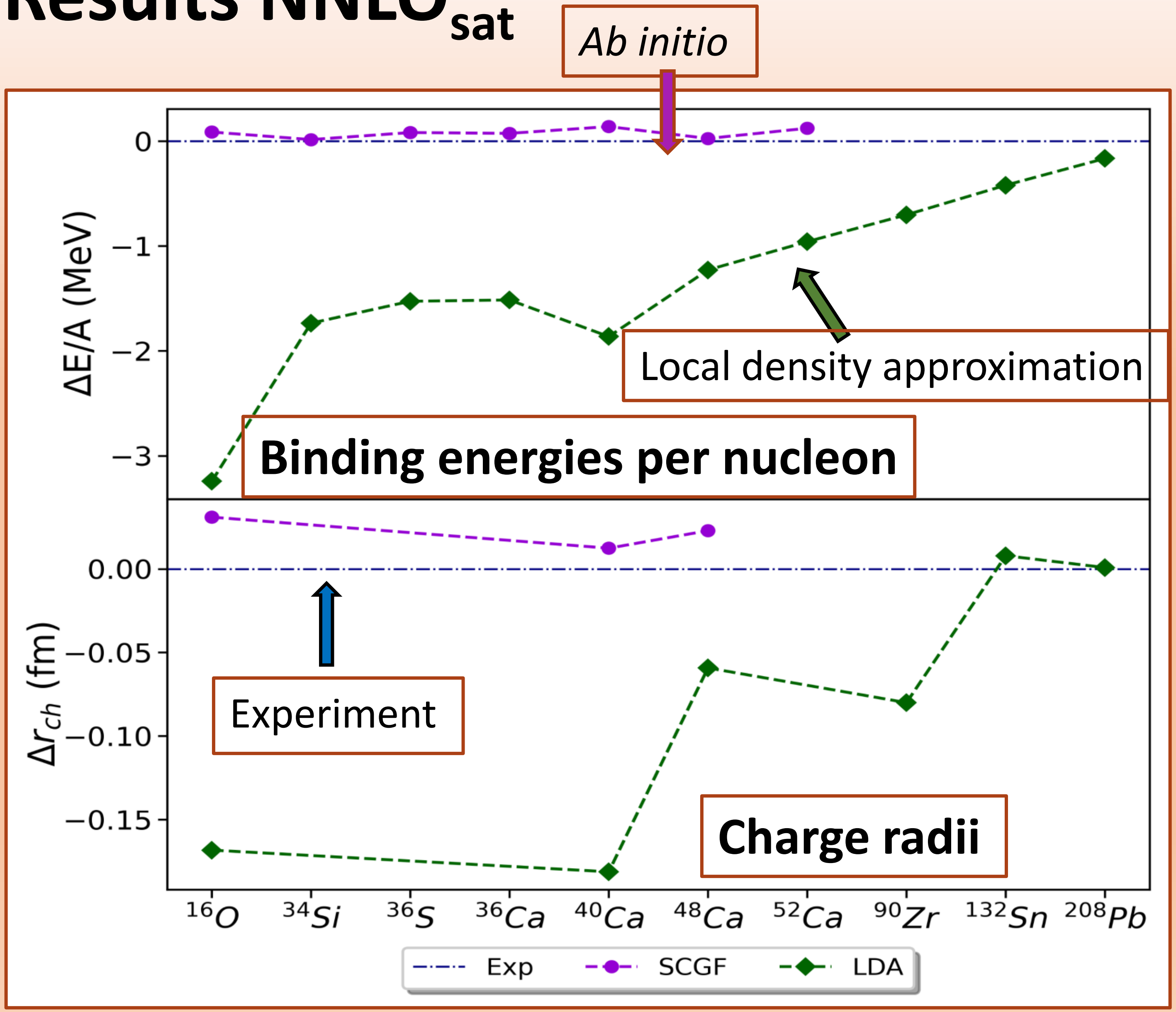


First results:
ground state energies and radii of closed-shell nuclei with $NNLO_{sat}$ and SCGF

Phys. Rev. C **104**, 024315 (2021)

