Ab initio-based nuclear energy functionals: Constraints from the nuclear matter response

Francesco Marino

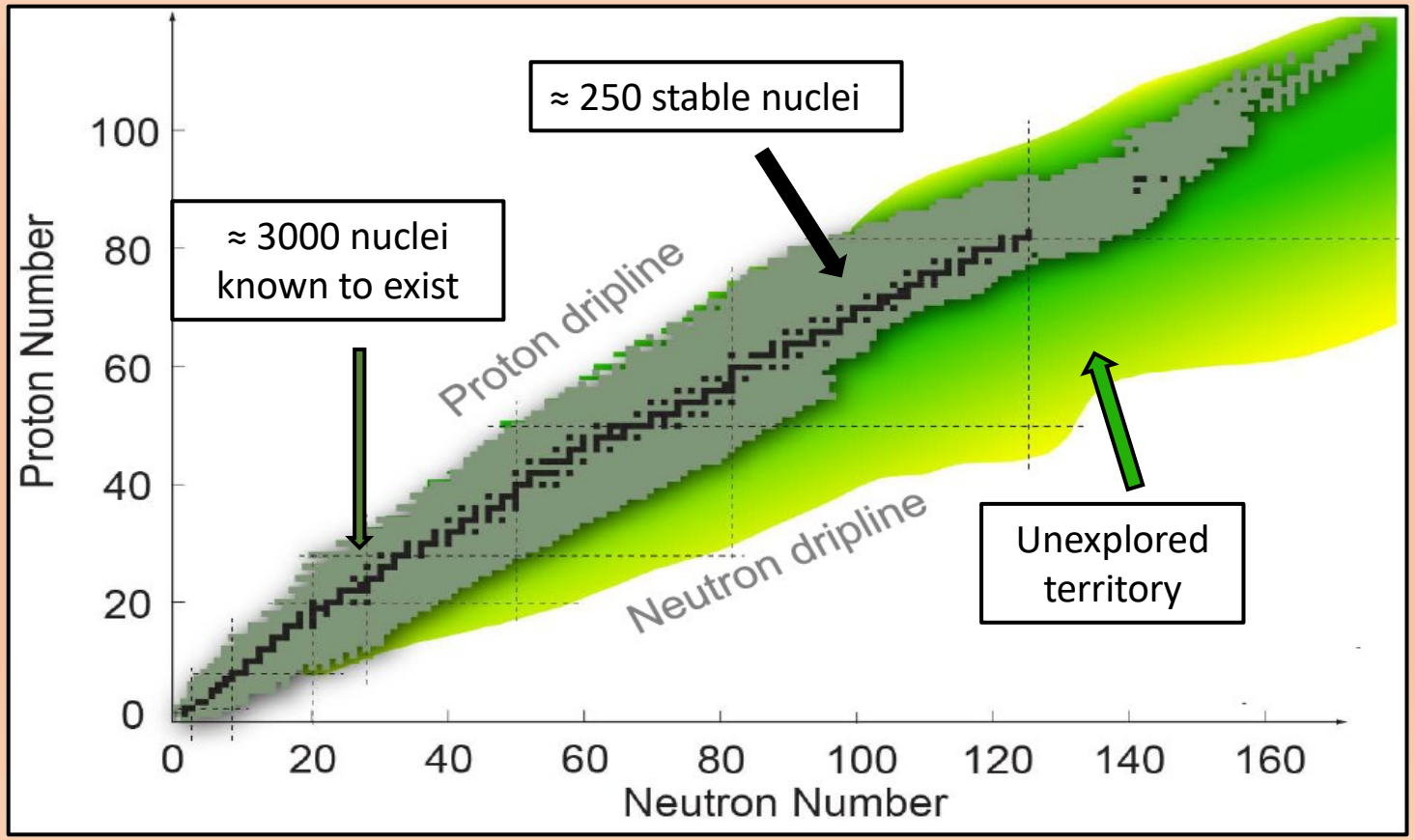
Recent Progress in Many-Body Theories XXI

Università di Milano and INFN

Introduction

Introduction

Ab initio → **Density functional theory**



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both infinite matter and finite nuclei

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

Examples: **Quantum Monte Carlo**, **Self-consistent Green's functions**, Coupled-cluster, …

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Ab initio theory is viable only for relatively **small systems**

But it is rapidly advancing, see Barbieri, Hagen etc.

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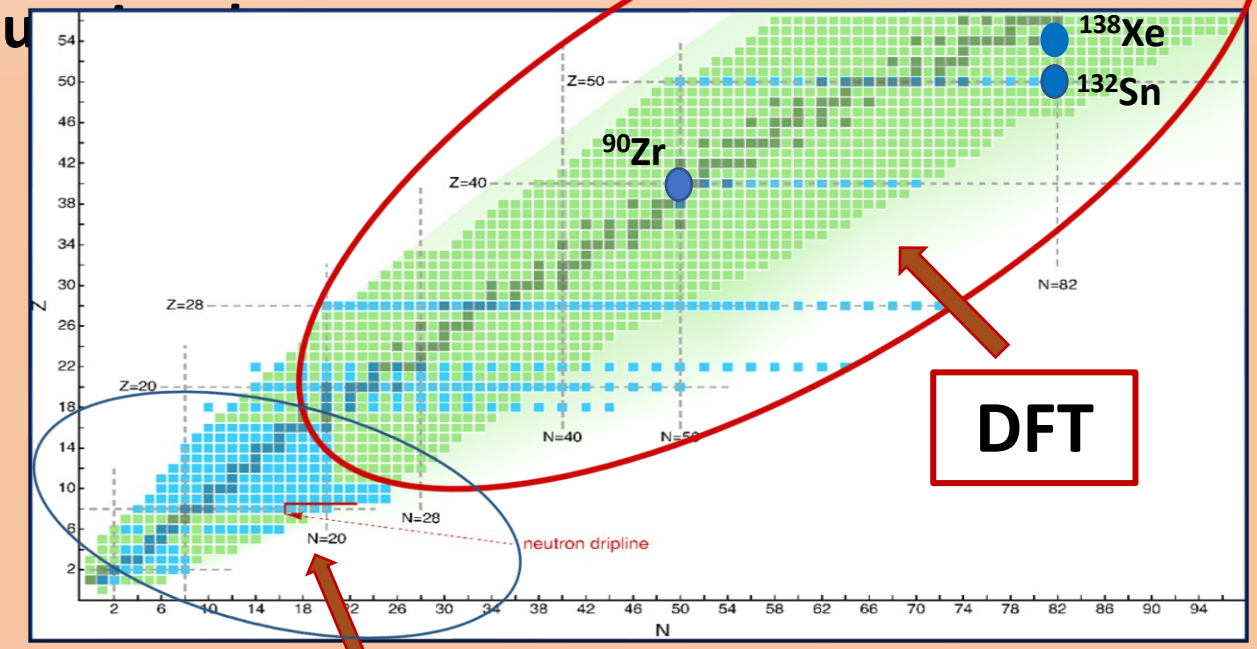

DFT

Ab initio

Arthuis, Phys. Rev. Lett. **125**, 182501 (2020)

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

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Nuclear density functional theory 1

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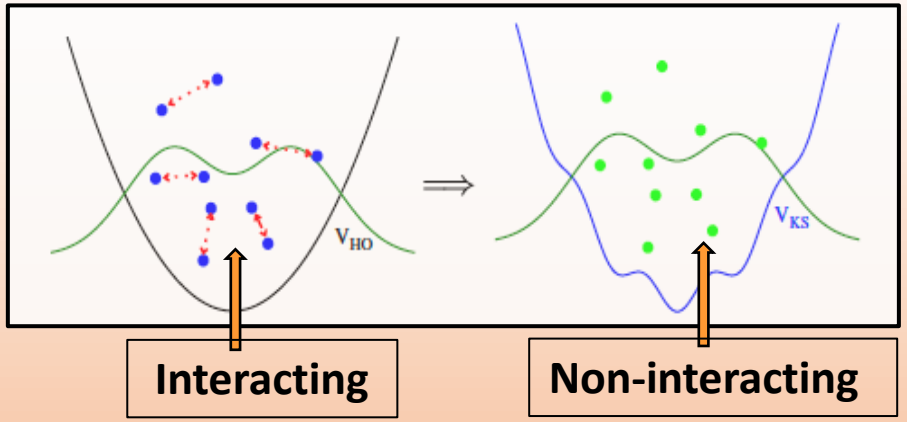

The key object in DFT is the **energy density functional** (EDF) $E[\rho]$

$\delta E = 0$ determines the **ground state** through the **self-consistent** single-particle equations: $h[\rho]\phi_j(\boldsymbol{x}) = \epsilon_j\, \phi_j(\boldsymbol{x})$

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

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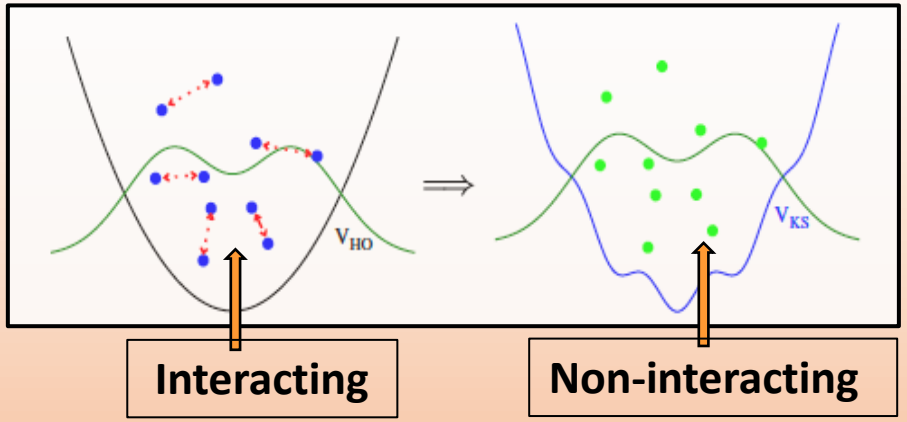

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$$E = \int d\boldsymbol{x} \left[\frac{\hbar^2}{2m}\tau + \sum_{\gamma} c_\gamma(\beta)\rho_0^{\gamma+1} + \sum_{t=0,1} C_t^{\tau}\rho_t\tau_t + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\nabla J}\rho_t\nabla\cdot\boldsymbol{J}_t \right]$$

