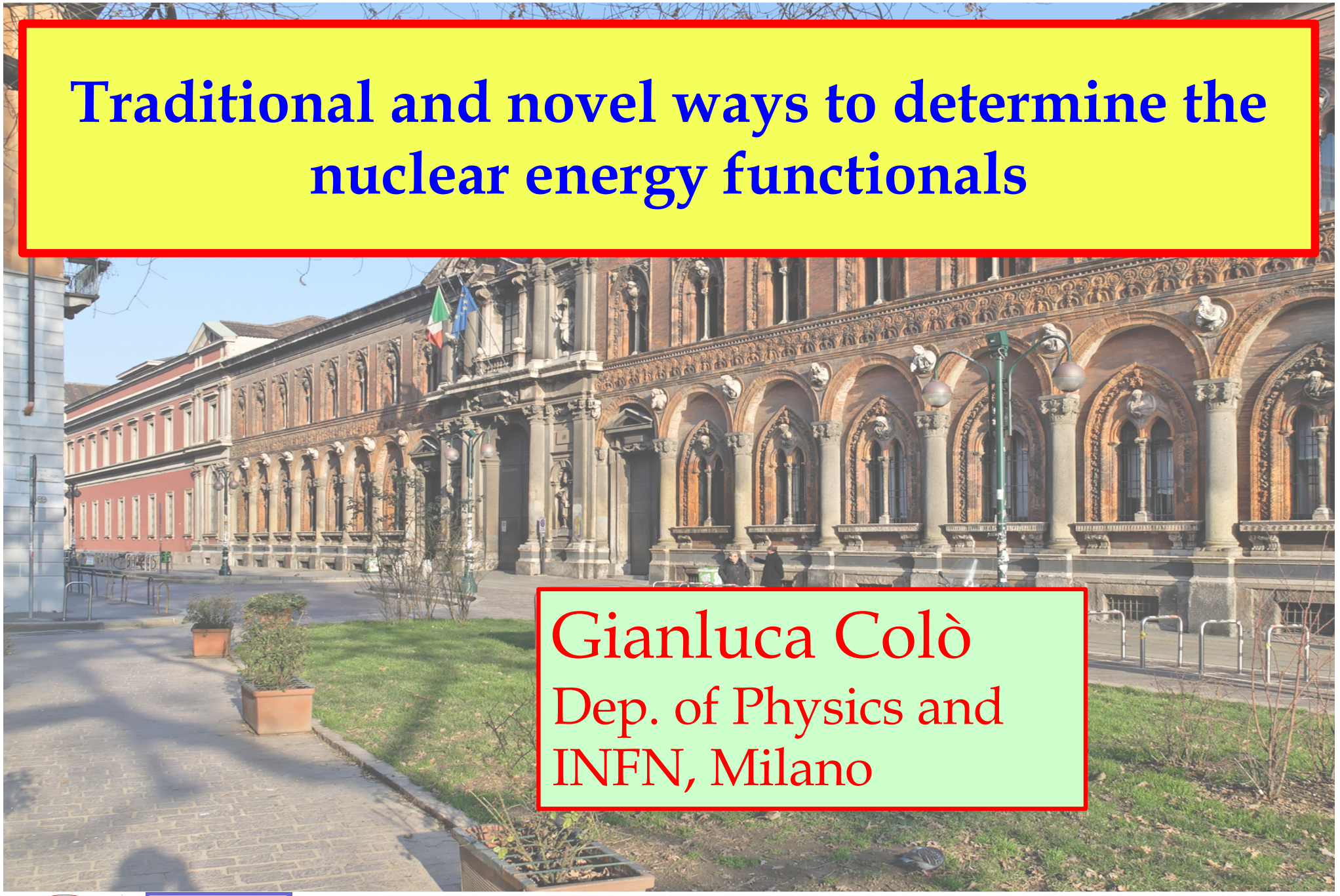
Traditional and novel ways to determine the nuclear energy functionals



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Outline of the talk

- Nuclear Density Functional Theory (DFT) and its current status (brief)
- "Tensions" in current energy functionals (EDFs)
- Novel ideas
- The inverse Kohn-Sham problem
- *Ab initio*-based EDFs

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(Nuclear) Density Functional Theory

$$E = \int \mathcal{E}[\rho]\ d^3r$$

Energy density = $\mathcal{E}$

E is a functional called **EDF**

$$E_{\text{ground state}} = \min_\rho E[\rho]$$

The **exact** functional has a **minimum** at the exact ground-state density, where it assumes the exact E as a value.

- Existence is guaranteed by the Hohenberg-Kohn theorem.
- It gives access, in principle, to all properties of the system.

- The theorem does **not** tell what the EDF looks like.
- Starting from current EDFs, the road for improvement is not fully clear.

- Alternative ways to proceed: highly welcome!

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The Kohn-Sham scheme

We assume that the density can be expressed in terms of **single-particle orbitals**, and that the kinetic energy has the simple form:

$$\rho(\vec{r}) = \sum_i \phi_i^*(\vec{r})\phi_i(\vec{r}) \qquad T = \sum_i \int d^3r\ \phi_i^*(\vec{r}) \left(-\frac{\hbar^2 \nabla_i^2}{2m} \right) \phi_i(\vec{r})$$

We have said that the energy must be minimized, but we add a constraint associated with the fact that we want **orbitals that form an orthonormal set** (Lagrange multiplier):

$$E - \sum_i \varepsilon_i \int d^3r\ \phi_i^*(\vec{r})\phi_i(\vec{r}) = T + F[\rho] + \int d^3r\ V_{\text{ext}}(\vec{r})\rho(\vec{r}) - \sum_i \varepsilon_i \int d^3r\ \phi_i^*(\vec{r})\phi_i(\vec{r})$$

The variation of this quantity, ($\delta/\delta\phi^*$)... = 0 produces a Schrödinger-like equation:

$$\left(-\frac{\hbar^2 \nabla_i^2}{2m} + \frac{\delta F}{\delta \rho} + V_{\text{ext}} \right) \phi_i(\vec{r}) = \varepsilon_i \phi_i(\vec{r}) \qquad v[\rho] = U[\rho] = \frac{\delta F}{\delta \rho}$$

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"DFT is an exactification of Hartree-Fock" (W. Kohn).

Nuclei are spin-1/2 fermions and the EDFs can depend on **number or spin densities**.

Generalised densities are obtained by the systematic use of derivative operators.

$$\rho(\mathbf{r}) = \rho(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}}$$

~~$$\mathbf{s}(\mathbf{r}) = \mathbf{s}(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}}$$~~

~~$$\mathbf{j}(\mathbf{r}) = \frac{1}{2i}(\nabla - \nabla')\,\rho(\mathbf{r},\mathbf{r}')\Big|_{\mathbf{r}'=\mathbf{r}}$$~~

$$\tau(\mathbf{r}) = \nabla\cdot\nabla'\rho(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}}$$

$$\mathbf{J}(\mathbf{r}) = \frac{1}{2i}(\nabla - \nabla')\otimes\mathbf{s}(\mathbf{r},\mathbf{r}')\Big|_{\mathbf{r}'=\mathbf{r}}$$

~~$$\mathbf{T}(\mathbf{r}) = \nabla\cdot\nabla'\mathbf{s}(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}}$$~~

Kinetic energy density

$$T = \int d^3r\ \frac{\hbar^2}{2m}\tau(\mathbf{r})$$

$$\mathbf{J}_{\mu\nu} = \frac{1}{3}\delta_{\mu\nu}J^{(0)} + \frac{1}{2}\sum_{\kappa}\epsilon_{\mu\nu\kappa}J^{(1)}_{\kappa} + J^{(2)}_{\mu\nu}$$

Spin-orbit density

Skyrme EDFs (even-even nuclei)

Local functionals depending on the various densities just introduced.

Proton/neutron labels are omitted for the sake of simplicity.

$$E = \int d^3r \ \left[\mathcal{E}^{\rm kin} + \mathcal{E}^{\rm Skyrme} + \mathcal{E}^{\rm pairing} + \mathcal{E}^{\rm Coulomb}\right]$$

$$\mathcal{E}^{\rm Skyrme} = C^{\rho\rho}[\rho]\rho^2 + C^{\rho\tau}\rho\tau + C^{J^2}\vec{J}^{\,2} + C^{(\nabla\rho)^2}\left(\vec{\nabla}\rho\right)^2 + C^{\rho\vec{\nabla}\cdot\vec{J}}\rho\vec{\nabla}\cdot\vec{J}$$

The quadratic form ensures the respect of the symmetries.

$$C^{\rho\rho}[\rho] = A + B\rho^{\gamma}$$

Parameters are determined by a **fit to data** (or pseudo-data).

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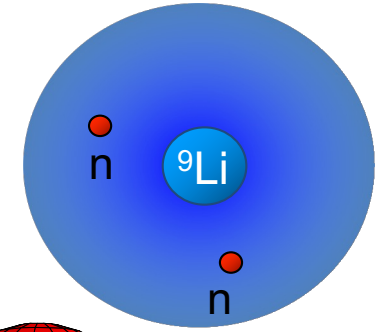
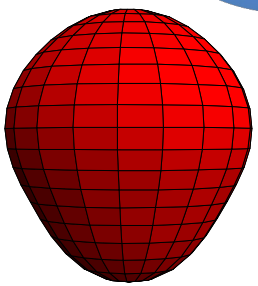
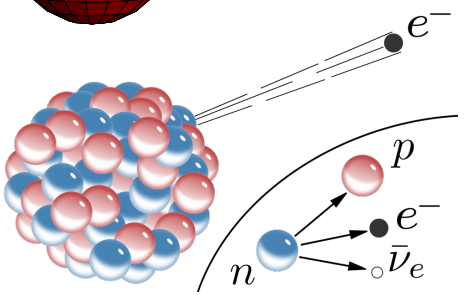
Status of nuclear DFT (very brief...)