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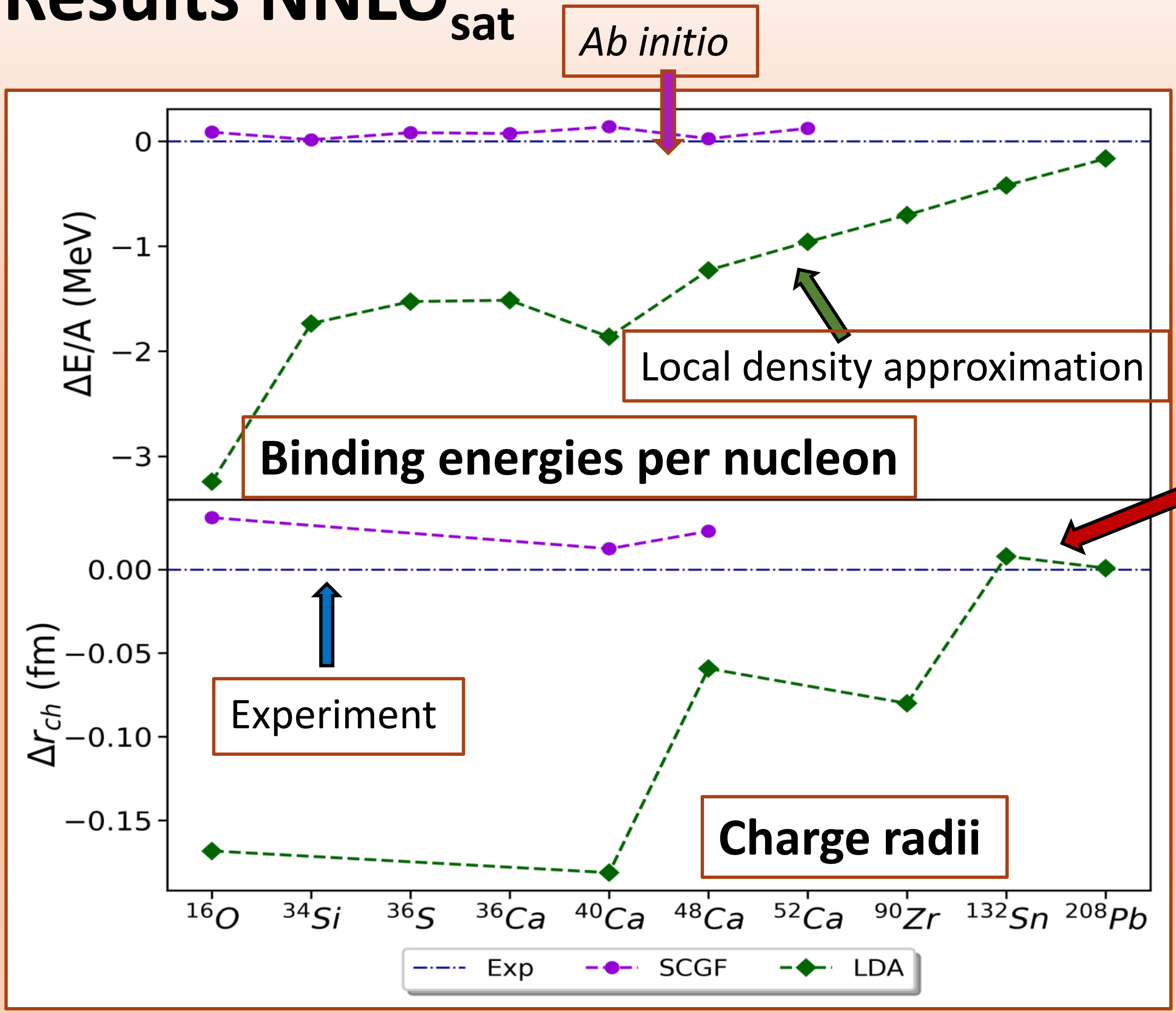


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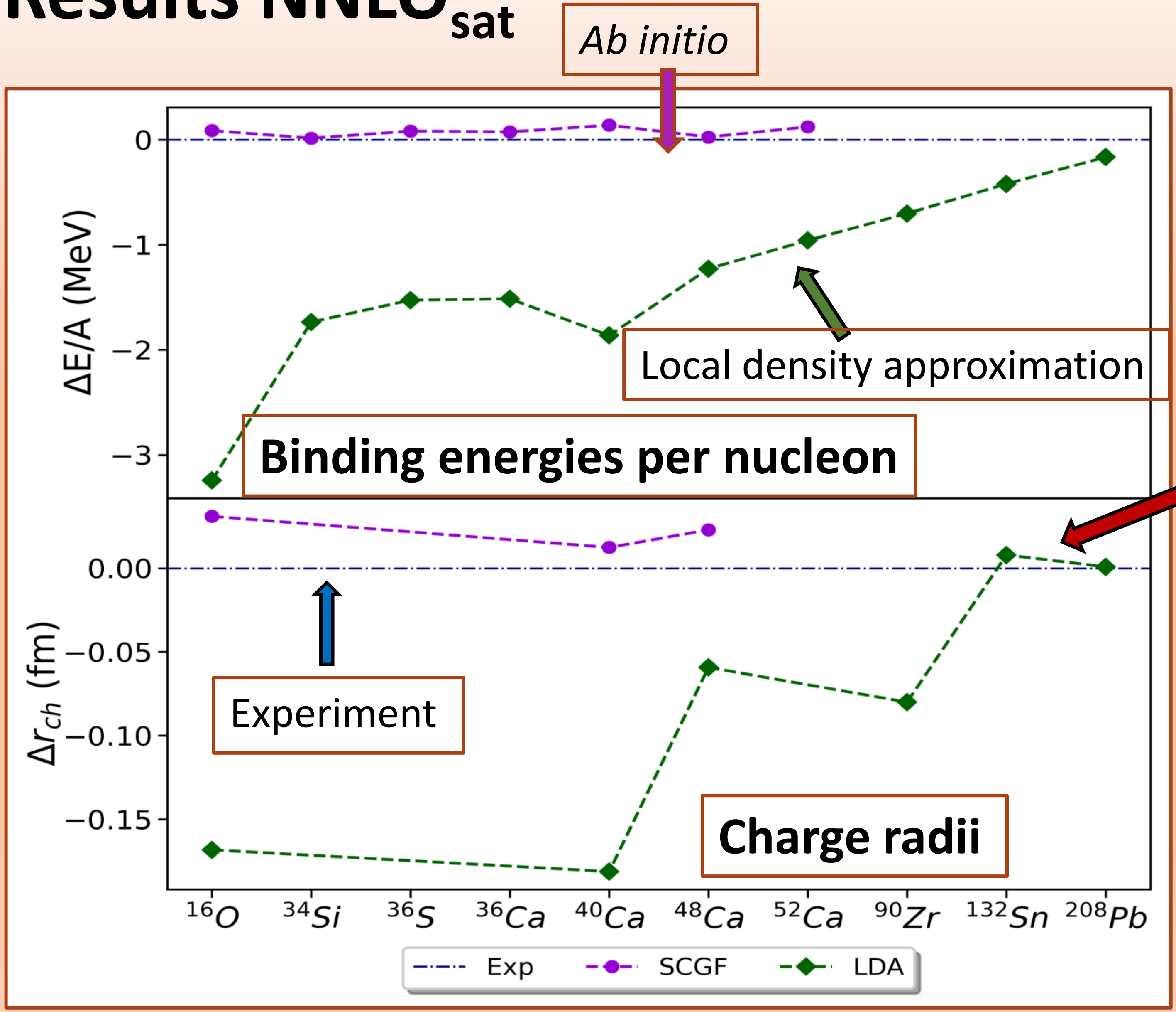


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Local density approximation is reasonable, but not highly accurate.
What is missing?