Kinetic Density-dependent Effective mass Gradient Spin-orbit

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

$t = 1$: isovector channel $\rho_1 = \rho_n - \rho_p$

ρ: number density

τ: kinetic energy density

J: spin-orbit density

$\beta = \rho_1/\rho_0$: isospin asymmetry

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

Nuclear DFT 2

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

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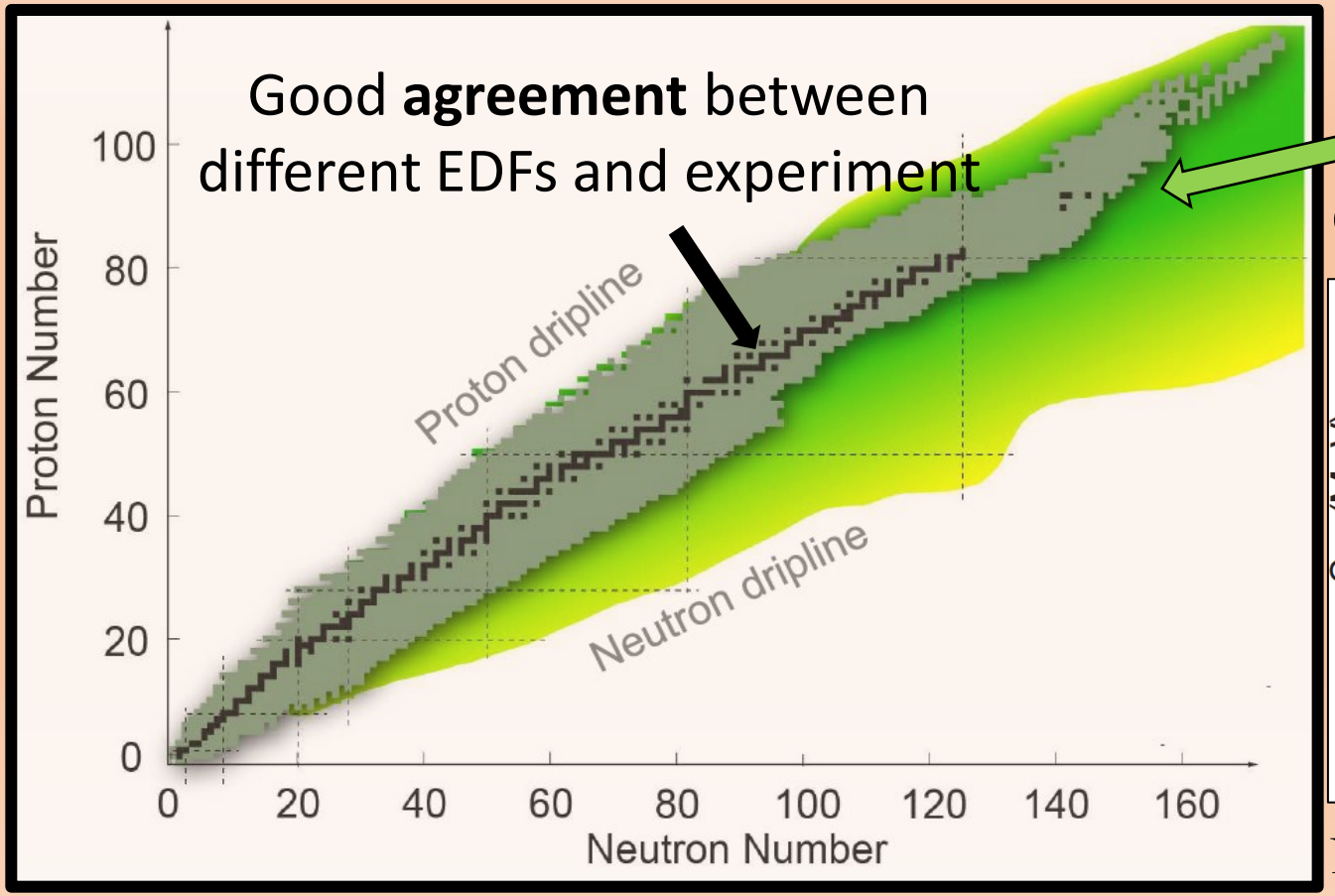
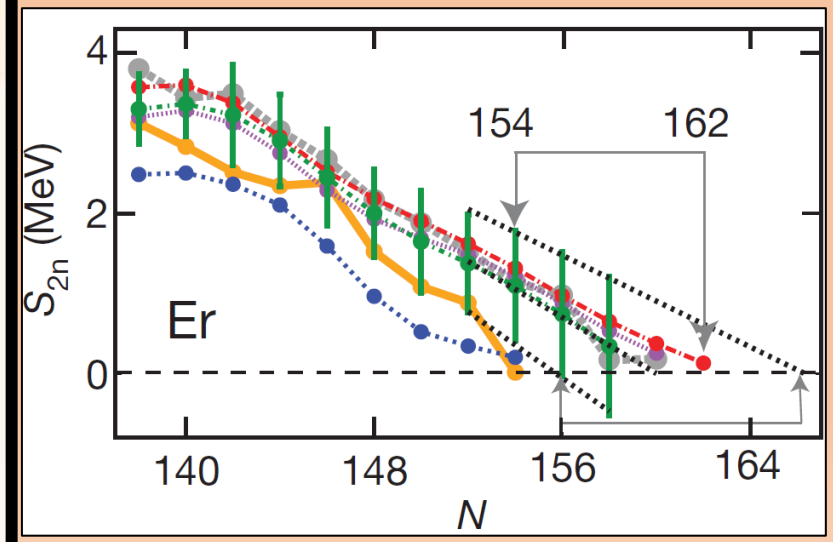


The predictions of different EDFs **disagree** more when one **extrapolates** towards the dripline

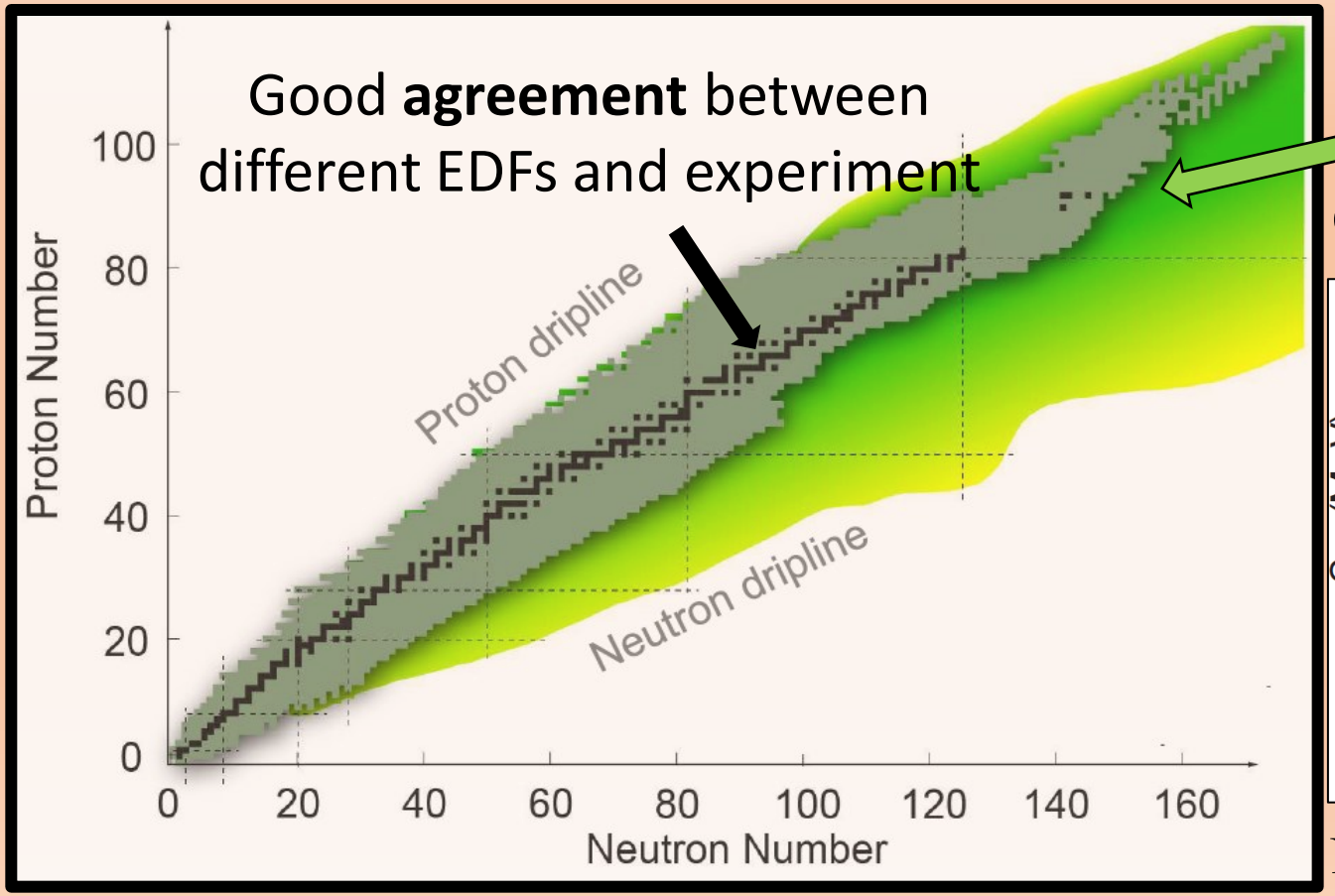


No clear consensus on the position of the **neutron dripline**

Nature **486**, 509–512 (2012)

Nuclear DFT 2

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



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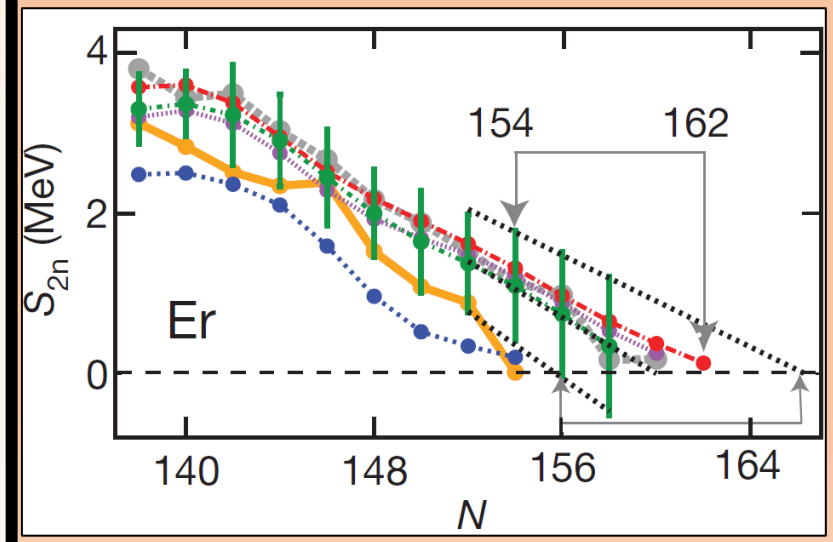

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Combining DFT and *ab initio*

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✓ fundamental and unbiased

DFT

✓ universally applicable

Can we use *ab initio* to inform nuclear DFT?

Ab initio → **Density functional theory**

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Can we use *ab initio* to inform nuclear DFT?