- Error on **masses** of the order of 1 MeV.
- Predictions of **drip lines** and **super heavy** nuclei.
- Trends of **charge radii and deformations** fairly well reproduced.
- Advanced (multi-reference) techniques based on **symmetry restoration.**
- **Giant resonances, charge-exchange states and β-decay.**
- Current interest in **large amplitude motion, reactions** etc.

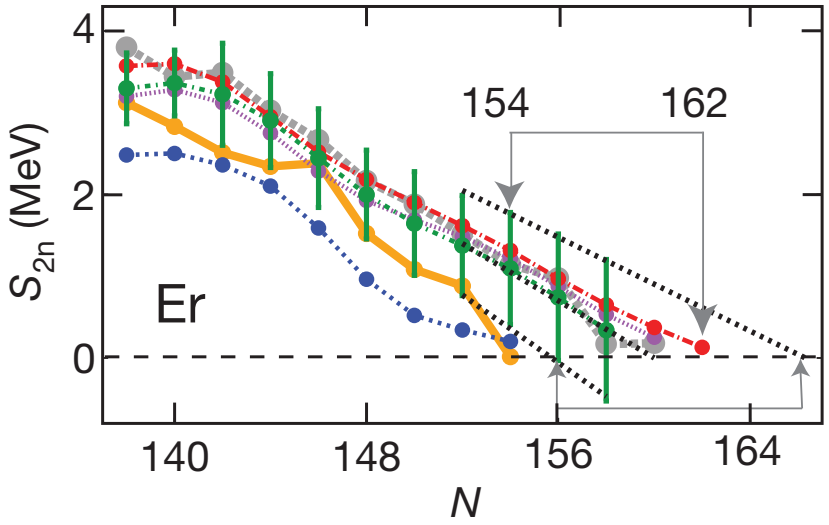






- There is no clear path for improving EDFs.

- Extrapolation of current EDFs towards the drip lines is a typical issue.



J. Erler *et al.*, Nature 486, 509 (2012)

- Other kinds of “tensions” exist...

Higher-order derivative terms

- The UNEDF collaboration **claimed that the standard Skyrme EDF has reached its limits** [M. Kortelainen *et al.*, Phys. Rev. C89, 054314 (2014)].
- Derivative operators up to fourth order have been introduced later on.
- There is no sign of a big improvement (yet one should mention the elimination of instabilities, and perhaps other weaker improvements).

PHYSICAL REVIEW C **96**, 044330 (2017)

Solution of Hartree-Fock-Bogoliubov equations and fitting procedure using the N2LO Skyrme pseudopotential in spherical symmetry

P. Becker,[1,*] D. Davesne,[1,†] J. Meyer,[1] J. Navarro,[2,‡] and A. Pastore[3,§]
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CNRS-IN2P3, UMR 5822, Institut de Physique Nucléaire de Lyon
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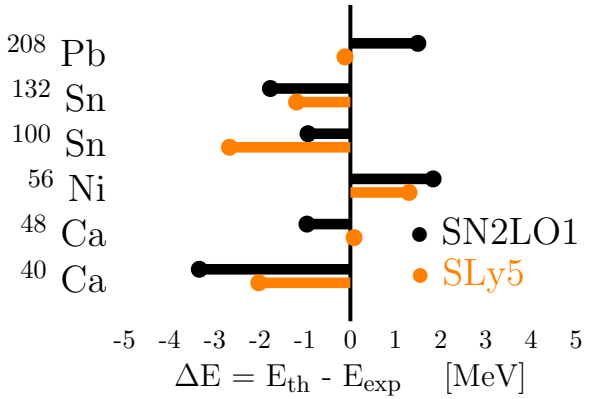
(Received 26 July 2017; published 26 October 2017)



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Recent results from PREX and CREX

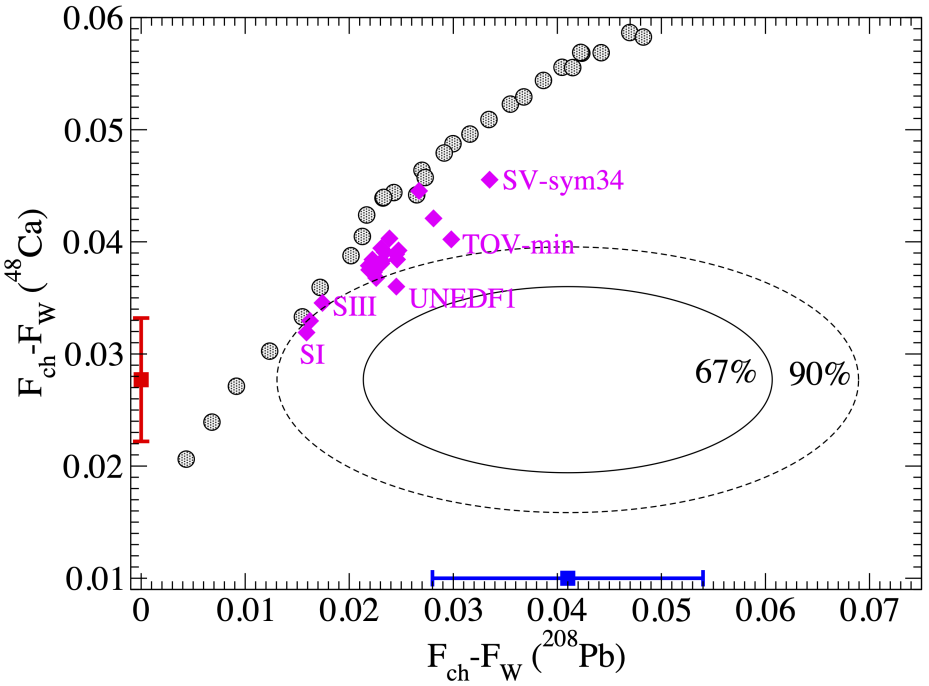
Parity-violating asymmetry measured in electron scattering is a probe of the neutron distribution (in principle, a model-independent probe).

Precision Determination of the Neutral Weak Form Factor of ^{48}Ca

(The CREX Collaboration)

Fig. 2 from
arXiv:2205:11593v1 [nucl-exp]

Results from nonrelativistic EDFs (magenta) and relativistic EDFs (grey) are displayed



New avenues

- Bayesian inference, machine learning...

- Reverse engineering: deduce EDFs from reliable energies/densities (i.e. the inverse KS problem).

- Building the EDFs from *ab initio*.

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- **The inverse Kohn-Sham problem**

G. Accorto *et al*., Phys. Rev. C101, 024315 (2020).

A. Liardi *et al*., Phys. Rev. C105, 034309 (2022).

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General formulation

Direct problem

$$F[\rho] \rightarrow v[\rho] \rightarrow \rho$$

Inverse problem

$$\rho \rightarrow v[\rho] \rightarrow F[\rho]$$

Y. Wang and R.G. Parr, Phys. Rev. A47, R1591 (1993).

R. Van Leeuwen and E.J. Baerends, Phys. Rev. A49, 2421 (1994).

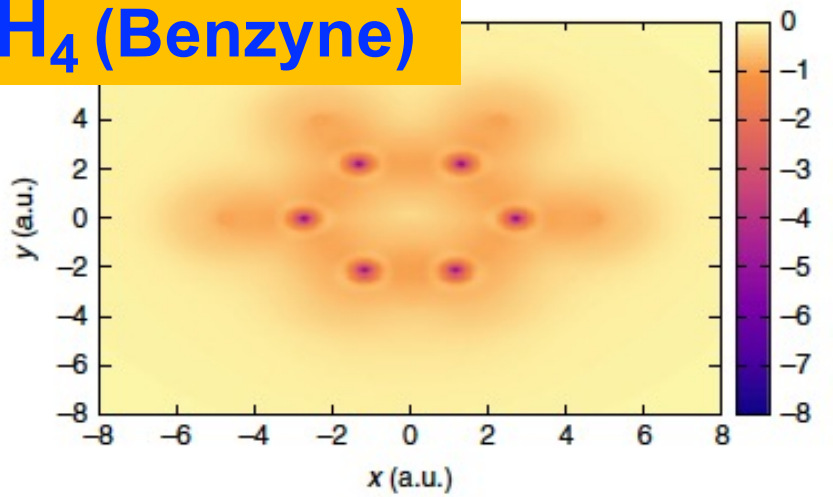
D.S. Jensen and A. Wassermann, Int. J. Quant. Chem. 118, e25425 (2018).

B. Kanungo, P.M. Zimmermann, V. Gavini, Nature Communications 10, 4497 (2019).

Some attempts have been made in the case of electronic systems, but not yet for atomic nuclei.