Phys. Rev. C **104**, 024315 (2021)

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**Nuclear matter perturbed by a periodic potential**

Other options:

- Neutron-proton drops [Phys. Rev. C 87, 054318 (2013)]
- Semi-infinite matter [Nucl. phys. A 818.1 (2009): 36–96]

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**Nuclear matter perturbed by a periodic potential**

**Static response** problem

**Static response** —GA→ $\boldsymbol{E}[\boldsymbol{\rho}, \boldsymbol{\nabla\rho}, \boldsymbol{J}]$

See A. Gezerlis works, e.g.
Phys. Rev. C **95**, 044309 (2017)
Phys. Lett. B **818**, 136347 (2021)

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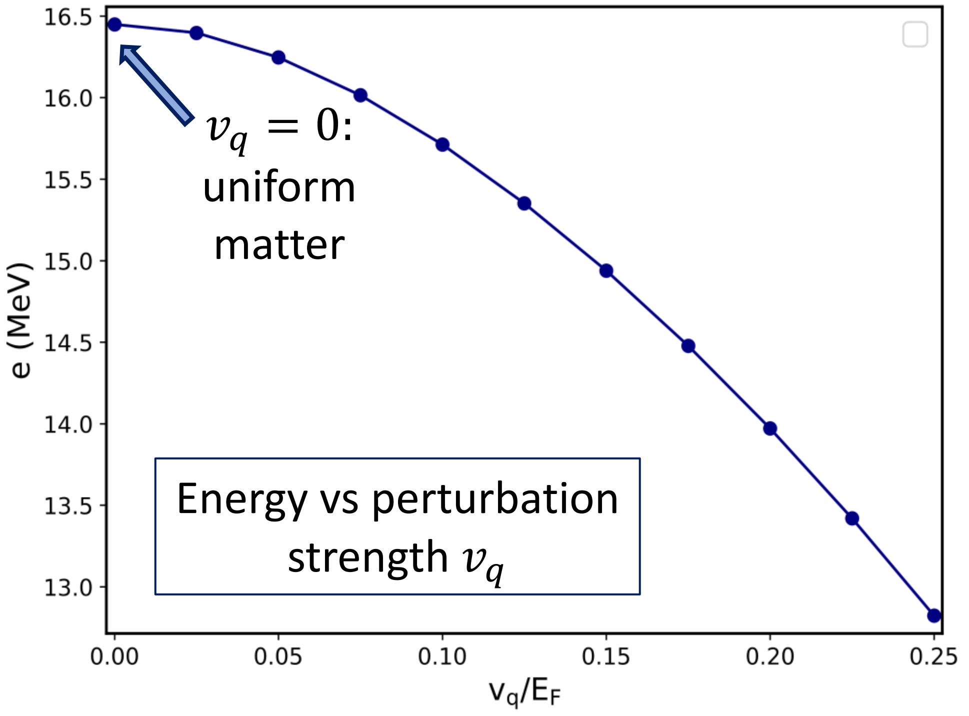
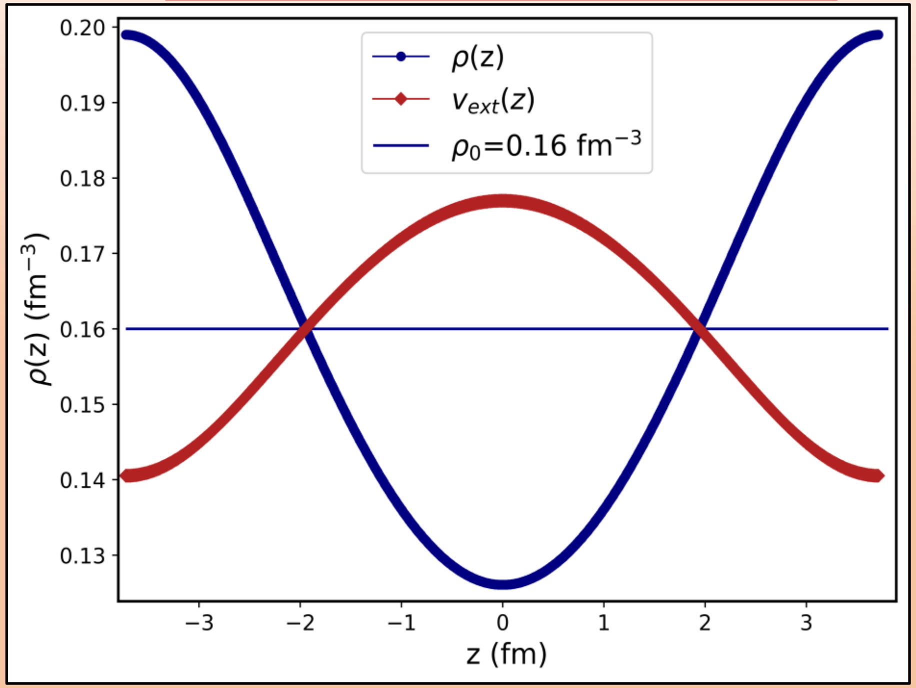
In linear response, $\delta\rho(\boldsymbol{x}) \propto v_q$ while $\delta e_v \propto v_q^2$




SLy4 EDF, $q/k_F$=0.5, $v_q/E_F$=0.1 in PNM (N=66 neutrons)