Ab initio → **Density functional theory**

Attempts at non-empirical EDFs:
EDF inspired by the unitary gas theory [Boulet, Phys. Rev. C **97**, 014301 (2018)]
Constraining the EDF by perturbing finite nuclei [Salvioni, J. Phys. G **47**, 085107 (2020)]
DFT and effective field theory [Furnstahl, Eur. Phys. J. A **56**, 85 (2020)]
Density matrix expansion [Zurek, Phys. Rev. C **103**, 014325 (2021)]

Our systematic strategy

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Strategy inspired by the **«Jacob's ladder»** of condensed matter DFT

Perdew, 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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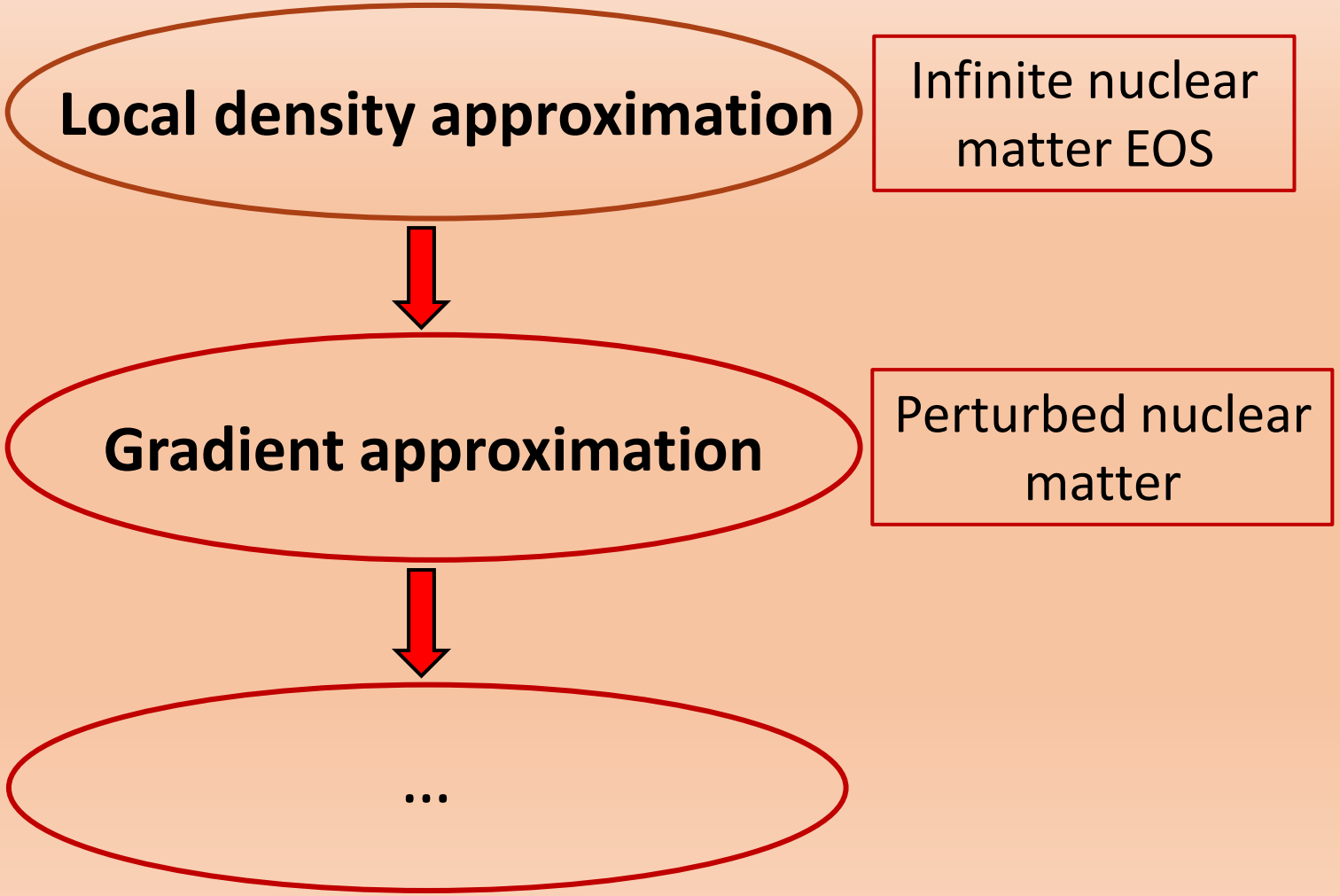

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Warning: the nuclear interaction is **not unique** and much more complicated than the Coulomb interaction

Local density approximation

Infinite nuclear matter EOS

Gradient approximation

Perturbed nuclear matter

...

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

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Local density approximation (LDA): The potential **energy density** in a generic system has the same expression as in **infinite matter**

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

Infinite nuclear matter EOS $\xrightarrow{\textbf{LDA}}$ $\boldsymbol{E[\rho_n, \rho_p]}$

e: energy per particle

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

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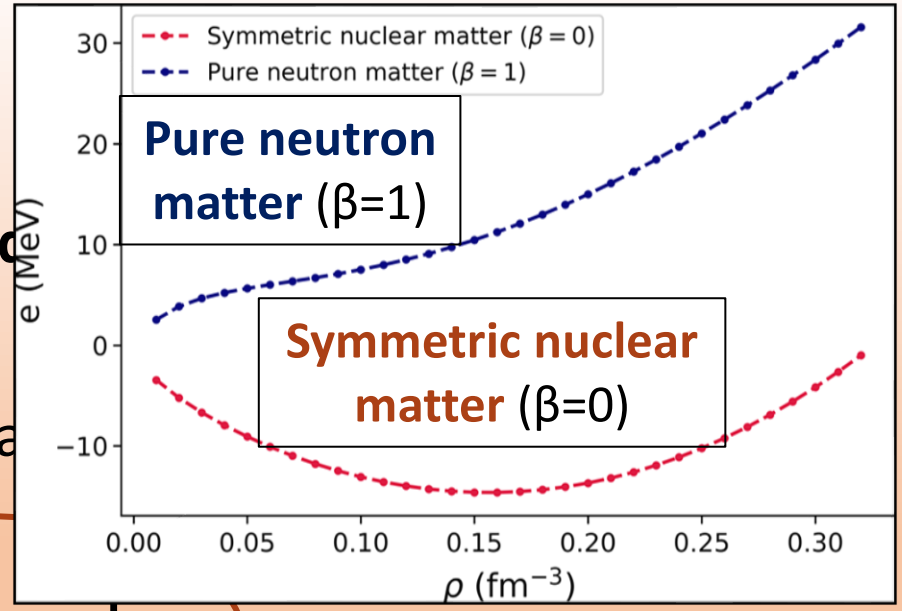

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Infinite matter *ab initio*

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Kinetic energy per nucleon

Potential energy per nucleon

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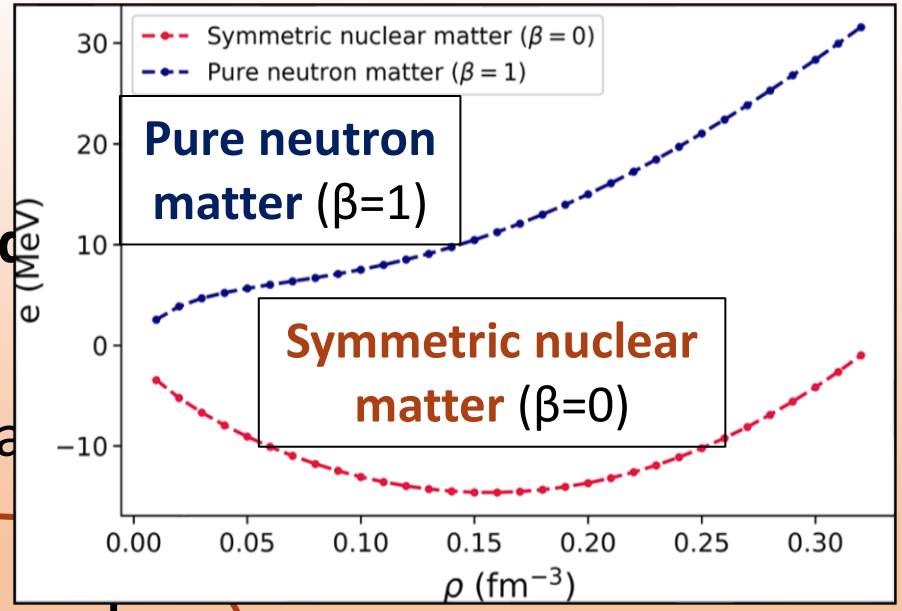

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EDF for **finite nuclei**

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

Equation of state 1

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Four-component system

The nuclear matter EOS has been computed *ab initio* in **symmetric nuclear matter** (β=0) and **pure neutron matter** (β=1).

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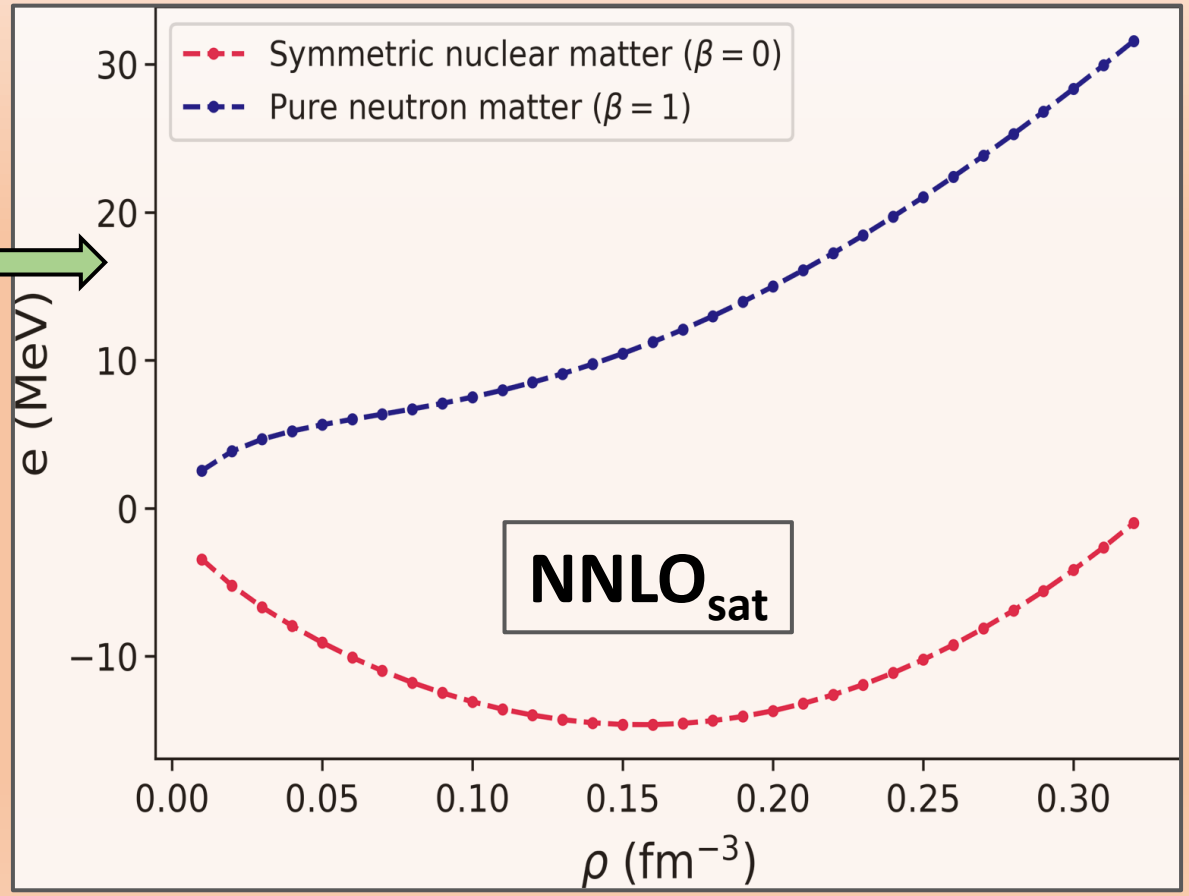
1. Self-consistent Green's function (**SCGF**) with $NNLO_{sat}$

Ladder approximation, finite-T formalism

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

2. Auxiliary field diffusion Monte Carlo (**AFDMC**) with AV4'+UIX_c

Gandolfi, Front. Phys. **8**, 00117 (2020)



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

Note: symmetric matter is essential for nuclei!