Input: target density $\tilde{\rho}(\vec{r})$

C_6H_4 (Benzyne)



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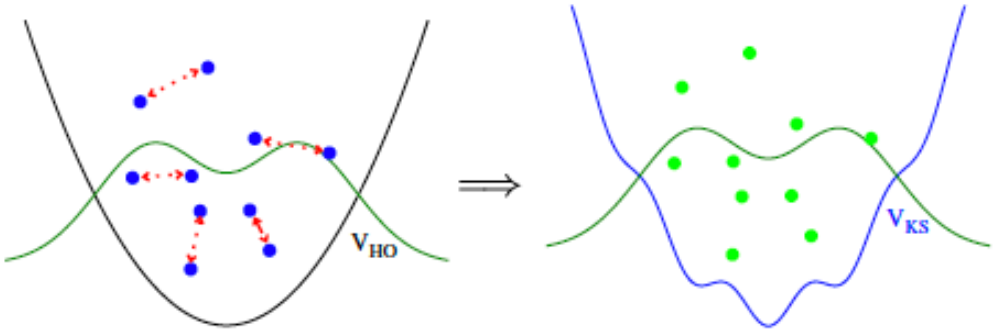
The constrained variational (CV) method



In the Kohn-Sham spirit, the system at hand is assumed to be equivalent to a **non-interacting system with the same density** $\Longrightarrow$ min. of the kinetic energy T

$$J = T_s\left[\{\phi_i\}\right] + \int d^3r\; U(\vec{r})\rho(\vec{r}) - \sum_{i=1}^{N_{\rm orb}}\sum_{j=1}^{i}\epsilon_{ij}\int d^3r\;\phi_i^*(\vec{r})\phi_j(\vec{r}).$$

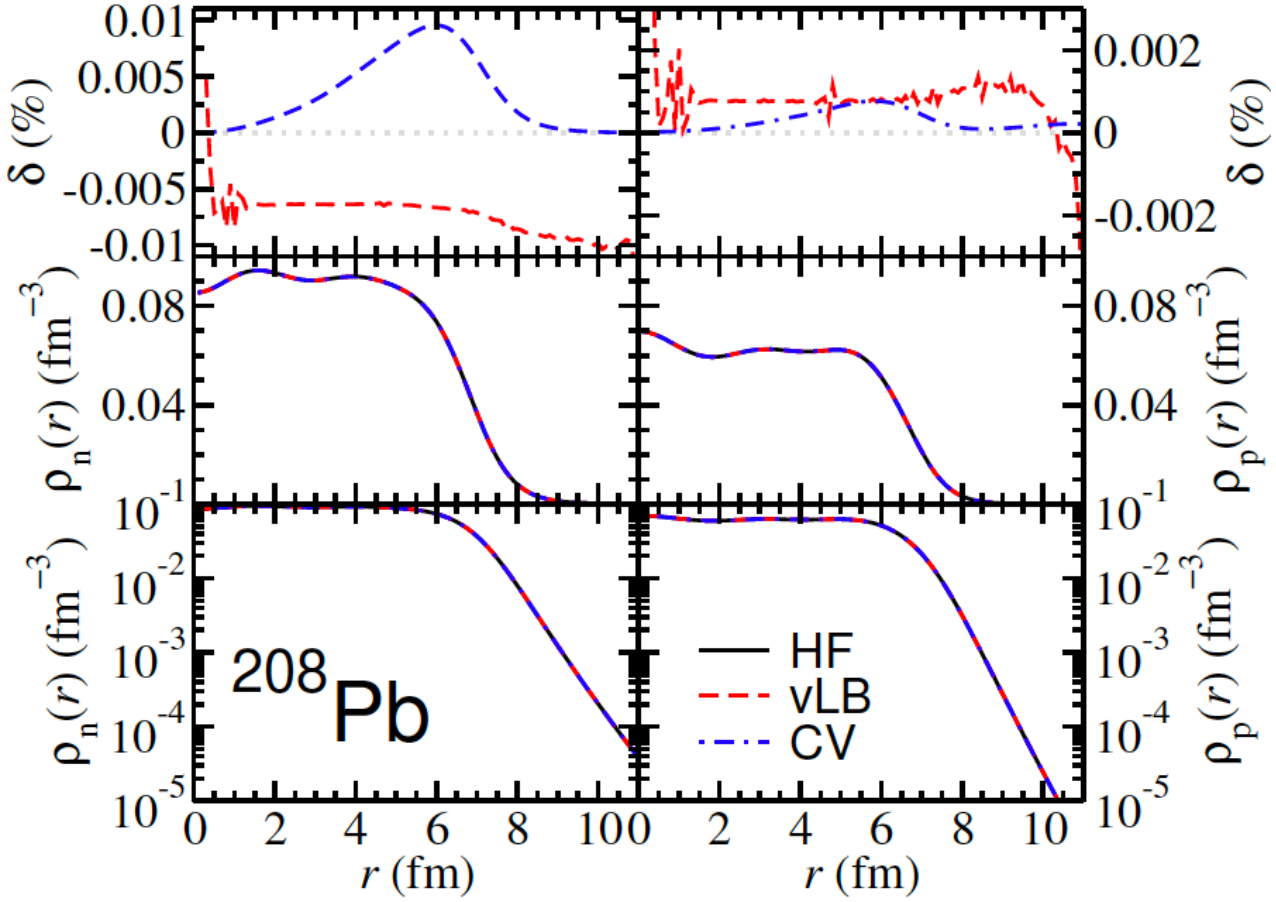
Constraints for: reproduction of target density plus orthonormality of the orbitals

$$\delta J = 0$$

The method is general/unbiased.

It relies on the IPOPT library

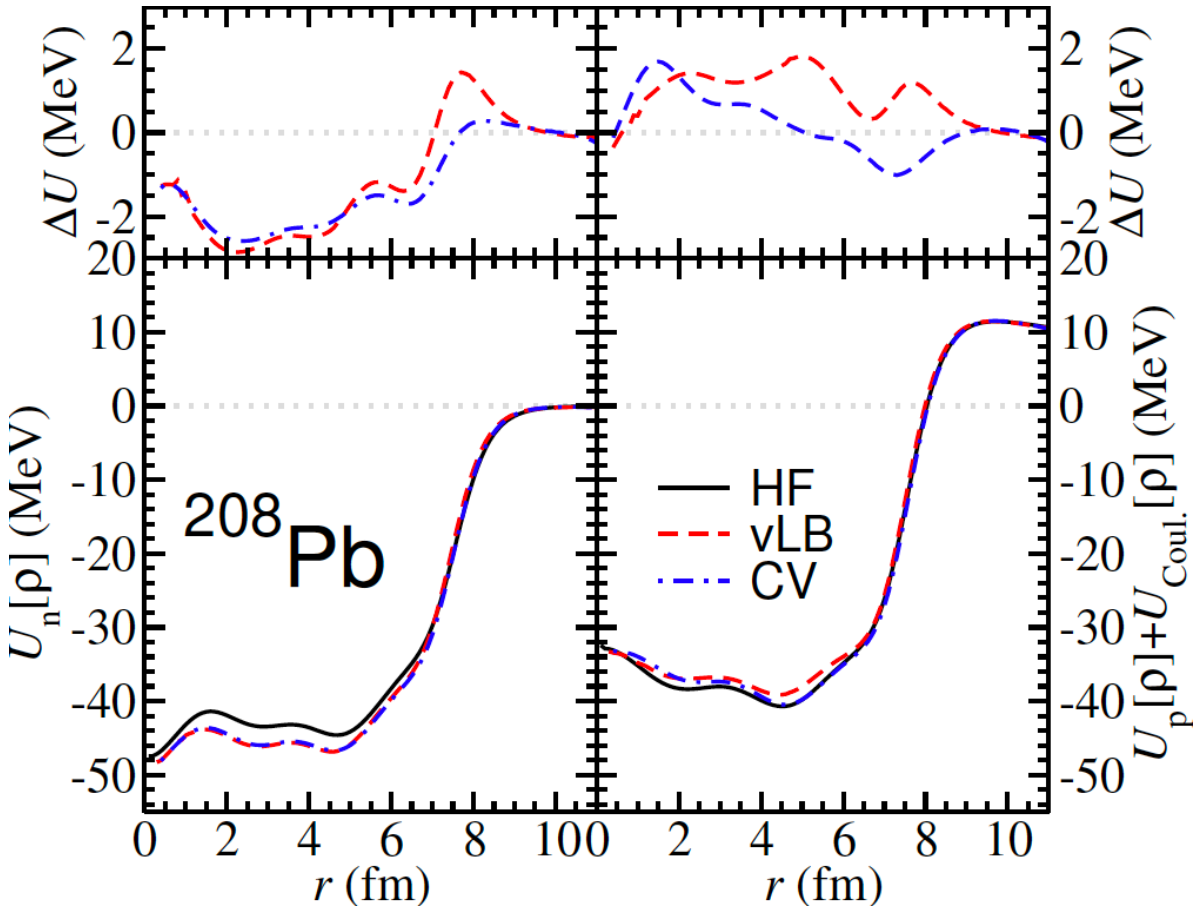
Reproduction of the target densities



The target densities are reproduced with a quite high accuracy.