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

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

$\chi(q)$ is the **static response function**

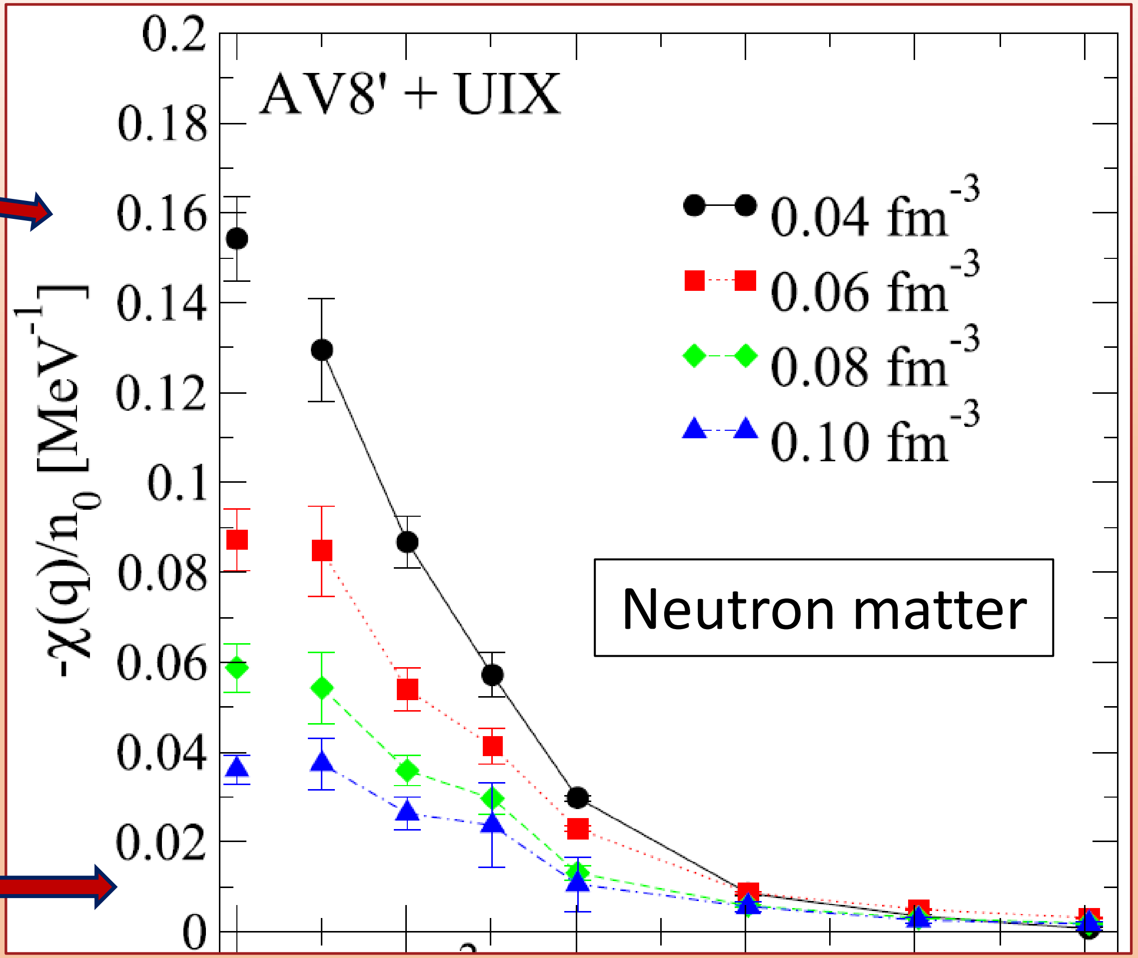
# Static response

# Static response

Auxiliary Field Diffusion Monte Carlo calculations of the static response of neutron matter

Results are extrapolated from **N=66** neutrons under **periodic boundary conditions** to the the thermodynamic limit

The momentum
*q* is quantized

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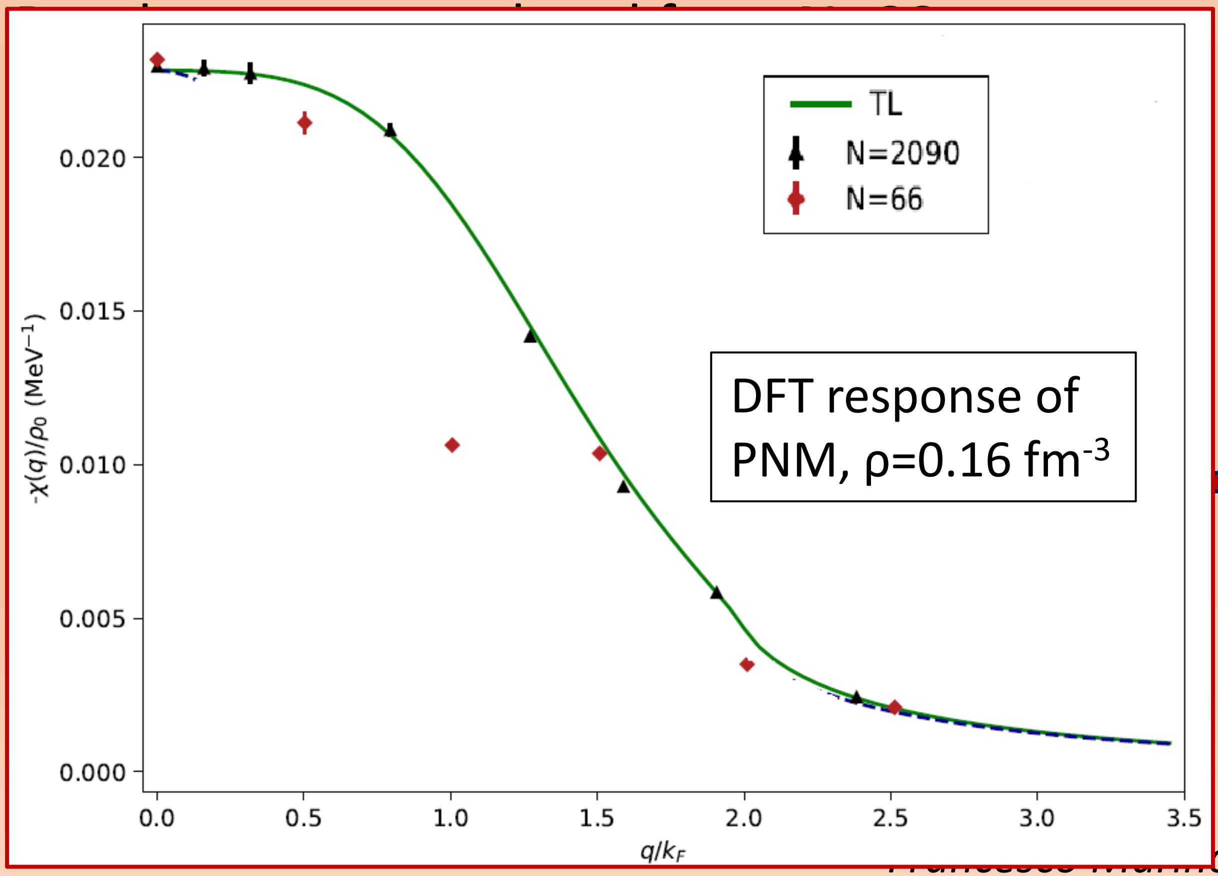