Equation of state 2

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3. The optimal set of powers {γ} is chosen by **model selection** with cross-validation

NNLO$_{sat}$ $\{\gamma\} = \frac{2}{3}, 1, \frac{4}{3}, \frac{5}{3}, 2$

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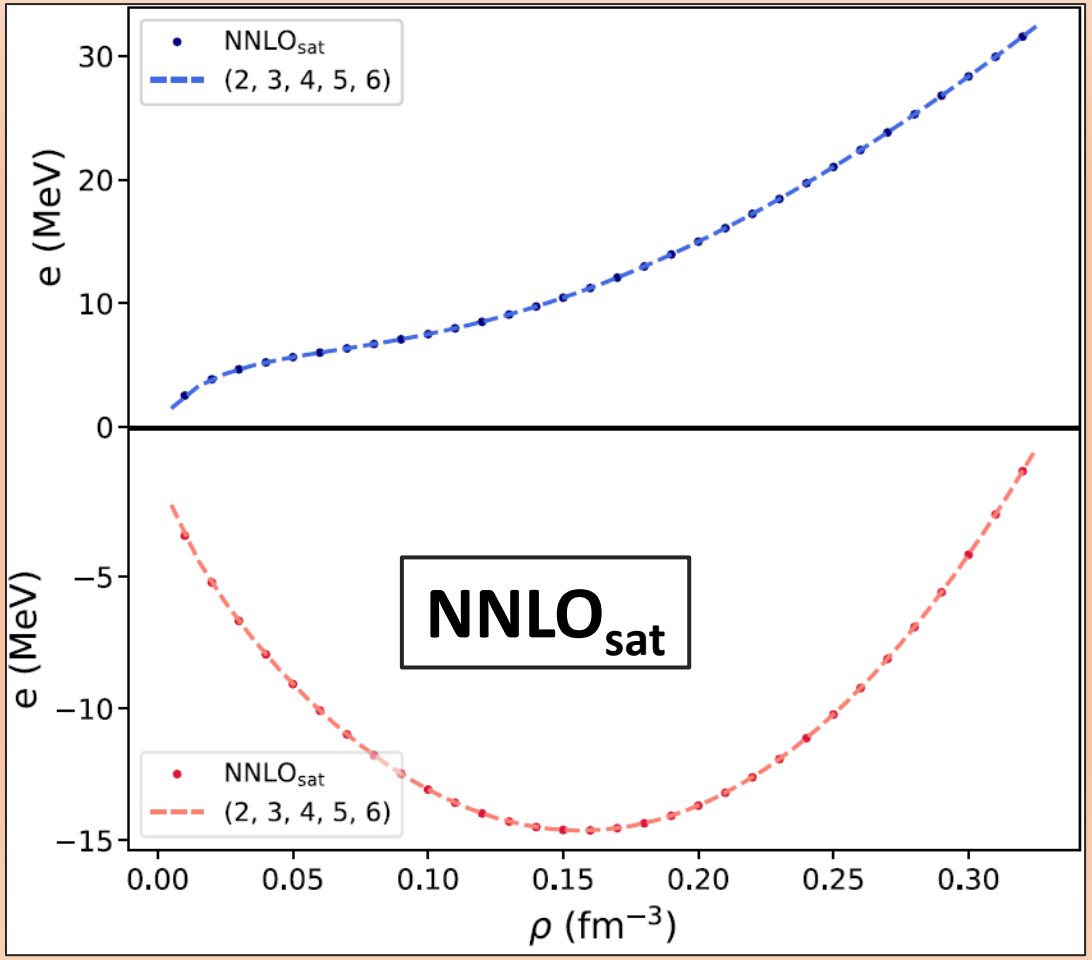

Results $NNLO_{sat}$

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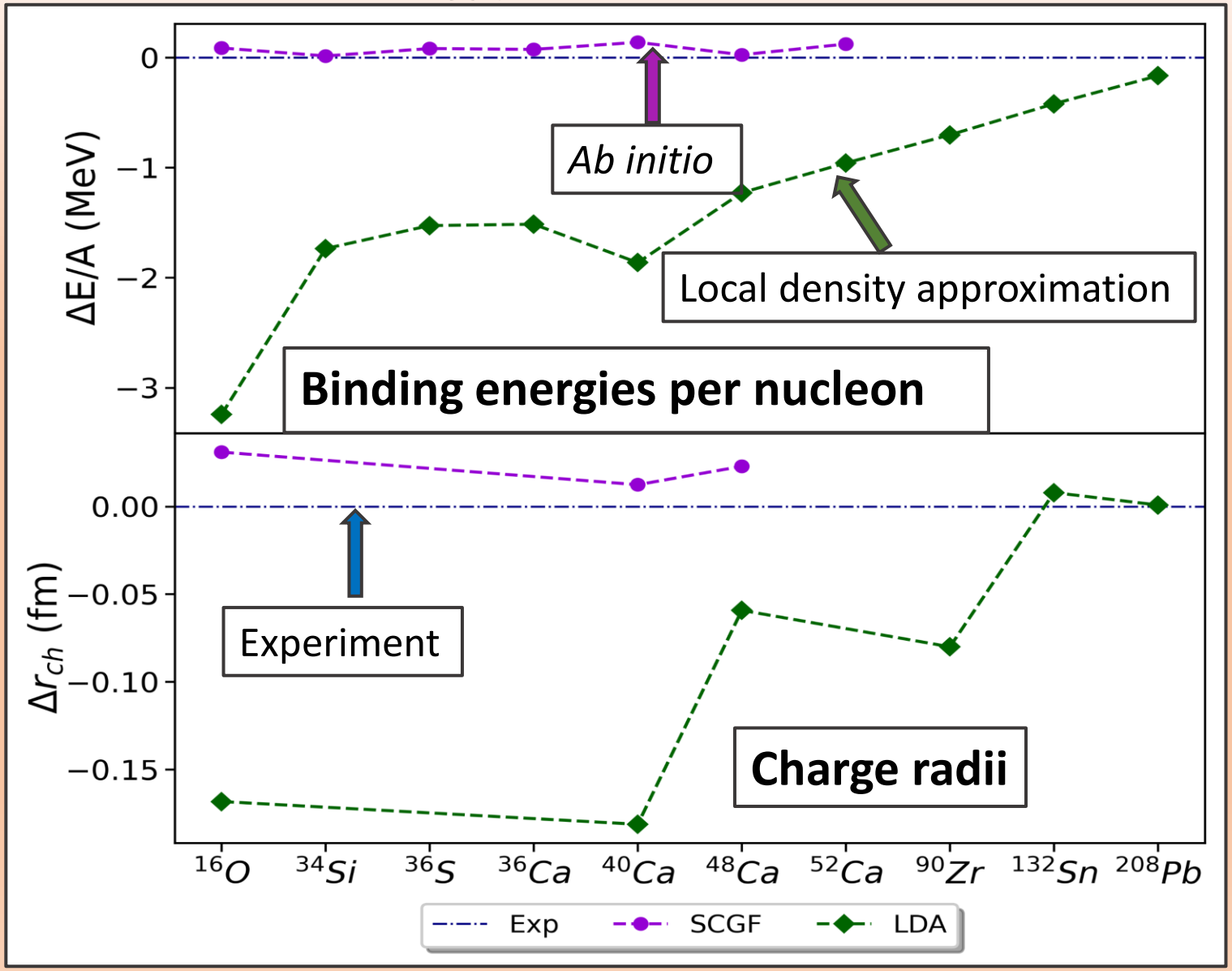

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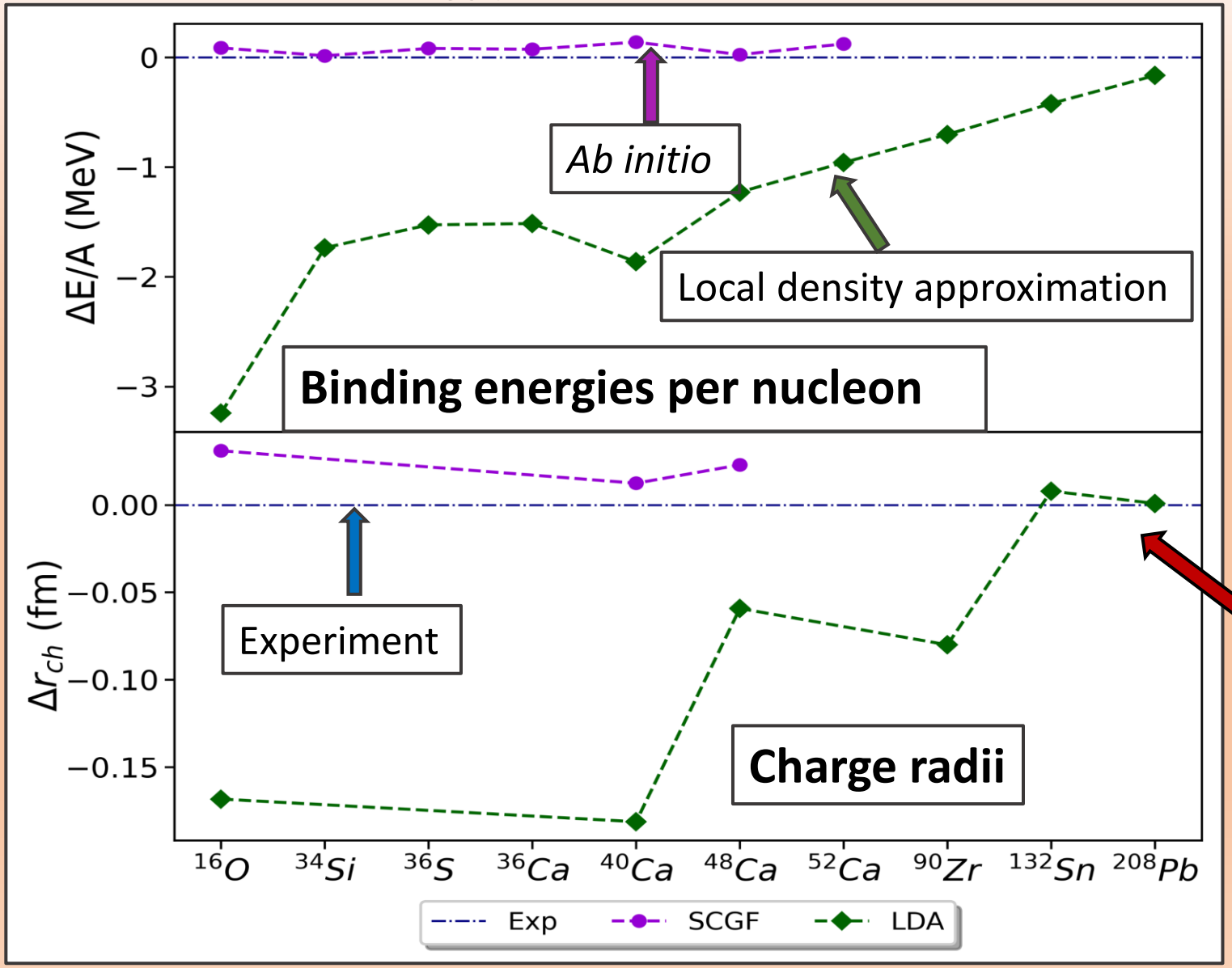