This paves the way for the **introduction of densities either from experiment or *ab initio* approaches.**

Results for the effective potential

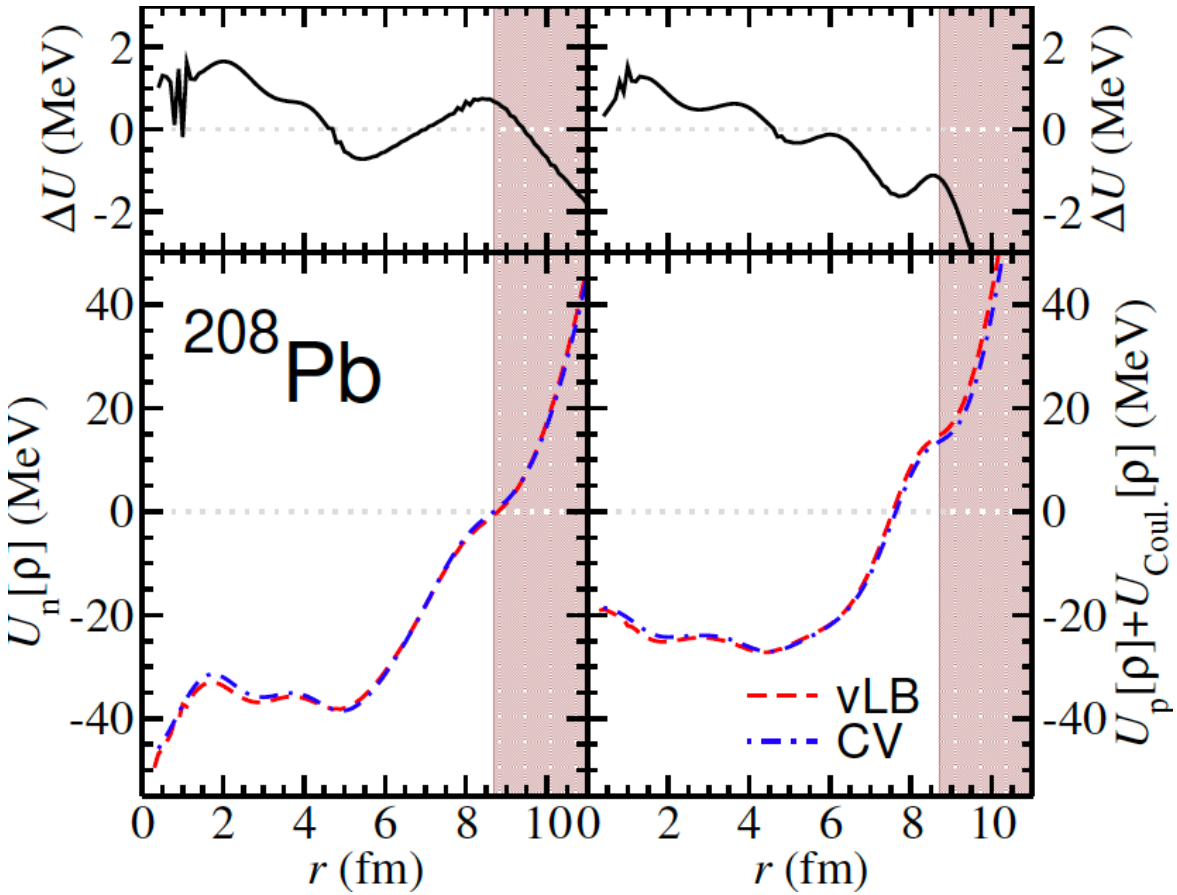


SkX has an effective mass close to 1 (within ≈ 5%)

Still, **"errors"** are also associated with the fact that the problem is not well defined according to Hadamard's definition.

Coulomb tail is fairly well extracted!

Effective potential from experimental densities



Critical point:
Experimental densities are written in terms of a **sum of Gaussians.**

$$\sum_{i=1}^{N} \frac{A_i^{(p,n)}}{\gamma^3} \left\{ e^{-\frac{(r-R_i)^2}{\gamma^2}} + e^{-\frac{(r+R_i)^2}{\gamma^2}} \right\}$$

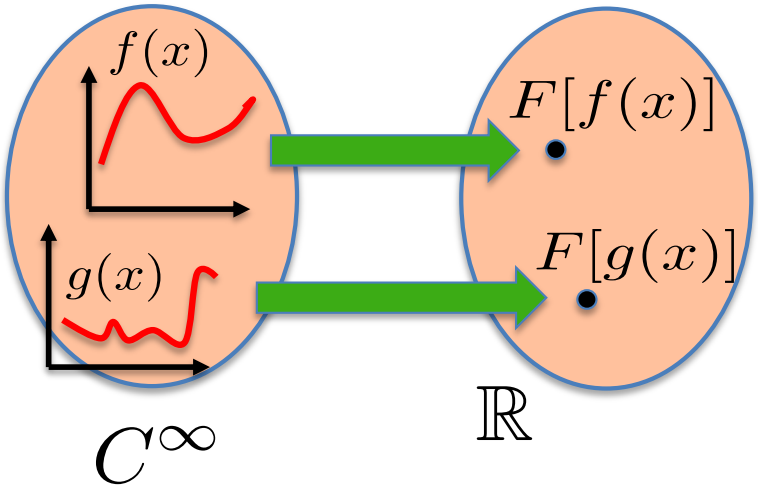
For radii larger than the radius of the last Gaussian, the IKS sees the **tail** of the density as caused by a **HO potential**.

Nevertheless, the two methods give consistent results.

How to deduce the EDF?

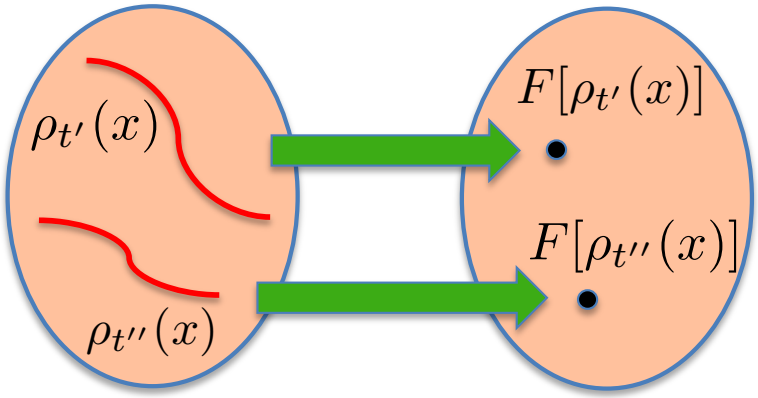
$$v[\rho] = \frac{\delta F}{\delta \rho}$$

Some kind of **functional integration** is called for.



A **line integration formula** has been proposed by Van Leeuwen and Baerends [PRA 51, 170 (1995)]

$$F[\rho_B] - F[\rho_A] = \int_A^B dt \int d^3r \; v[\rho_t] \frac{d\rho_t(\vec{r})}{dt}$$



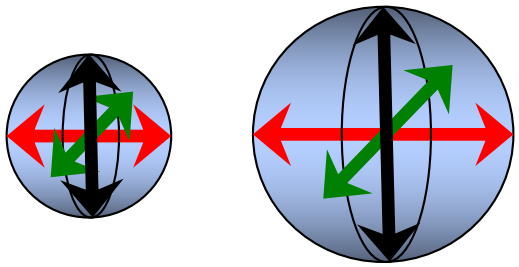
Which path of densities?

In the works by A. Gaiduk *et al.*, **possible choices are discussed** [cf. e.g. J. Chem. Theory Comput. 5, 699 (2009)].

t - scaling

$$\rho_t(\vec{r}) = t^3 \rho(t\vec{r})$$

This looks familiar to nuclear physicists as the **scaling model for the GMR**.



In principle, it can be generalised to other shapes.

We have applied the line-integration formula **for the first time in the nuclear case.**

We have shown that we can indeed reconstruct the EDF.

Simple Skyrme (t_0-t_3) EDF.

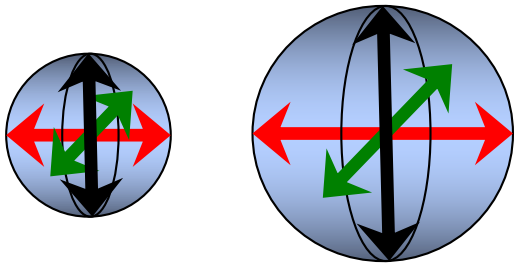
$$\left(-\frac{\hbar^2\nabla_i^2}{2m}+v[\rho]+v_{\rm ext}\right)\phi_i(\vec{r})=\varepsilon_i\phi_i(\vec{r})$$

When we invert the relation between densities and potentials we obtain: $v = v[\rho] + v_{\rm ext}$

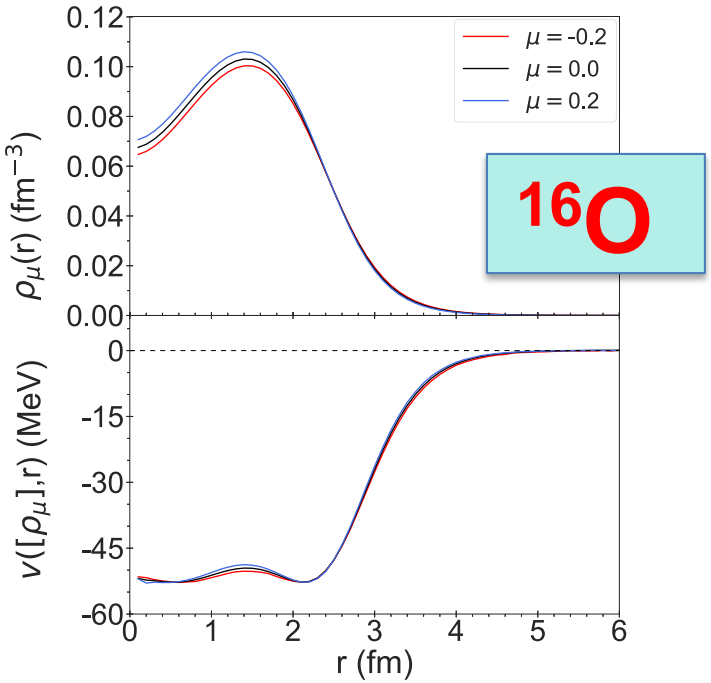
The relevant information is $v[\rho] = \dfrac{\delta F}{\delta \rho}$