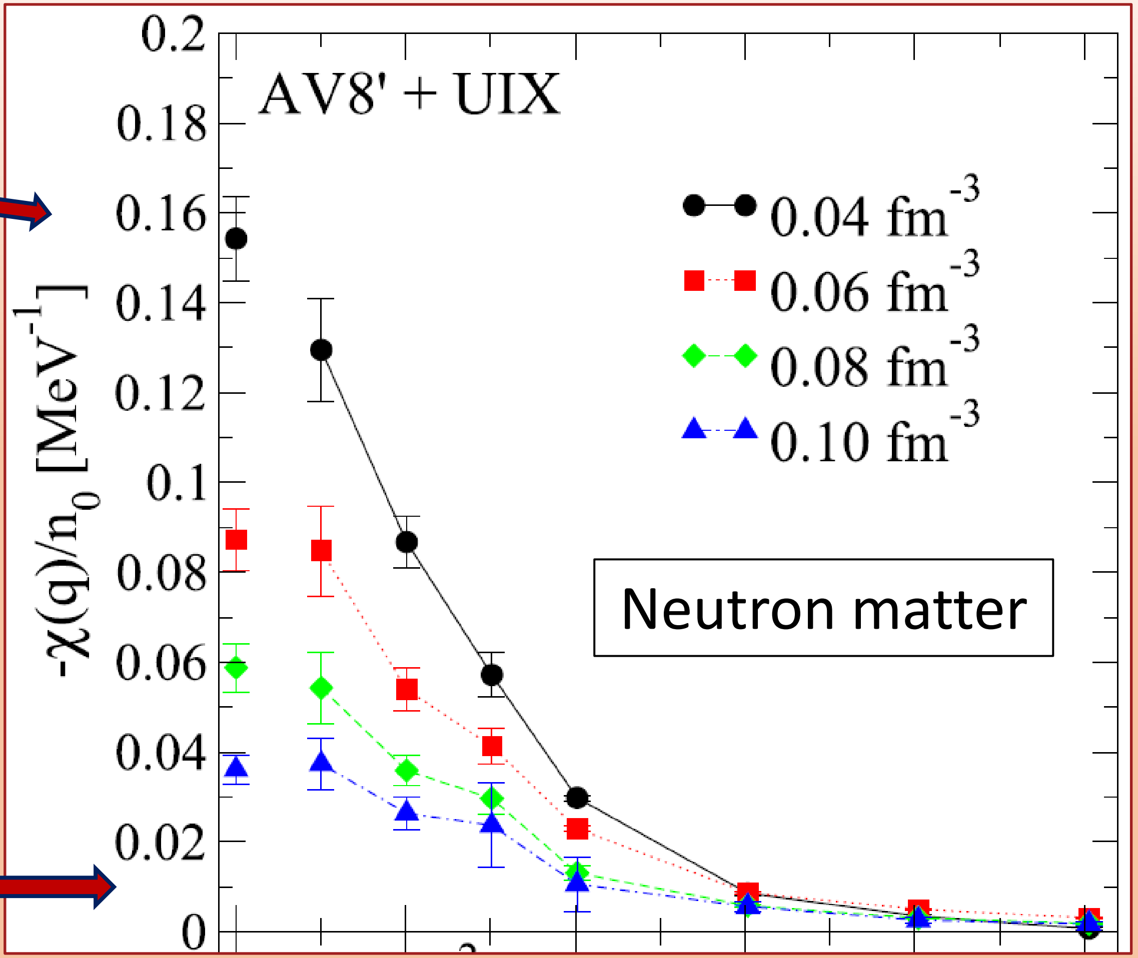


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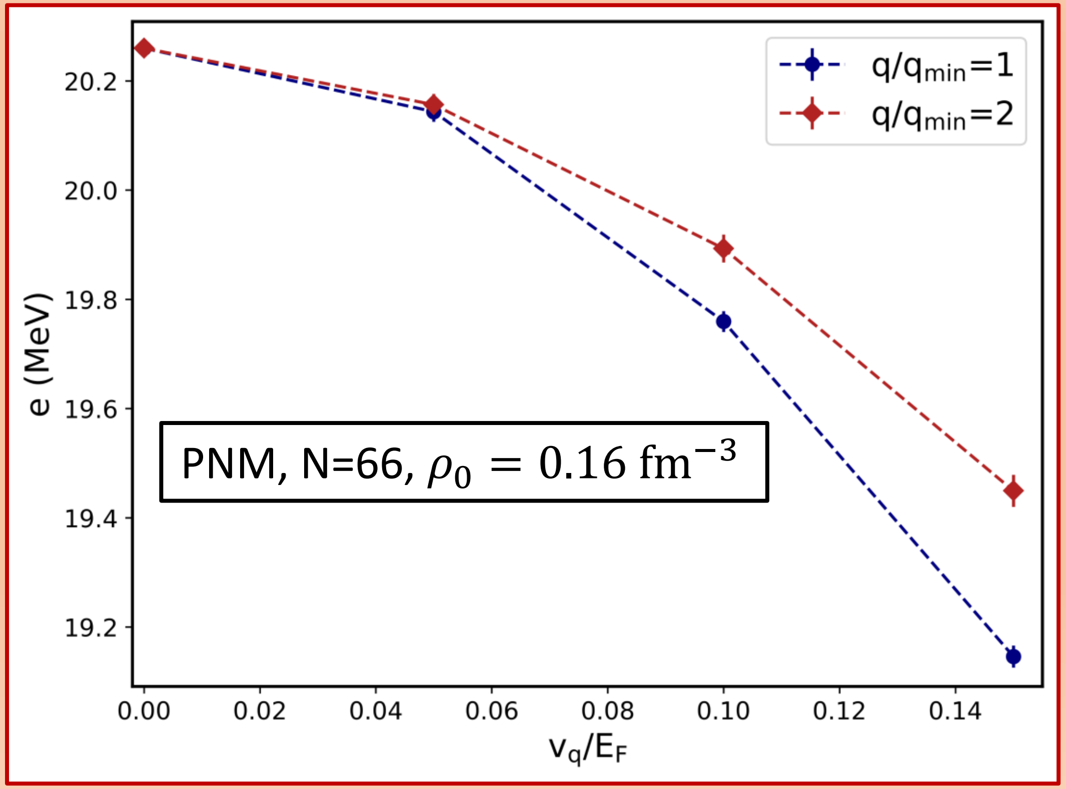
**Work in progress!**