Ground state energies and charge radii of closed-shell nuclei with $NNLO_{sat}$ and SCGF in the **ADC(3)** scheme

Local density approximation is reasonable especially for heavy nuclei

Somà, Front. Phys. **8**, 340 (2020)

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

Results AV4’+UIX$_c$

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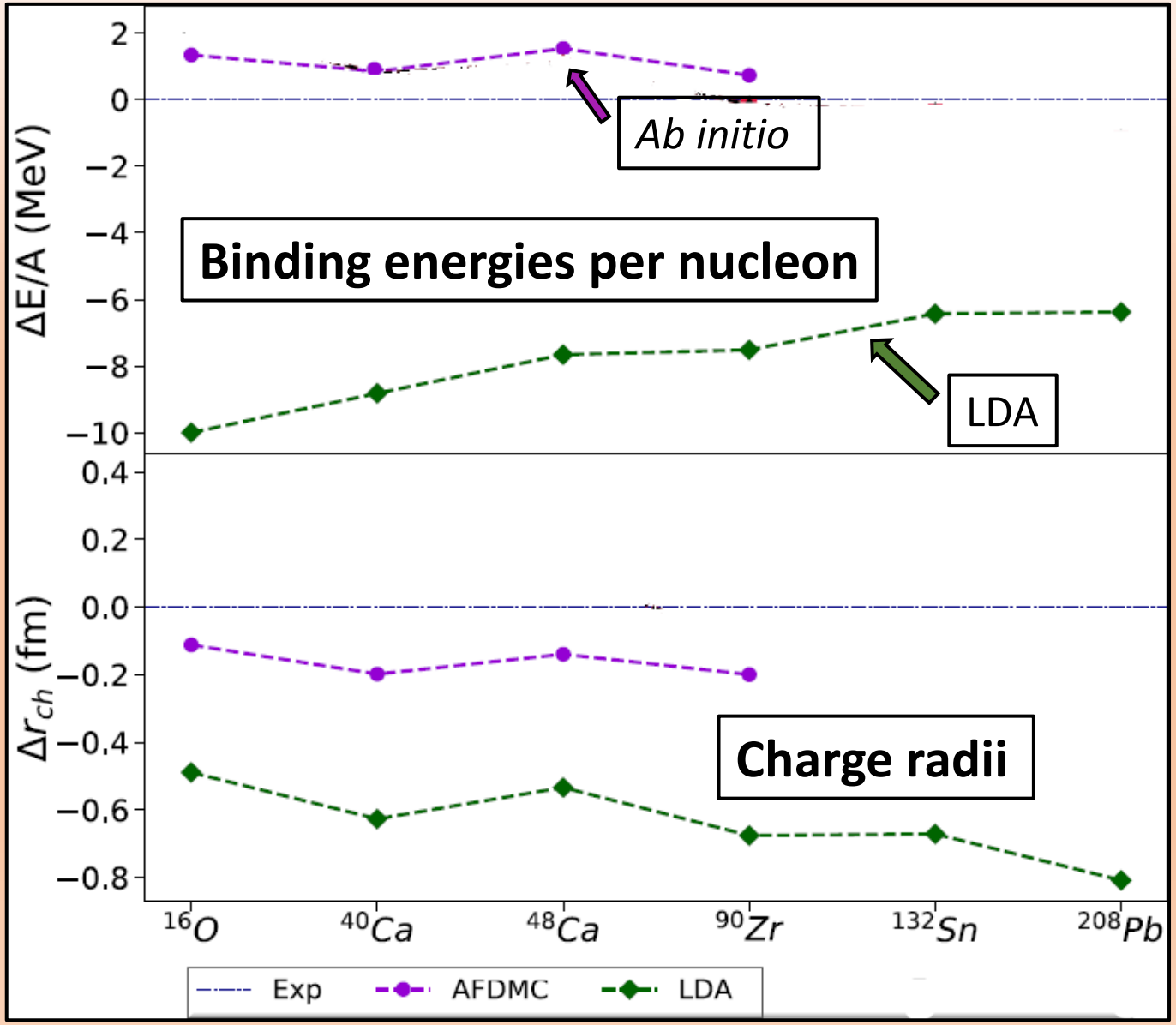

Ground state energies and charge radii of closed-shell nuclei with AFDMC and AV4'+UIX$_c$

Towards the gradient approximation 1

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Our approach → study **inhomogeneous model systems** *ab initio*

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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 $\xrightarrow{\textbf{GA}}$ $\boldsymbol{E[\rho, \nabla\rho, J]}$

See A. Gezerlis works, e.g.

Phys. Rev. C **95**, 044309 (2017)

Phys. Lett. B **818**, 136347 (2021)

The static response problem 1

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Uniform nuclear matter is perturbed by a **weak** external sinusoidal **potential**

$$v_{ext}(\boldsymbol{x}) = 2v_q \cos(\boldsymbol{q} \cdot \boldsymbol{x})$$

Perturbation of the number density

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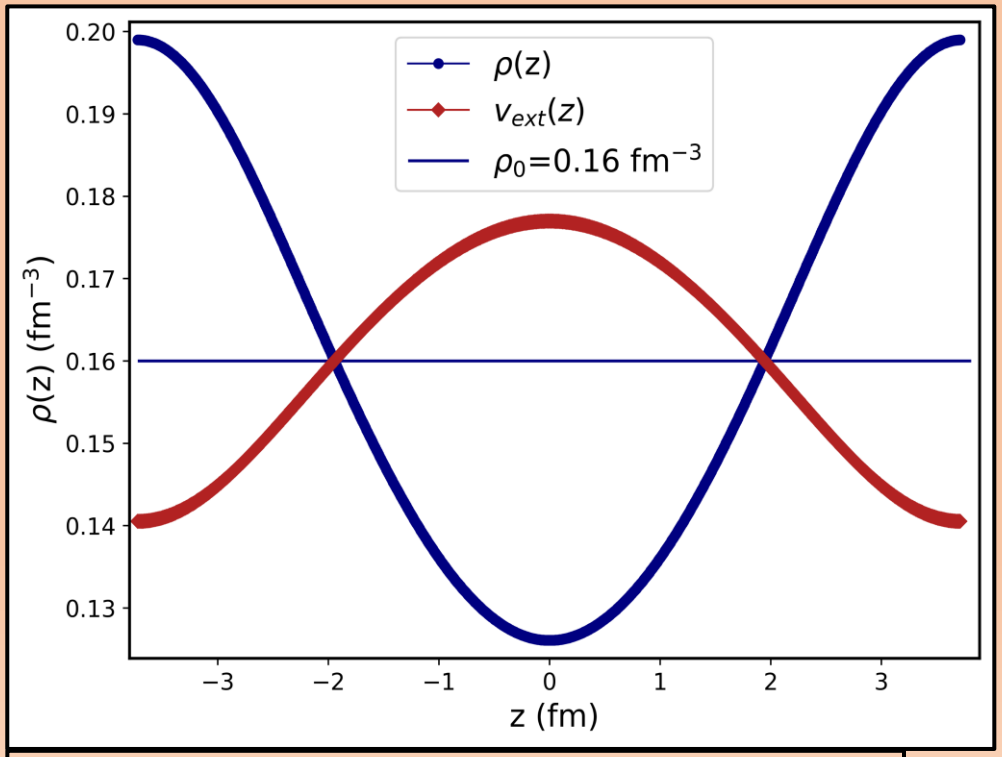
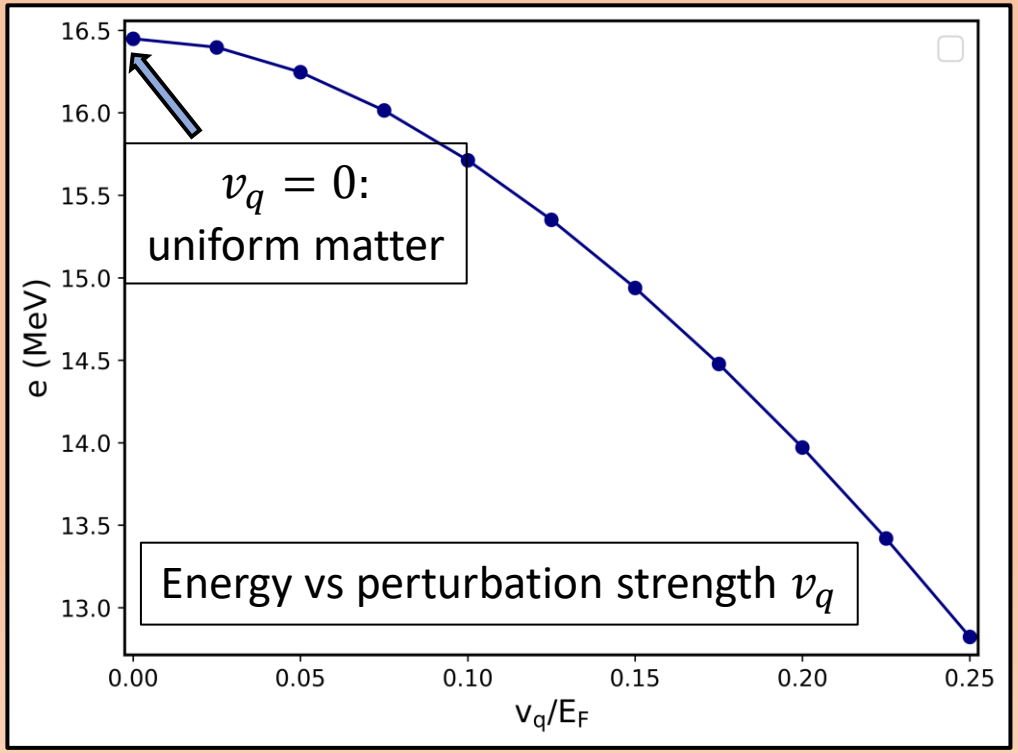
$$v_{ext}(\boldsymbol{x}) = 2v_q \cos(\boldsymbol{q} \cdot \boldsymbol{x})$$

Perturbation of the number density

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

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





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

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

The static response problem 2

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We perform calculations with a finite number of particles in a box with **periodic boundary conditions** (**N=66** neutrons, **A=132** nucleons)