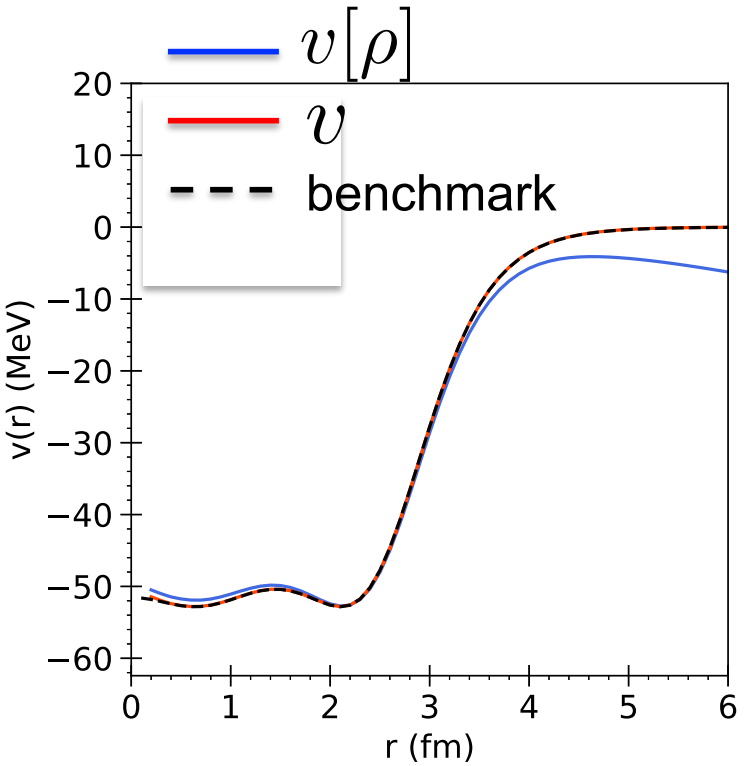
We must use a density path in which the external potential is known along with the density

$$v_{\rm ext} = \mu r^2$$



Reproduction of (scaled) densities and potentials

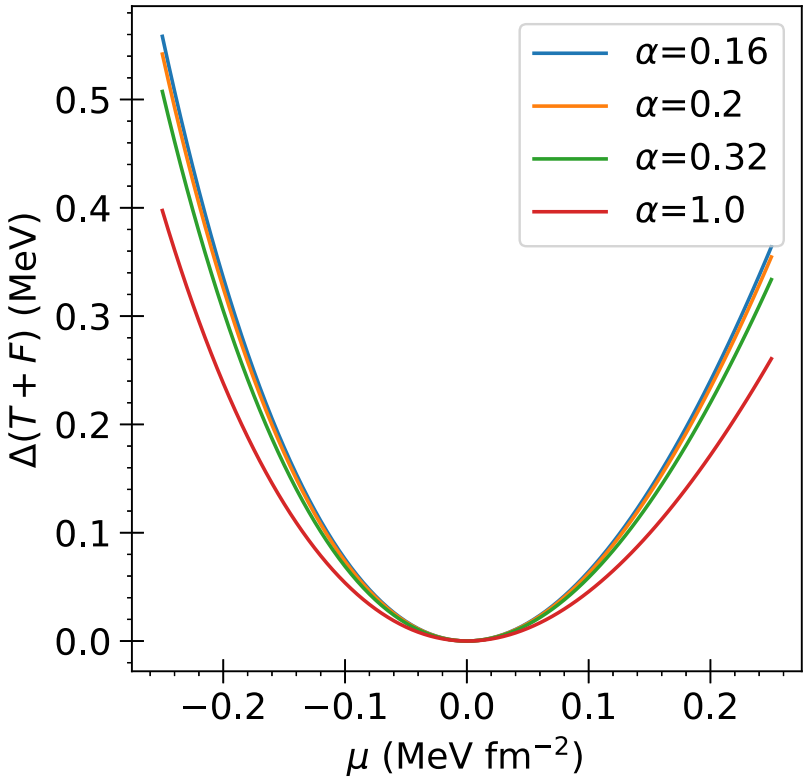




The "external" potential produces a small, but still detectable, effect.

We can accurately **produce the potential v** and distinguish it from the external potential.

Reconstruction of E[ρ]



What information do we get when we reconstruct the energy?

In the **case at hand**, we have correctly reproduced the EDF.

$$\mathcal{E} = \frac{1}{2}\left(t_0 + \frac{t_3}{6}\rho^\alpha\right)\left(\rho^2(\vec{r}) - \frac{1}{2}\rho_p^2(\vec{r}) - \frac{1}{2}\rho_n^2(\vec{r})\right)$$

We are indeed **sensitive to the exponent α.**

Appropriate strategies must be devised if we start from *ab initio* results.

Conclusions

- **The full inversion of the Kohn-Sham problem, from density to Kohn-Sham potential and to the energy functional, has been shown to be feasible and robust.**
- Experimental densities parametrized as a sum of Gaussians are an issue.
- **The method can be applied having at one's disposal accurate densities from more fundamental theories.**
- The spherical symmetry assumption can be overcome.
- The open question is how to infer the gradients terms, the spin-orbit terms etc.

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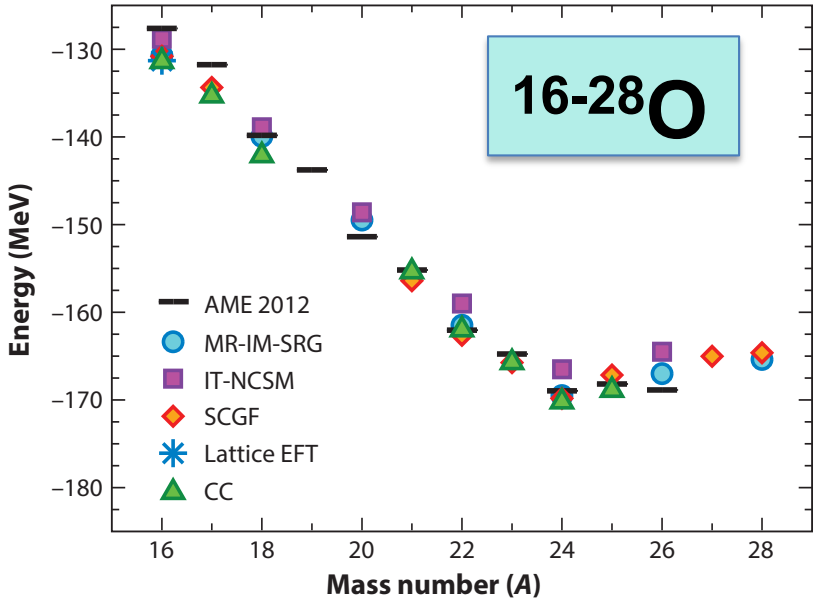
- ***Ab initio*-based EDFs**

F. Marino *et al*., Phys. Rev. C104, 024315 (2020).

Ab initio approaches

They aim at solving the nuclear many-body problem using a **realistic Hamiltonian** and a **many-body method that is in principle exact** (or whose uncertainty can be quantified).

H is a larger source of uncertainties than the MB method.



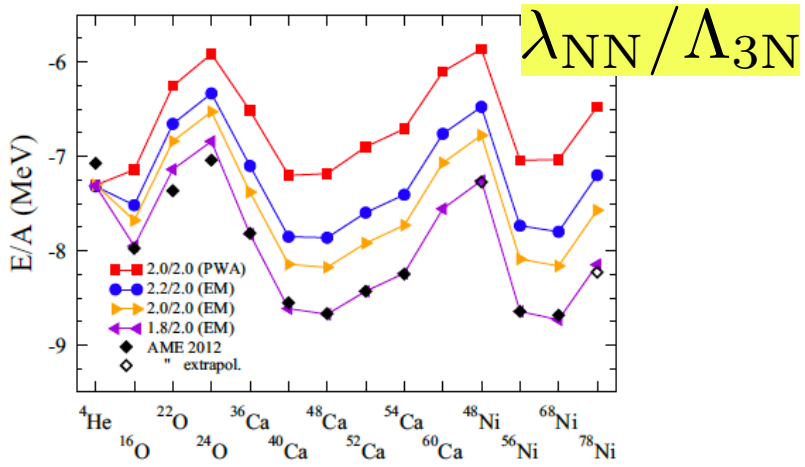


FIG. 5. Systematics of the energy per nucleon E/A of closed-shell nuclei from ^{4}He to ^{78}Ni calculated with the IM-SRG for the four Hamiltonians considered. The results are compared against experimental ground-state energies from the AME 2012 [40] (extrapolated for ^{48,78}Ni).