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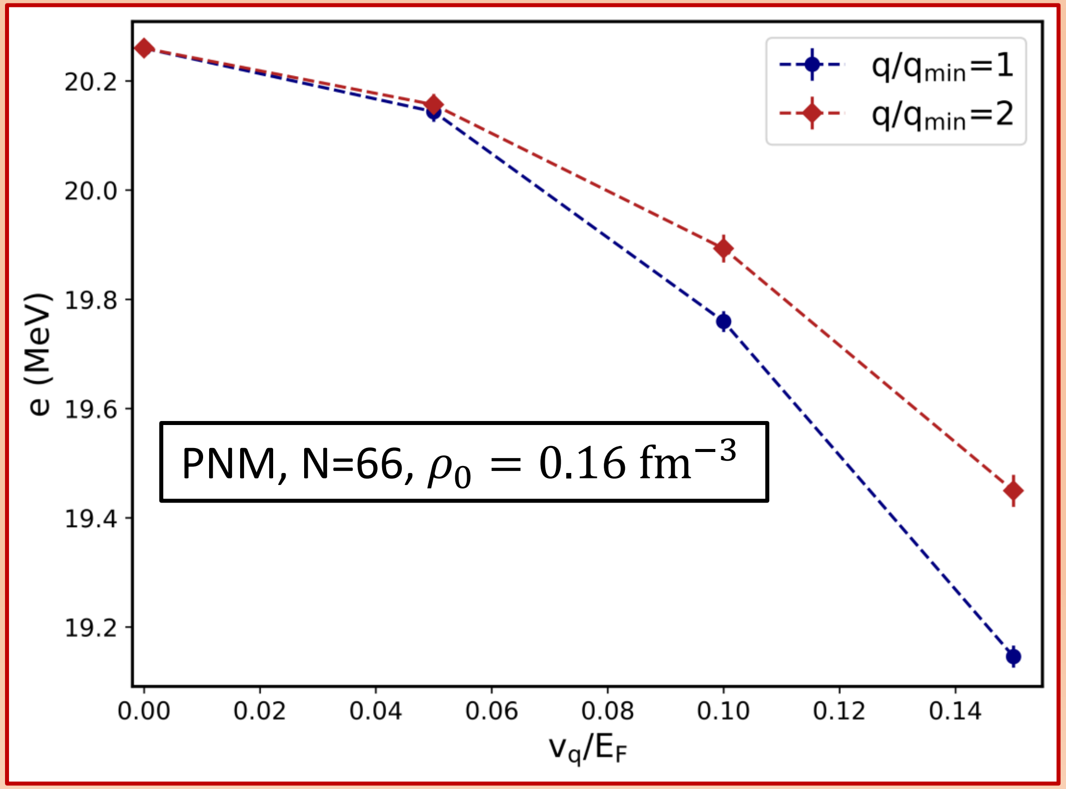
$$E_{GA} = E_{LDA} + \int d\boldsymbol{r} \sum_{t=0,1} \left[ C_t^{\Delta\rho} \rho_t \Delta\rho_t + C_t^{\nabla J} \rho_t \nabla \cdot \boldsymbol{J}_t \right]$$

**Work in progress!**

**Static response of perturbed matter** → **GA** → $\boldsymbol{E}[\boldsymbol{\rho}, \boldsymbol{\nabla\rho}, \boldsymbol{J}]$

Energies $e_v$ at different strengths and momenta → $C_t^{\Delta\rho}$ and $C_t^{\nabla J}$ parameters

Match energies at a finite number of nucleons



# Conclusion and perspectives

- We are developing a **ladder** of ***ab initio*-constrained** nuclear EDFs
- The first rung (**local density approximation**) has been implemented
- Gradient terms are currently being constrained on **response of nuclear matter** to a weak static perturbation
- Near-term goals are completing the gradient approximation and **applying** the new EDFs to collective states (RPA)