DFT, AFDMC and (in progress) SCGF

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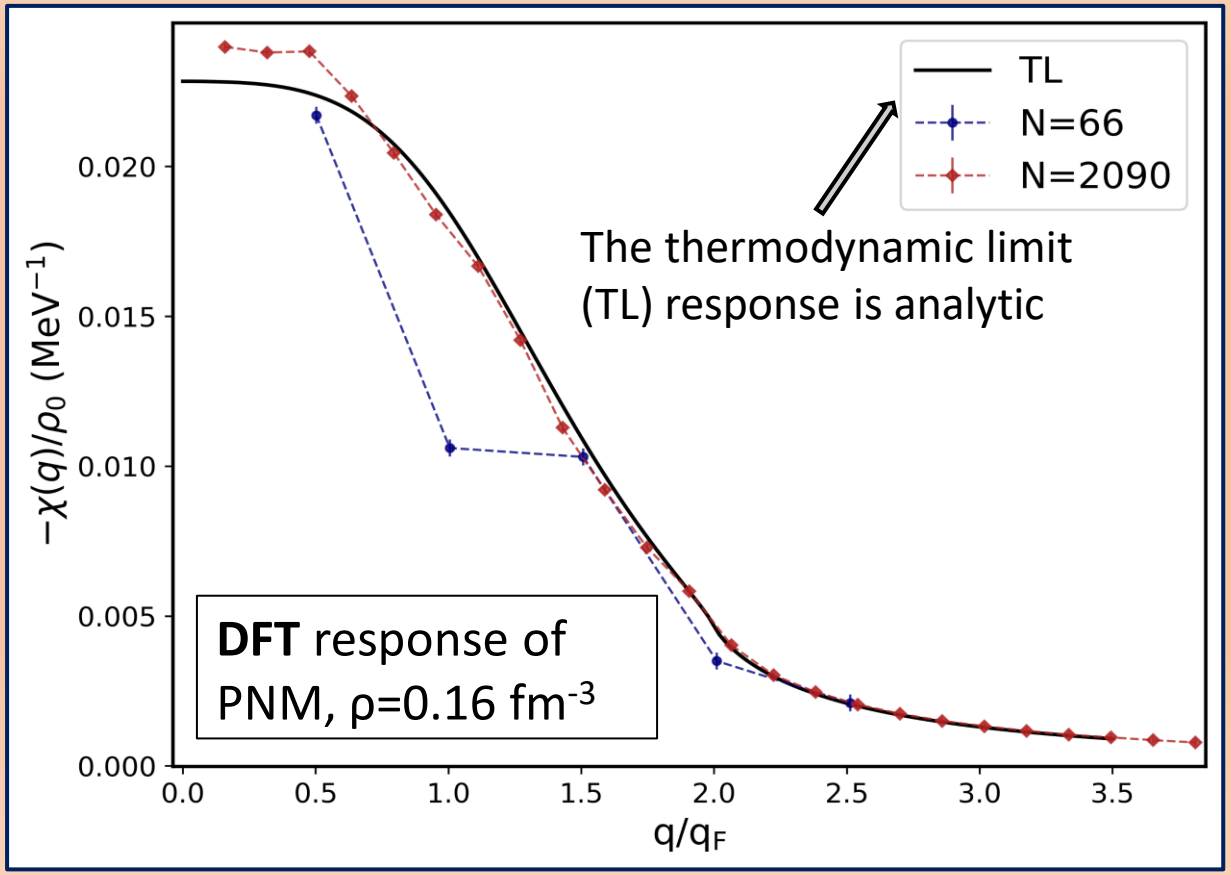
The momentum q is quantized
Strong finite-size effects on $\chi(q)$

$\chi(q)$ is extracted by fitting the energies $\delta e_v(v_q)$ at fixed q



AFDMC 1

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Diffusion Monte Carlo is an exact method for the many-body ground state

$$\Psi_0(X) = \lim_{\tau\to+\infty} \Psi(X,\tau) = \lim_{\tau\to+\infty} e^{-(\hat{H}-E_T)\tau}\, \Psi_T(X)$$

Imaginary-time **projection** of a trial state

$$E_0 = \lim_{\tau\to+\infty} \frac{\langle \Psi_T | \hat{H} | \Psi(\tau) \rangle}{\langle \Psi_T | \Psi(\tau) \rangle} = \frac{1}{M} \sum_{i=1}^{M} \frac{(H\Psi_T)(X_i)}{\Psi_T(X_i)}$$

Stochastic estimate of the energy

Gandolfi, Phys. Rev. C **90**, 061306 (2014)
Gezerlis, Phys. Rev. C **95**, 044309 (2017)

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Stochastic estimate of the energy

The AV4' interaction contains four operators

$$O_{ij}^p = 1, \sigma_i\cdot\sigma_j, \tau_i\cdot\tau_j, (\sigma_i\cdot\sigma_j)(\tau_i\cdot\tau_j)$$

$$\Psi_T(X) = \prod_{i<j} f(r_{ij})\left(1+\sum_{i<j}\sum_{p=1}^{4} f_p(r_{ij})O_{ij}^p\right)\Phi(X)$$

Jastrow correlations

Linear operator correlations

Mean field state

Gandolfi, Phys. Rev. C **90**, 061306 (2014)
Gezerlis, Phys. Rev. C **95**, 044309 (2017)

AFDMC 2

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In uniform matter, $\Phi(X)$ is commmonly taken to be a Slater determinant of plane waves

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Improved ansatz → start from **Mathieu orbitals**

$$-\frac{\hbar^2}{2m}\psi''(x) + 2v_q \cos(qx)\,\psi(x) = \epsilon\,\psi(x)$$

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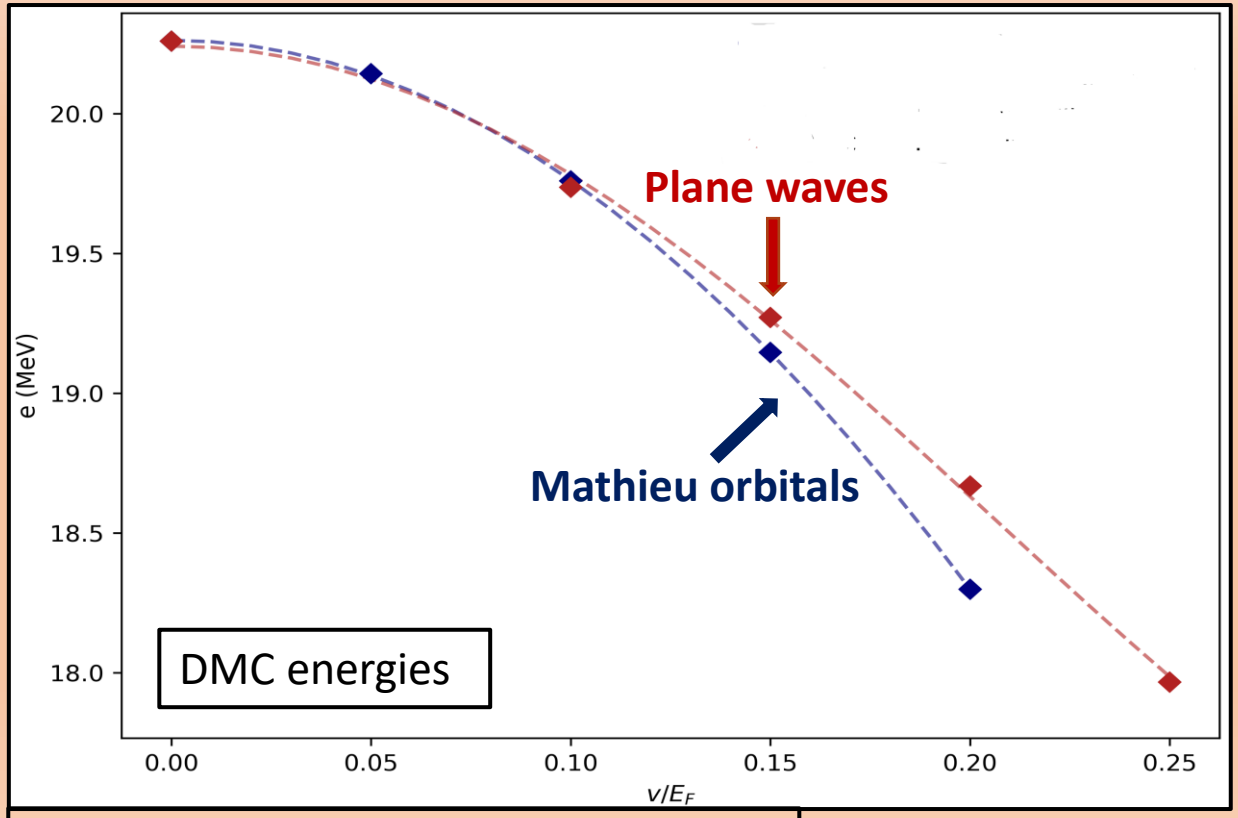
$$-\frac{\hbar^2}{2m}\psi''(x) + 2v_q \cos(qx)\,\psi(x) = \epsilon\,\psi(x)$$

The effect of the perturbation is accounted for and the energy is **lowered**



PNM, N=66, $\rho_0 = 0.16\ \mathrm{fm}^{-3}$, q/q_{min}=1

Gezerlis, Phys. Rev. C **95**, 044309 (2017)