J. Simonis et al., Phys. Rev. C 96, 014303 (2017)

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

Nuclear energy density functionals grounded in *ab initio* calculations

F. Marino,[1,2,*] C. Barbieri,[1,2] A. Carbone,[3] G. Colò,[1,2] A. Lovato,[4,5] F. Pederiva,[6,5] X. Roca-Maza,[1,2] and E. Vigezzi[2]

[1]*Dipartimento di Fisica "Aldo Pontremoli," Università degli Studi di Milano, 20133 Milano, Italy*
[2]*Istituto Nazionale di Fisica Nucleare, Sezione di Milano, 20133 Milano, Italy*
[3]*Istituto Nazionale di Fisica Nucleare–CNAF, Viale Carlo Berti Pichat 6/2, 40127 Bologna, Italy*
[4]*Physics Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*
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Quantum Monte Carlo (QMC)

Self-consistent Green's Function (SCGF) method

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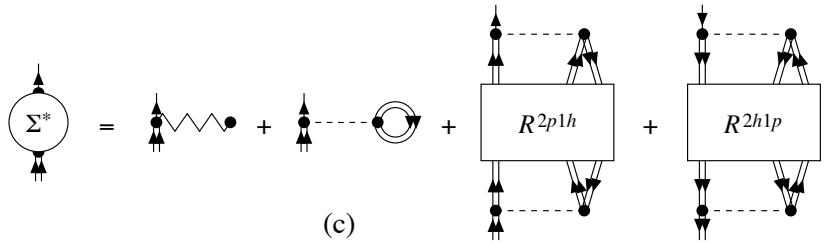
Self-consistent Green's functions (SCGF) approach

The **Green's function** represents the probability amplitude that a particle is found in state α at time t after having been introduced in the system at time t' in state β

$$g_{\alpha\beta}(t-t') \quad \rightarrow \quad g_{\alpha\beta}(\omega)$$



W.H. Dickhoff and C. Barbieri, PPNP 52, 377 (2004)

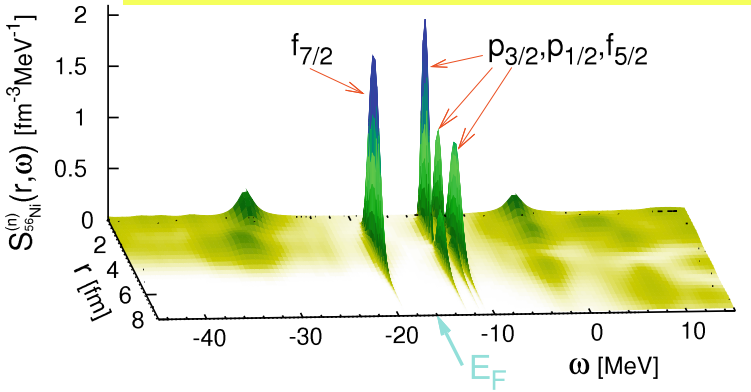
It obeys the **DYSON EQUATION:**

$$g_{\alpha\beta}(\omega) = g^{(0)}_{\alpha\beta}(\omega) + \sum_{\gamma\delta} g^{(0)}_{\alpha\gamma}(\omega)\Sigma_{\gamma\delta}(\omega)g_{\delta\beta}(\omega)$$

V. Somà, Frontiers in Physics(2020)

The self-energy Σ is approximated by a set of diagrams. From the solution for *g*, one calculates the observables.

C. Barbieri, PRL 103, 202502 (2009)



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Quantum Monte Carlo

$$E = \min \frac{\langle \Psi_{\text{trial}} | H | \Psi_{\text{trial}} \rangle}{\langle \Psi_{\text{trial}} | \Psi_{\text{trial}} \rangle} \qquad |\Psi_{\text{trial}}\rangle = \hat{O}_{\text{corr}} |\Phi\rangle$$

Variational

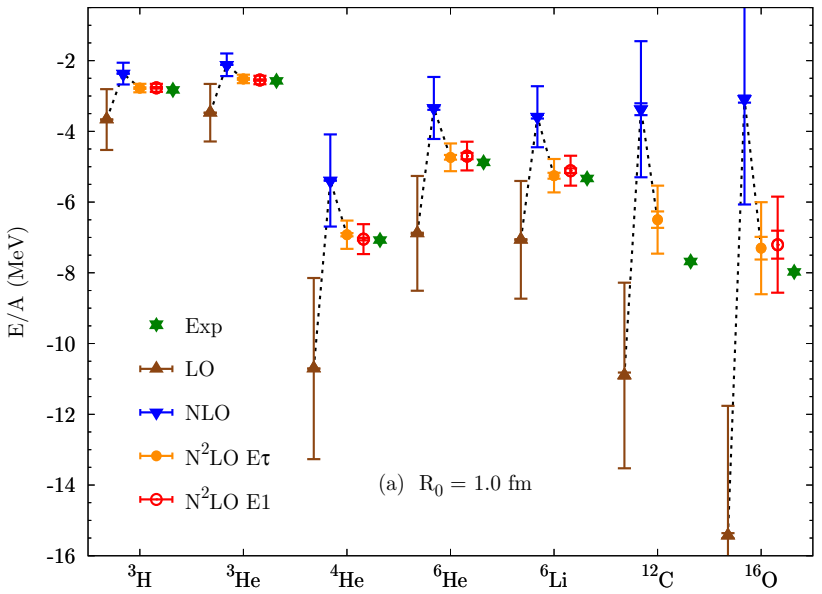
$$|\Psi_0\rangle = \lim_{\tau \to \infty} e^{-(H-E_0)\tau} |\Psi_{\text{trial}}\rangle$$

$$|\Psi(\tau)\rangle = \left[e^{-(H-E_0)\Delta\tau} \right]^n |\Psi_{\text{trial}}\rangle$$

Metropolis Monte Carlo algorithm

$$\tau = n\Delta\tau$$

Diffusion



Computationally very demanding. Nuclear matter and light nuclei.

J. Carlson et al., Rev. Mod. Phys. 87, 1067 (2015)
S. Gandolfi, D. Lonardoni, A. Lovato, and M. Piarulli, Front. Phys. 8, 00117 (2020).

D. Lonardoni *et al.*, PRC 97, 044318 (2018)

Building DFT from *ab initio*

$$\mathcal{E}^{\text{Skyrme}} = C^{\rho\rho}[\rho]\rho^2 + C^{\rho\tau}\rho\tau + C^{J^2}\vec{J}^{\,2} + C^{(\nabla\rho)^2}\left(\vec{\nabla}\rho\right)^2 + C^{\rho\vec{\nabla}\cdot\vec{J}}\rho\vec{\nabla}\cdot\vec{J}$$

We can start by sticking to the local ansatz.

The parameters are usually fit to experimental data, while we want to constrain them on *ab initio*.

There have been only partial attempts along this line.

J. Phys. G 47, 085107 (2020);
Eur. Phys. J. A 56, 85 (2020);
Phys. Rev. C 103, 014325 (2021).

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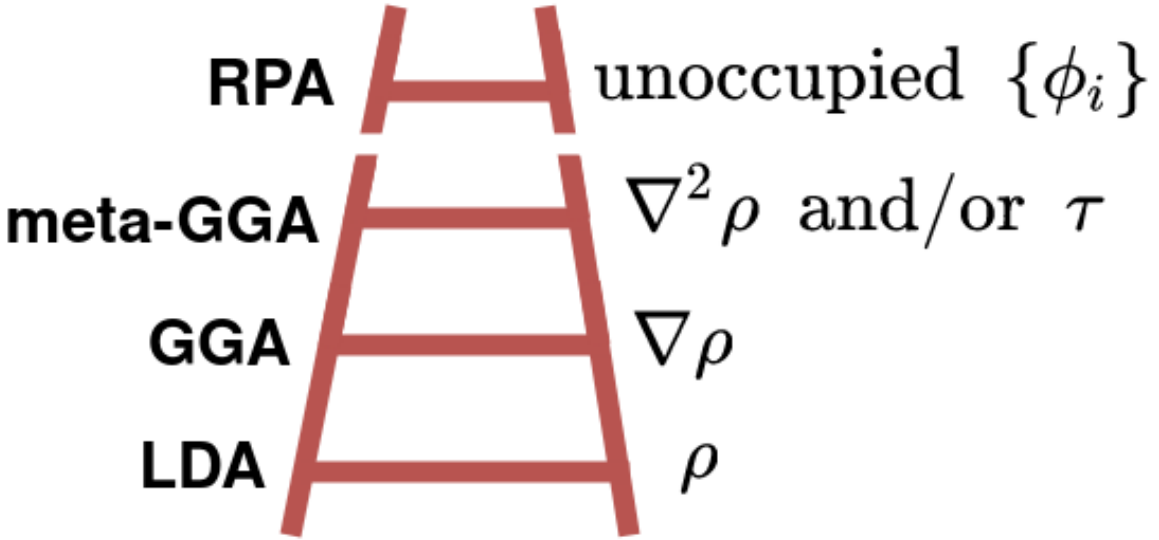
Our systematic ladder of approximations

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

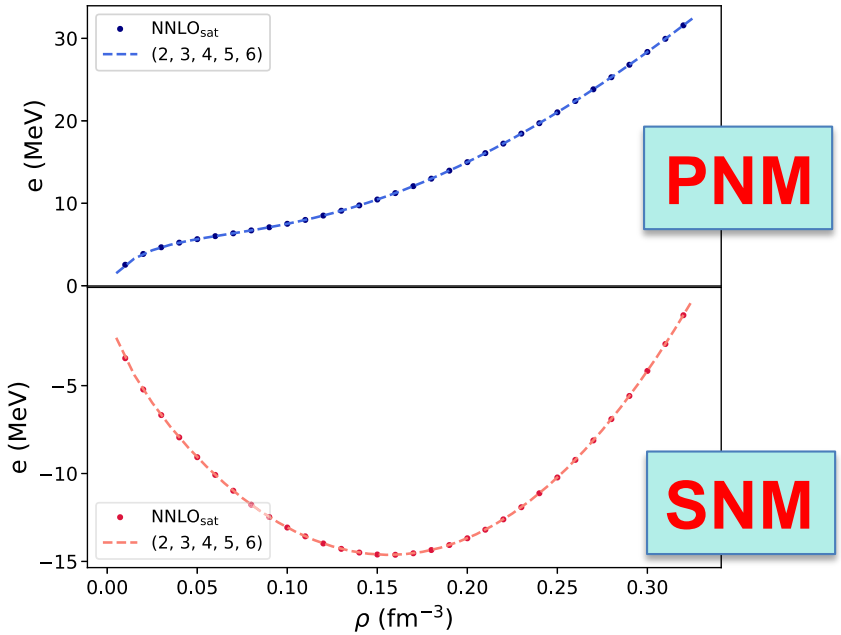
J. Perdew, K. Schmidt, AIP Conf. Proc. 577, 1 (2001).