# Thank you for your attention!

**Nuclear energy density functionals grounded in *ab initio* calculations**

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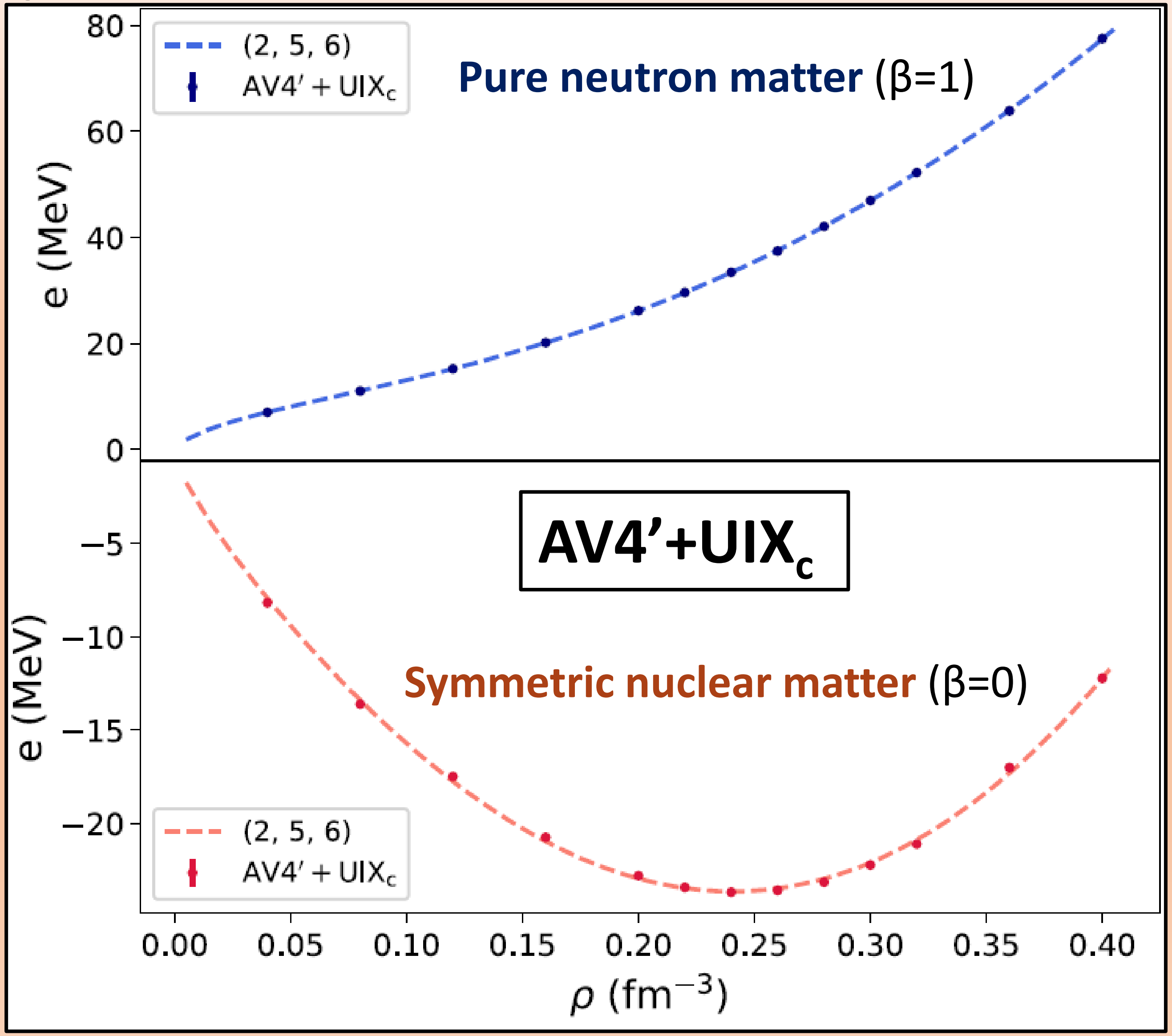
PHYSICAL REVIEW C **104**, 024315 (2021)