Results AFDMC

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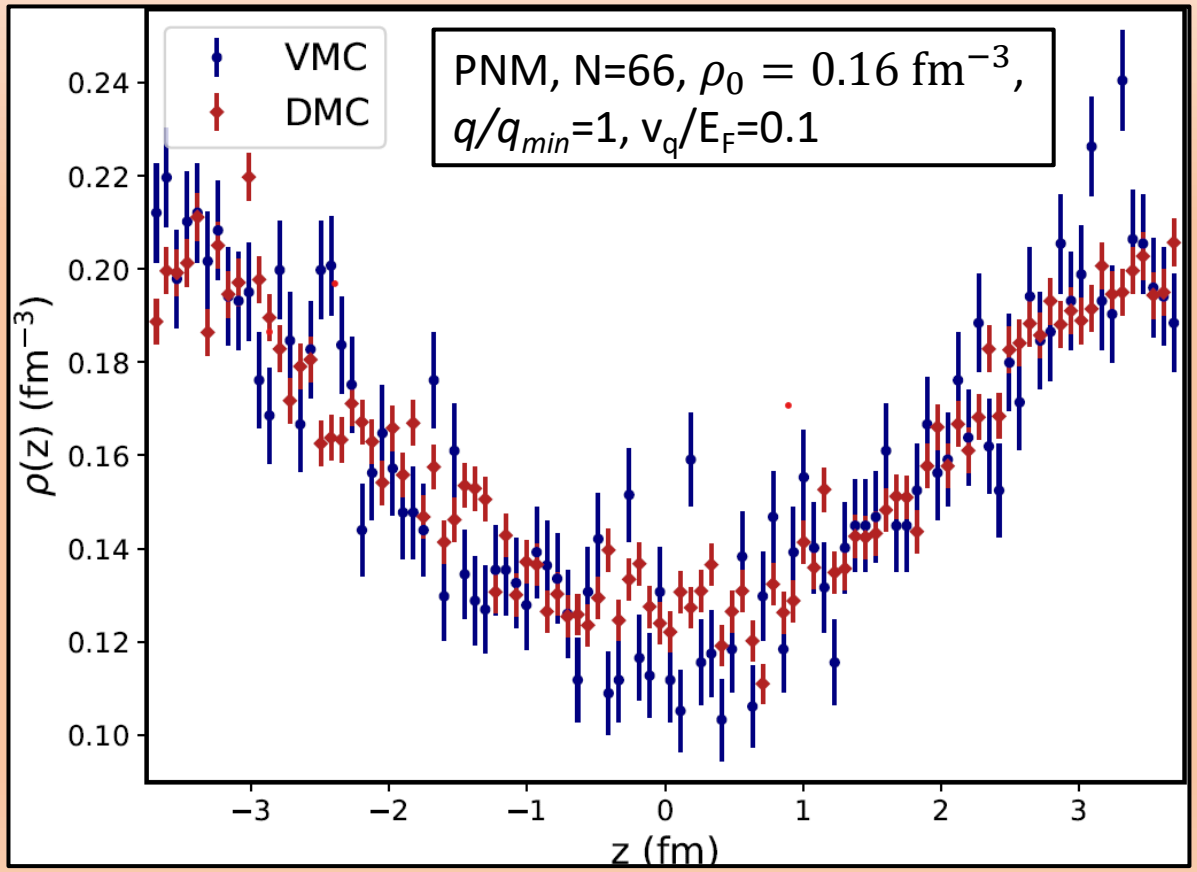
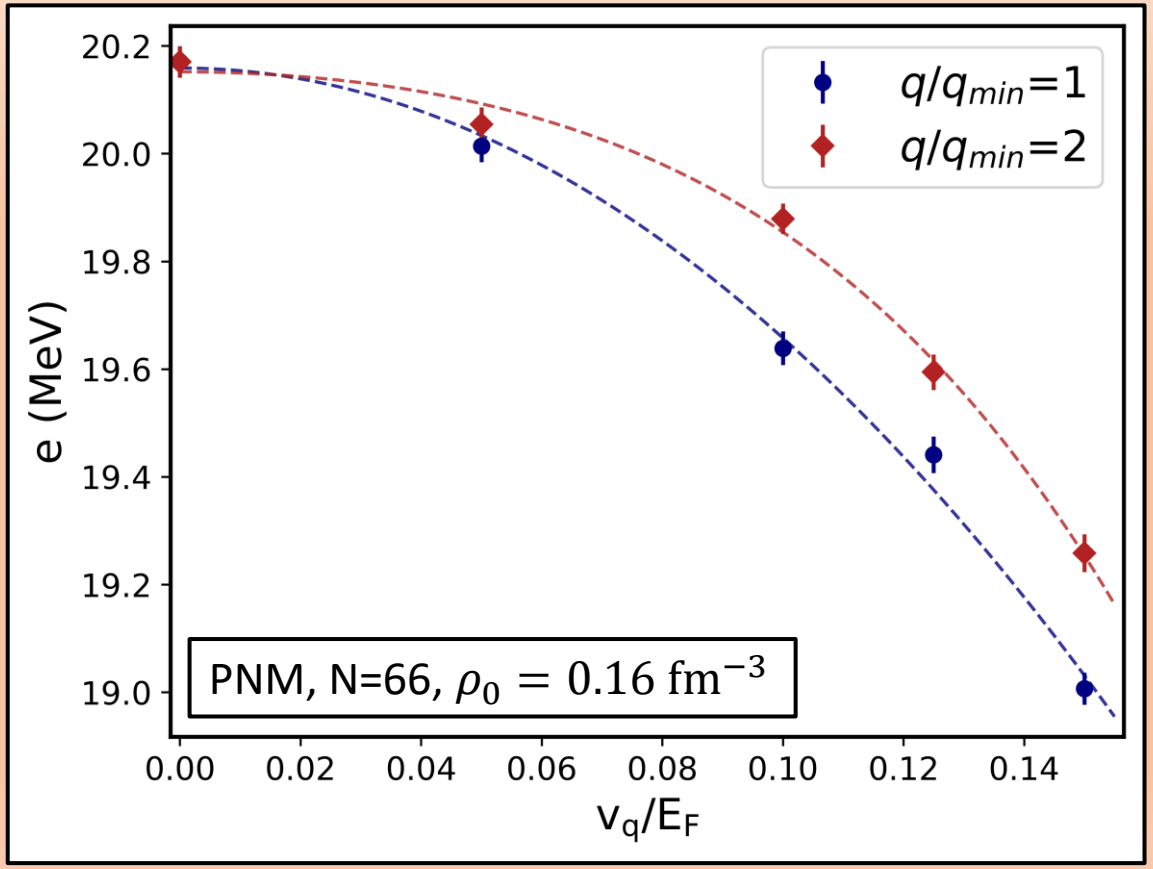
Results with the improved trial wave functions in PNM





Next steps: run at several momenta, complete SNM

Towards the gradient approximation 2

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Perturbed nuclear matter calculations in both **SNM** and **PNM**

Towards the gradient approximation 2

Perturbed nuclear matter calculations in both **SNM** and **PNM**

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

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

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

Match DFT and *ab initio* energies at a finite number of nucleons

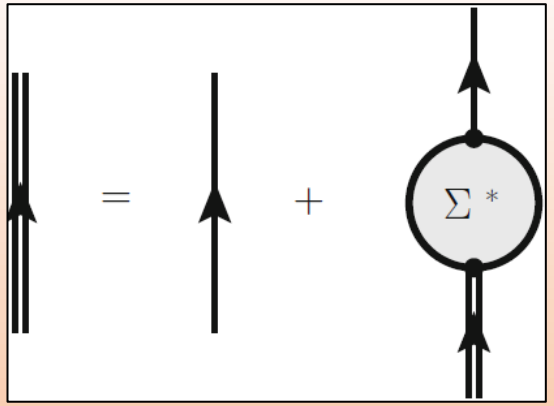
Self-consistent Green's functions

Self-consistent Green's functions

Dyson equation $$g_{\alpha\,\beta}(\omega) = g^{(0)}_{\alpha\,\beta}(\omega) + \sum_{\gamma\delta} g_{\alpha\,\gamma}(\omega)\Sigma^{*}_{\gamma\delta}(\omega)g^{(0)}_{\delta\,\beta}(\omega)$$

One-body propagator

Self-energy



See Carlo Barbieri's talk

$g_{\alpha\,\beta}(\omega)$ gives access to total energy, addition/removal energies, single-particle observables, spectral functions…

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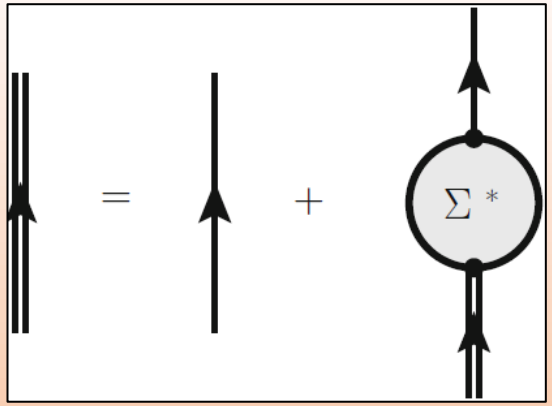

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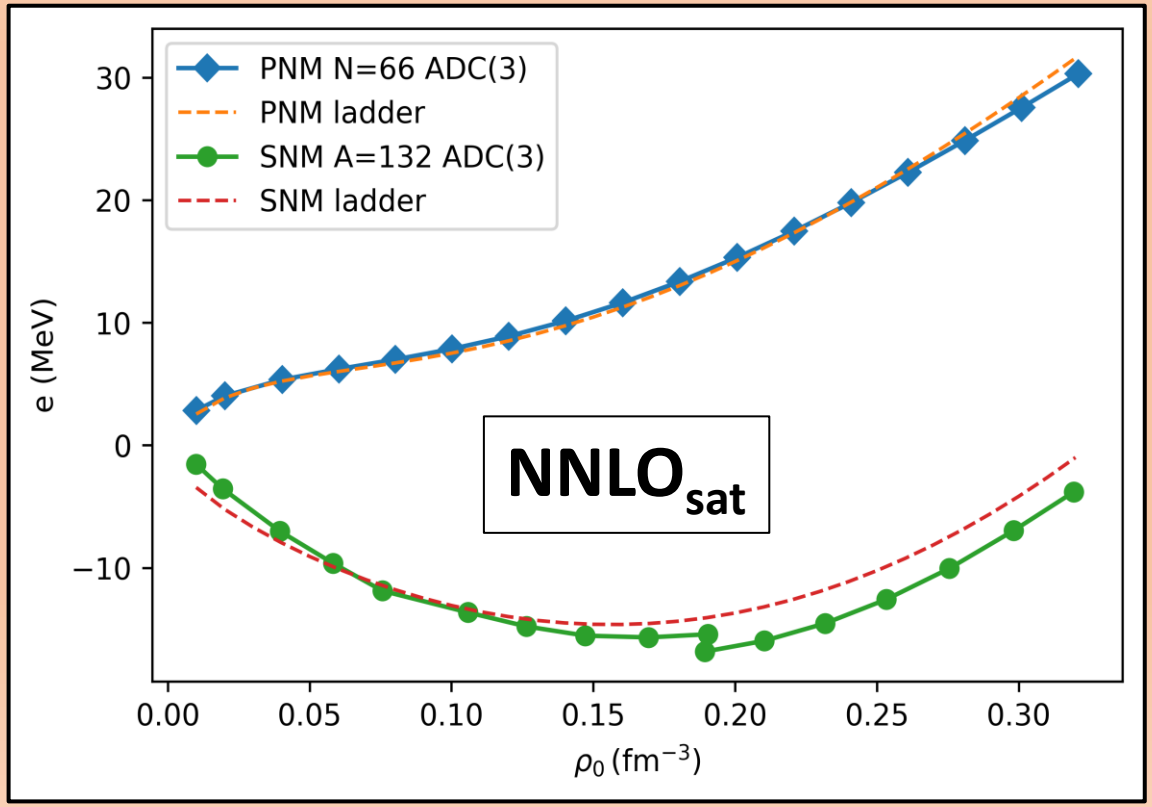
Currently implementing **ADC(3)** in infinite nuclear matter



Preliminary!

C. Barbieri and A. Carbone, Lect. Notes Phys. **936**, 571 (2017)
C. McIlroy, Ph.D. thesis, University of Surrey (2020)

Conclusion and perspectives

- We are developing a **ladder** of ***ab initio*-constrained** nuclear EDFs
- We have implemented the first rung, the **local density approximation**
- Calculations of the **response of nuclear matter** to a static perturbation are being performed.
- Completing the **gradient approximation** and **applying** the new EDF to collective states (RPA) are our near-term goals

Thank you for your attention!