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

Local Density Approximation (LDA)

We start from the Equation of State (EoS) of nuclear matter.



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.

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

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

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The Equation of State (EoS)

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

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

SCGF with NNLO$_{sat}$

QMC with AV4'

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.

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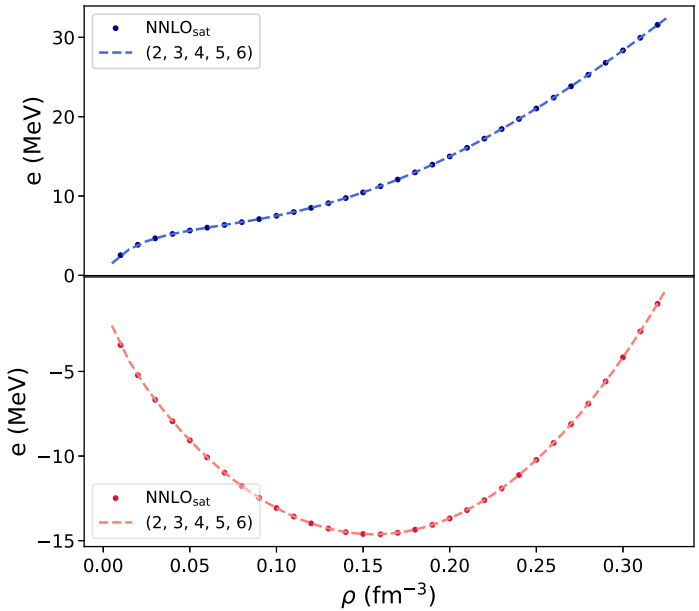
EoS with different Hamiltonians

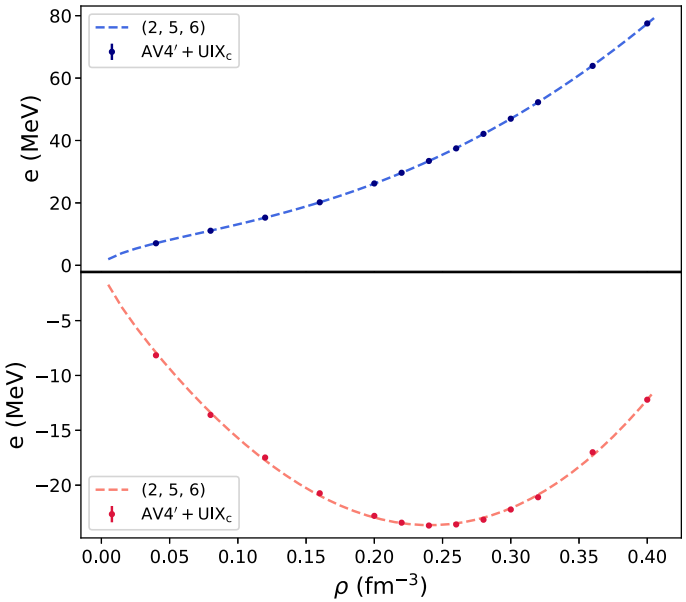
NNLO$_{sat}$



PNM

SNM

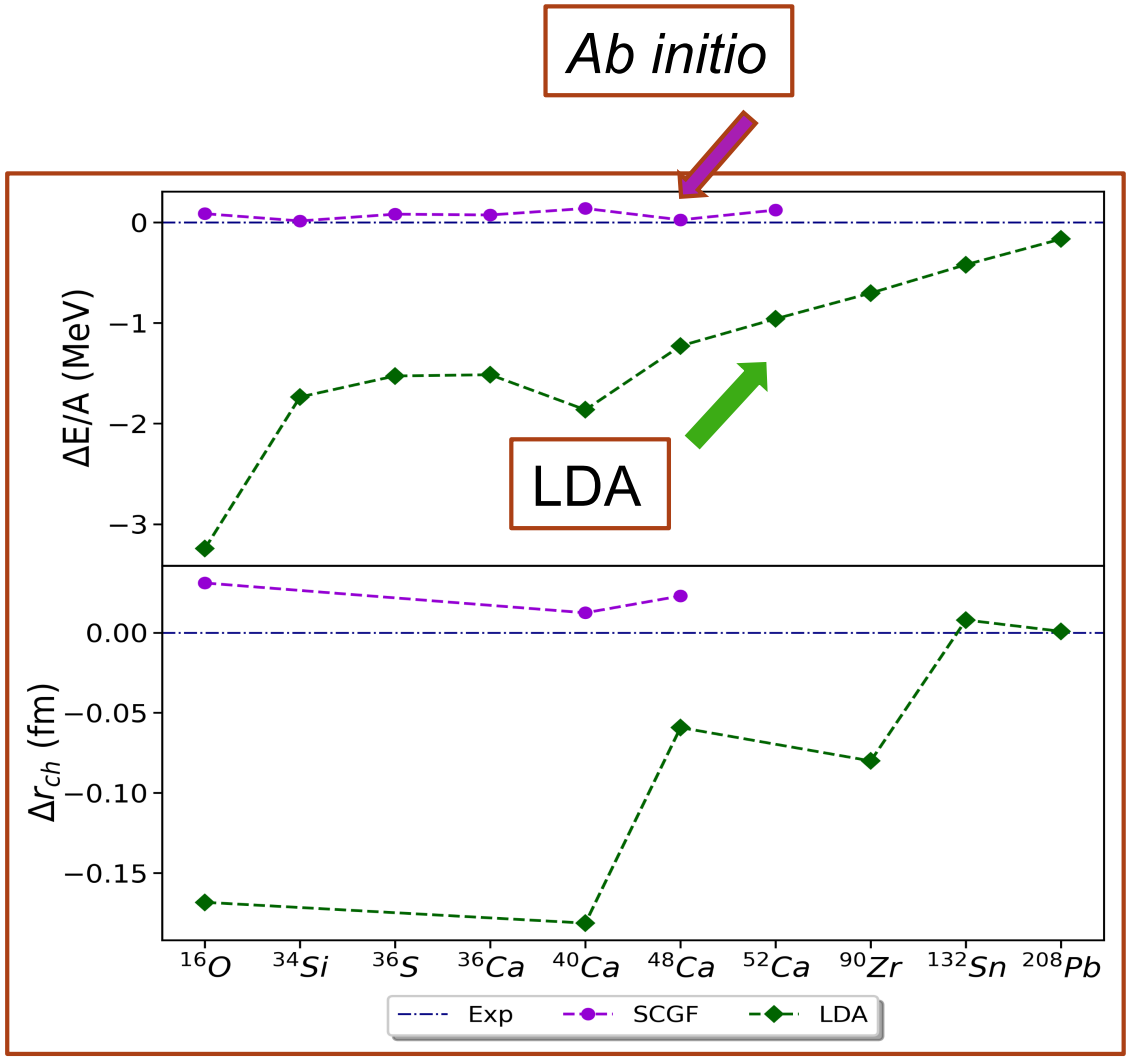
Av4'



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

$$\gamma = \frac{2}{3}, \frac{5}{3}, 2$$

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

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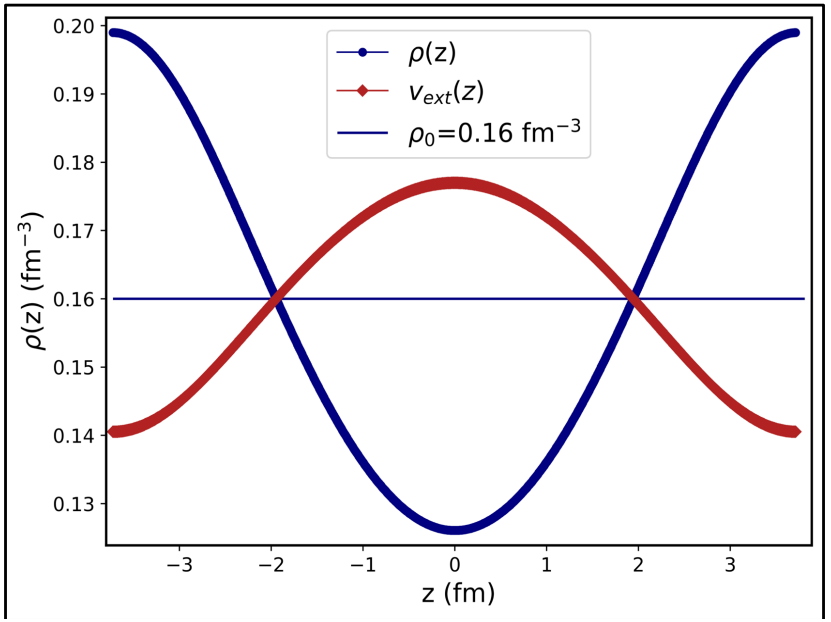
Towards the gradient approximation

$$\mathcal{E}^{\text{Skyrme}} = C^{\rho\rho}[\rho]\rho^2 + C^{\rho\tau}\rho\tau + C^{J^2}\vec{J}^{\,2} + C^{(\nabla\rho)^2}\left(\vec{\nabla}\rho\right)^2 + C^{\rho\vec{\nabla}\cdot\vec{J}}\rho\vec{\nabla}\cdot\vec{J}$$

Nuclei are finite systems and the dependence of the EDF on $\nabla\varrho$, τ and J is mandatory. These quantities vanish in uniform matter.