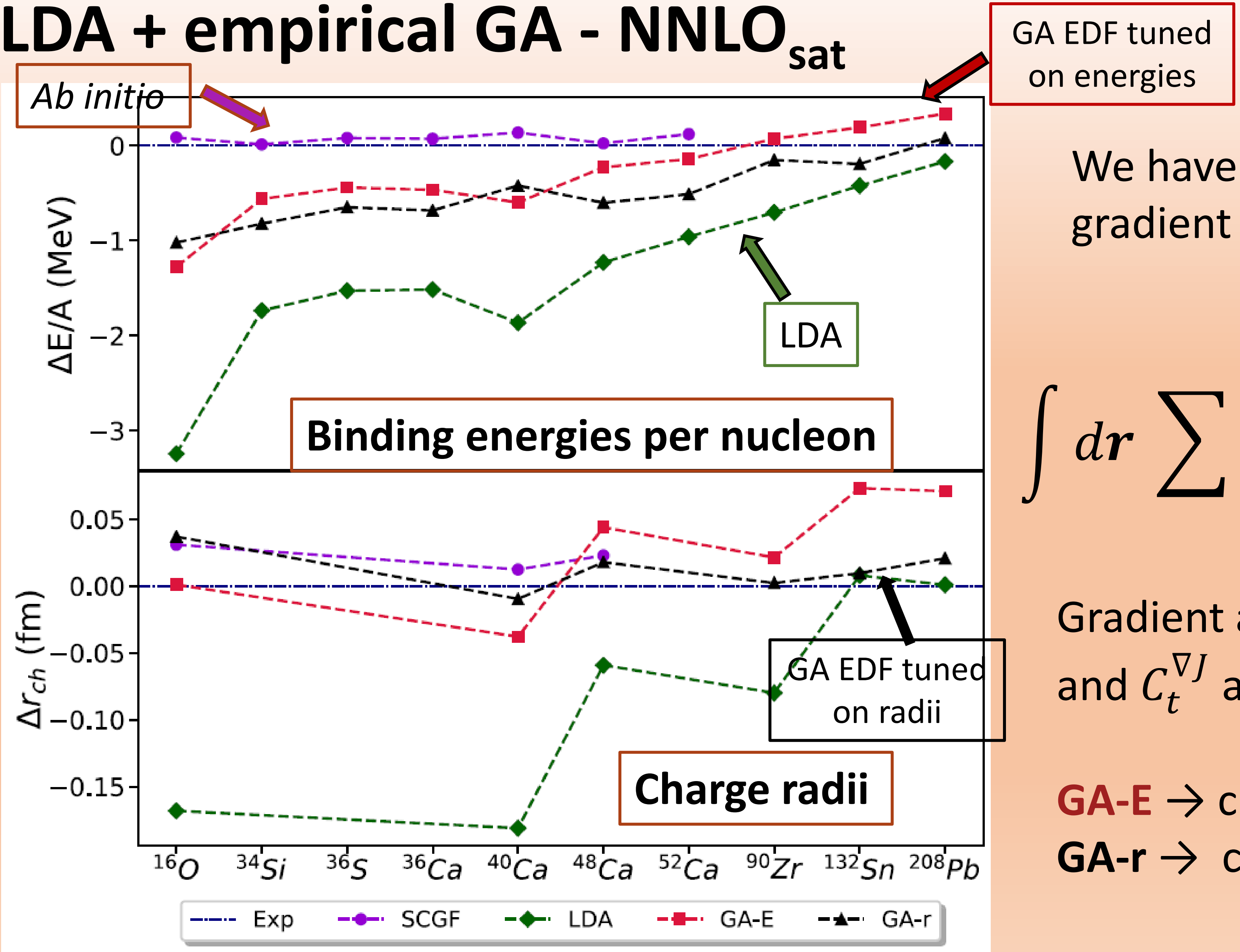
# Equation of state - AV4'+UIX$_c$

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

AV4'+UIX$_c$ $\{\gamma\} = \frac{2}{3}, \frac{5}{3}, 2$



# LDA + empirical GA - NNLO$_{sat}$




We have devised preliminary gradient approximation (GA) EDFs

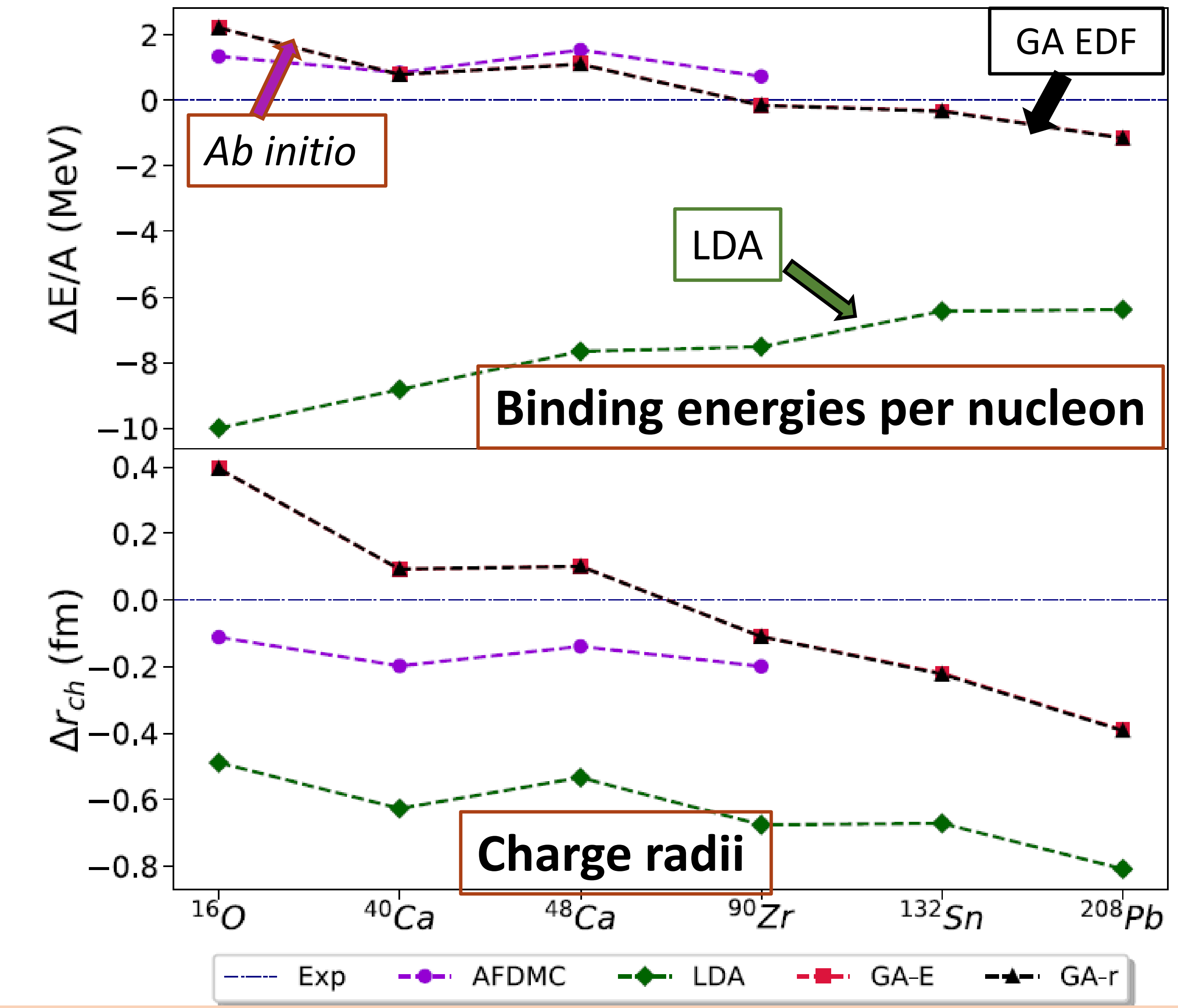
$$E_{GA} = E_{LDA} + \int d\boldsymbol{r} \sum \left[ C_t^{\Delta\rho} \rho_t \Delta\rho_t + C_t^{\nabla J} \rho_t \nabla \cdot \boldsymbol{J}_t \right]$$

Gradient and spin-orbit coefficients $C_t^{\Delta\rho}$ and $C_t^{\nabla J}$ are tuned on **empirical data**

**GA-E** → chosen to reproduce energies

**GA-r** → chosen to reproduce radii

# LDA + empirical GA - AV4'+UIX$_c$

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Match energies at a finite number of nucleons