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

Nuclear energy density functionals grounded in *ab initio* calculations

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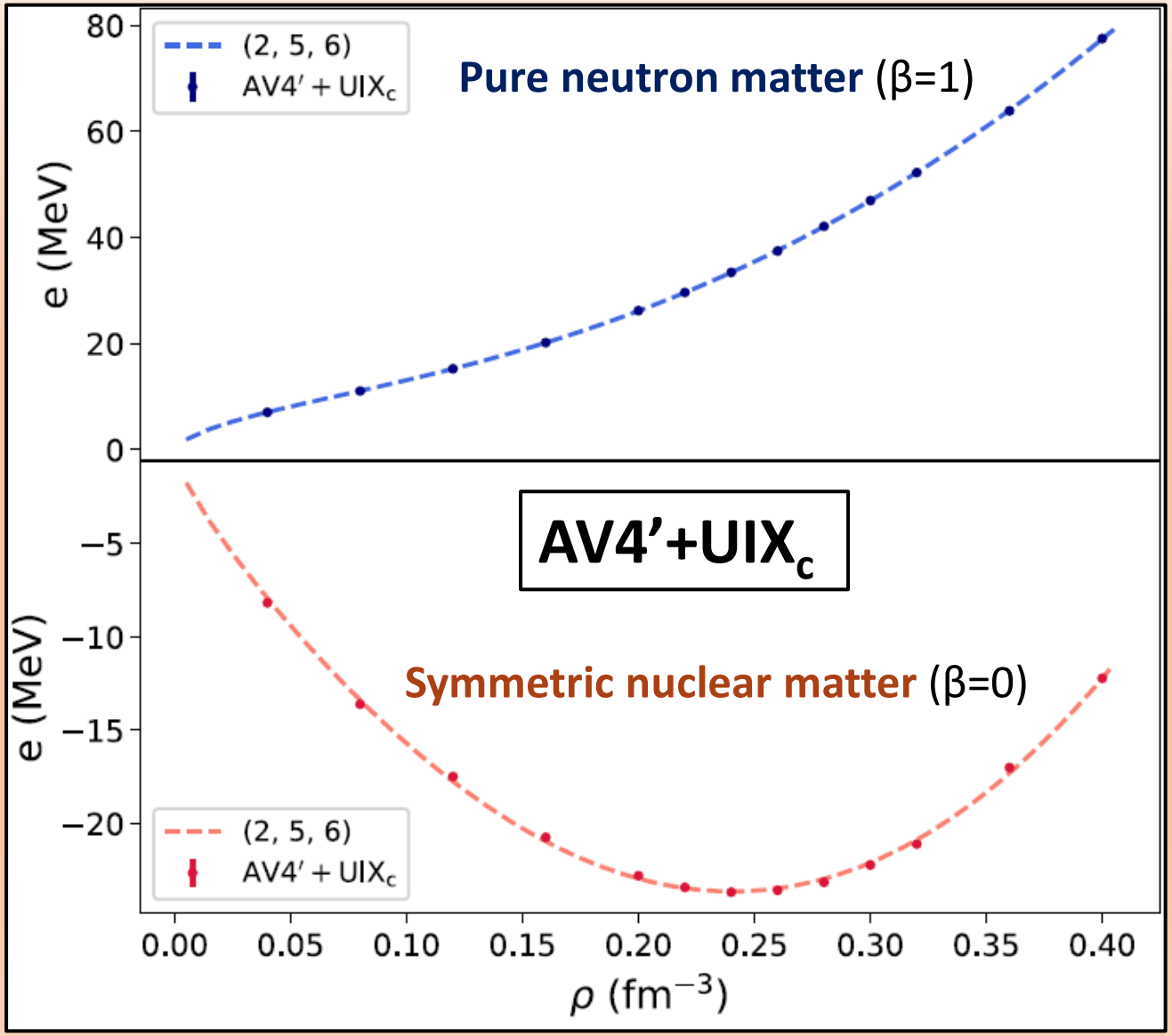
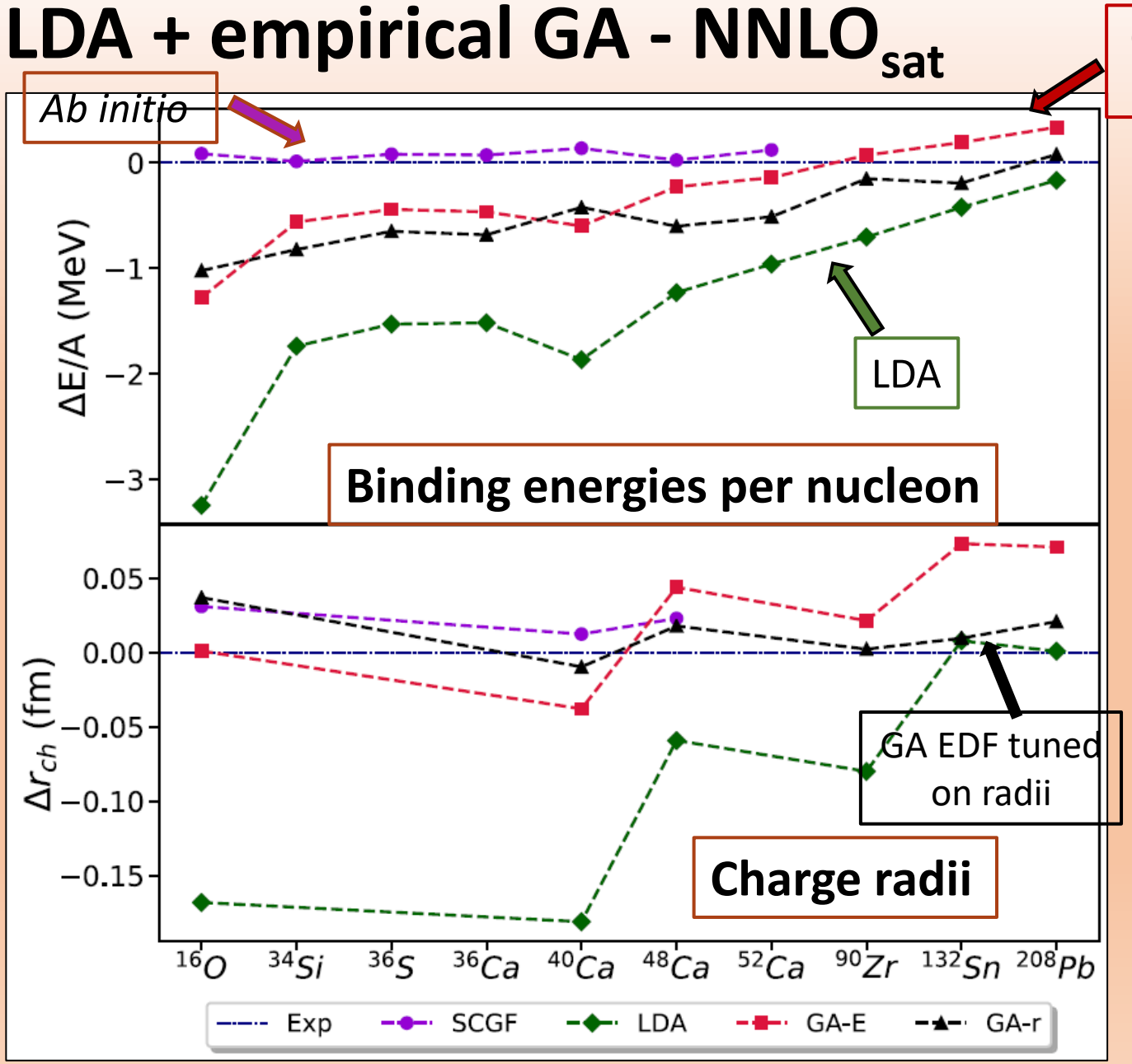
Equation of state - AV4'+UIX$_c$

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

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



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



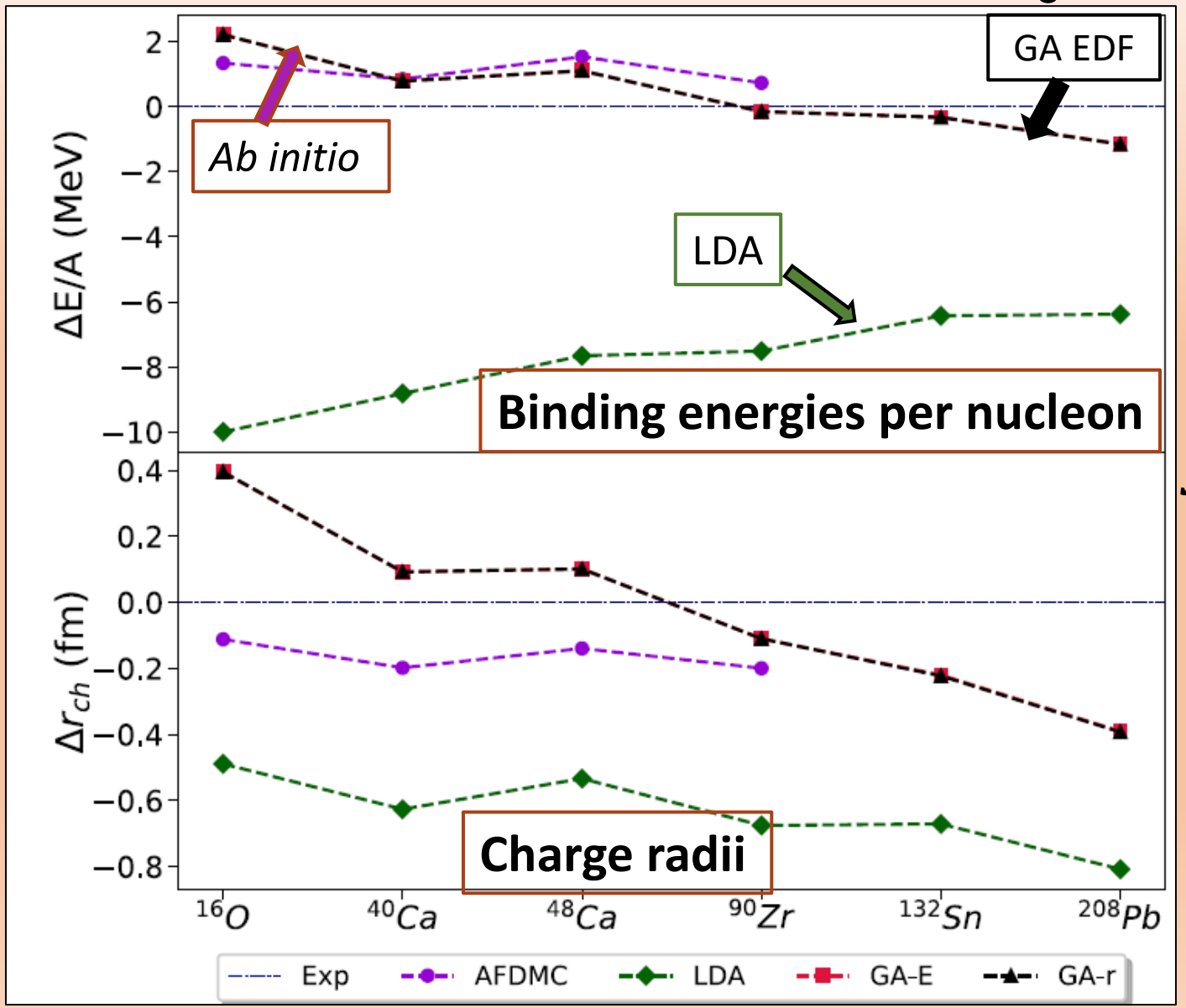
We have devised preliminary gradient approximation (GA) EDFs

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

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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