How can *ab initio* inform us about this dependence?

Uniform matter perturbed by a (weak) periodic potential



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Perturbed nuclear matter

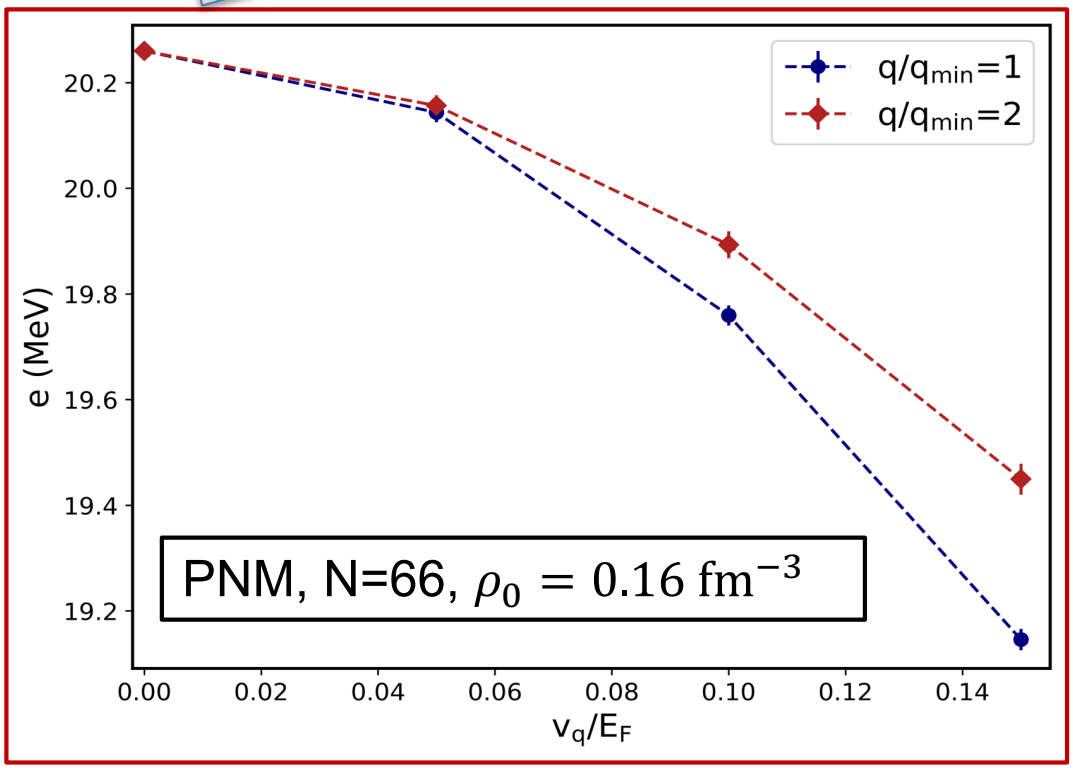
Add a **weak external potential** of the type: $v_{\rm ext} = 2v_q cos(\vec{q}\cdot\vec{r})$

In linear response:

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

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

WORK IN PROGRESS



Perturbing the system gives access to

$C^{\rho\tau}$ $C^{(\nabla\rho)^2}$ $C^{\rho\vec{\nabla}\cdot\vec{J}}$

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Conclusions

- **We are developing a ladder of *ab initio*-constrained nuclear EDFs.**
- The first rung of the ladder (LDA) has been already implemented.
- We have started from different Hamiltonians and many-body methods (there is no unique *ab initio* approach so far).
- **We are working to obtain gradient terms by exploiting the response of uniform matter to a weak perturbation.**
- Applications to ground-states and collective nuclear excitations (by means of RPA) are underway.

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- G. Accorto (Univ. Zagreb, Croatia)
- A. Liardi (Cambridge University, UK)
- A. Lovato (ANL, USA)

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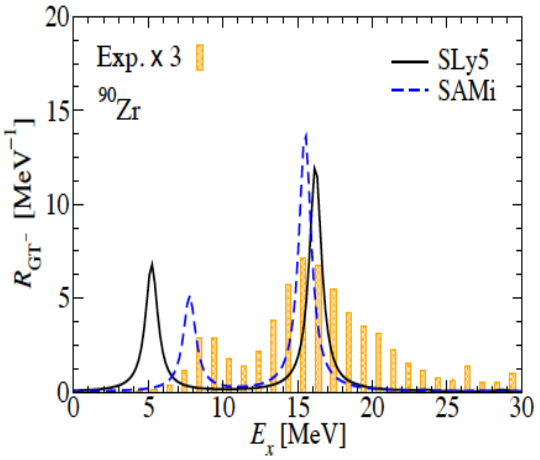
Backup slides

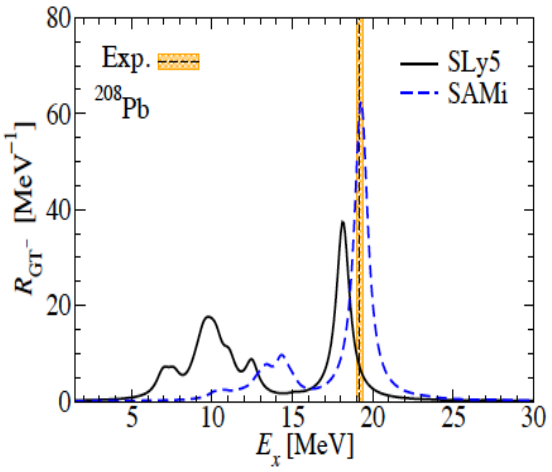
Spin-isospin terms, ISB terms

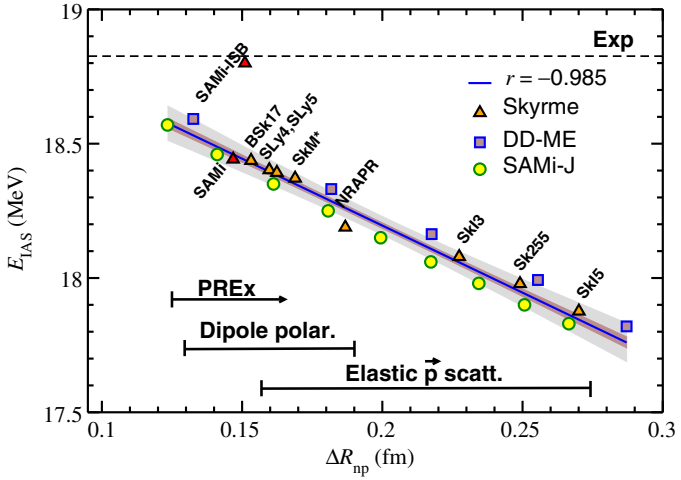
The **SAMi** functional has been introduced in Phys. Rev. C 86, 031306(R) (2012), and **provides a good description of Gamow-Teller resonances**.

It needs, however, to be complemented by **isospin symmetry breaking terms** (ISB)[1] **to provide a realistic value for the Isobaric Analog resonance energy.**

[1] Cf. T. Naito







X. Roca-Maza, G.C., H. Sagawa, PRC 86, 031306(R) (2012).

PRL 120, 202501 (2018).

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Many EDFs do not have realistic spin-isospin/ISB terms.

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Nuclear density functional theory

G. Colò

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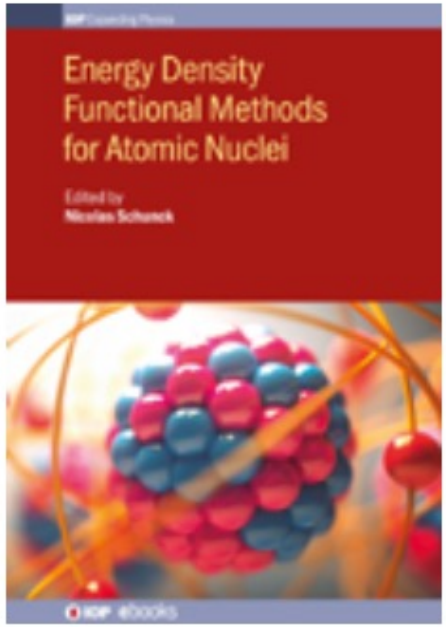

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