On the use of charge distribution in nuclei to constrain effective interactions (work in progress)

K. Bennaceur

IP2I, CNRS/IN2P3, Université Claude Bernard Lyon 1, France

June 12^{th}, 2024

PLATAN 2024 – University of Jyväskylä, June 9-14, 2024

Outline

Mean-field models

- Stationary Schrödinger equation for A particles

$$\hat{H}\Psi = \left(\hat{T} + \hat{V}_2 + \hat{V}_3 + \ldots\right)\Psi = E_0\Psi$$

- Mean-field approximation, Hartree-Fock(-Bogolyubov)

$$E = \langle\Phi|\hat{H}_{\mathrm{eff}}|\Phi\rangle \simeq E_0 = \langle\Psi|\hat{H}|\Psi\rangle$$

- Effective interaction $\hat{H}_{\mathrm{eff}} = \hat{T} + \hat{V}_{\mathrm{eff}}$

$$\hat{V}_{\mathrm{eff}} = \hat{V}_{\mathrm{eff}}(\mathbf{p})\,, \quad \mathbf{p} \in \mathbb{R}^n\,, \quad n \sim 10 \text{ to } 25$$

Details don't matter but:

- HF(B) equations are non linear and are solved iteratively
- Can be very time consuming when many symmetries are broken
- Fits often done using empirical properties and, often, spherical or even-even ones

Predictive power in uncharted territory?

Data and algorithm

Non-relativistic functionals, see for example:

- Fayans functionals:

  P.-G. Reinhard and W. Nazarewicz Phys. Rev. C 95, 064328 (2017).

- Regularized functionals:

  K.B., J. Dobaczewski, T. Haverinen, M. Kortelainen, JPG 47, 105101 (2020)

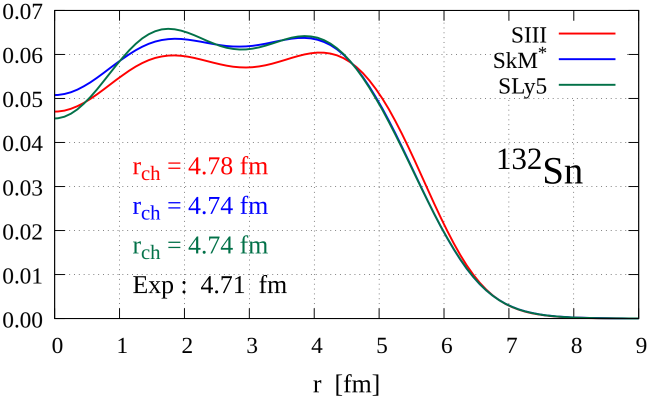
- Skyrme functionals:

  W. Ryssens, G. Scamps, S. Goriely, M. Bender, EPJA 59, 96 (2023).

- Gogny functionals:

  G. Zietek, thesis 2023, `https://theses.hal.science/tel-04394860`

Charge distribution in ^{132}Sn with Skyrme functionals



SIII	SkM*	SLy5	
$\rho_{\rm sat} = 0.145$	$\rho_{\rm sat} = 0.160$	$\rho_{\rm sat} = 0.160$	[fm^{-3}]

$\rho_{\rm sat} \leftrightarrow r_{\rm ch}$ but does not constrain oscillations in the inside

Finite size instabilities

Charge density oscillations are also related to the vicinity of **finite-size instabilities**.

- Oscillation of the isovector density $\rho_1(r) = \rho_n(r) - \rho_p(r)$ observed when we tried to modified the effective mass.

  T. Lesinski, K.B., T. Duguet, J. Meyer, Phys. Rev. C74, 044315 (2006)

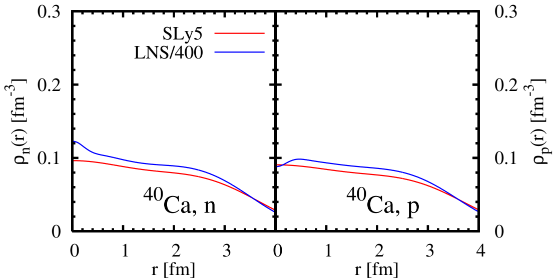
- Can also appear in the vector (spin) channels.
- Exist in the scalar-isoscalar channel as a physical phenomenon (spinodal instability).
- Also observed for some Gogny functionals.

  M. Martini, A. De Pace, K.B. EPJA 55, 150 (2019).

Example of instability in the isovector channel

T. Lesinski, K.B., T. Duguet, J. Meyer, PRC 74, 044315

- HF calculation for ^{40}Ca with SLy4 and LNS[1] parameterizations
- HF iterations do not lead to convergence with LNS



- Appearance of domains with asymmetric and/or polarized matter

[1] L.G. Cao, U. Lombardo, C.W. Shen, Nguyen Van Giai, PRC 73, 015313

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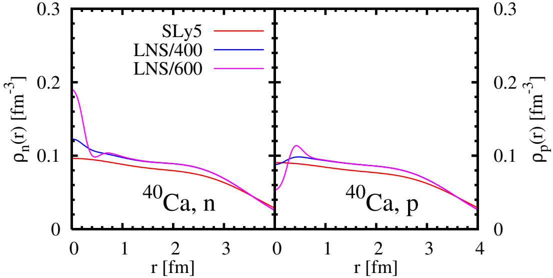

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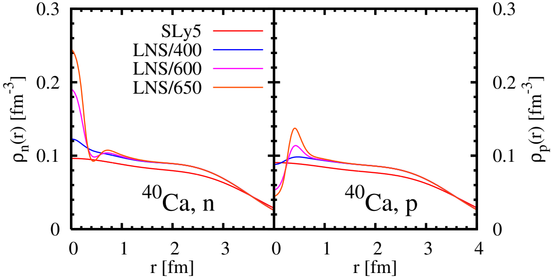

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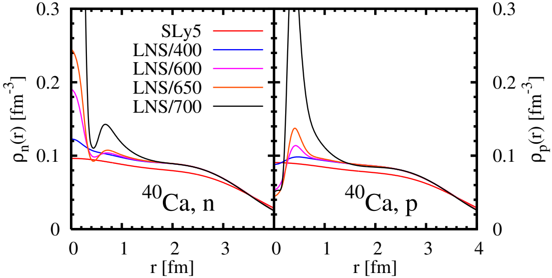


- Appearance of domains with asymmetric and/or polarized matter

[1] L.G. Cao, U. Lombardo, C.W. Shen, Nguyen Van Giai, PRC 73, 015313

Linear response method in infinite nuclear matter

C. Garcia-Recio, J. Navarro, Van Giai Nguyen, L.L. Salcedo, Ann. Phys. 214 (1992) 293

D. Davesne, M. Martini, K.B., J. Meyer, Phys. Rev. C80, 024314, errat.: Phys. Rev. C84, 059904[2]

- Excitation of the system with a perturbation $(\omega, \mathbf{q})$

$$\mathcal{Q}^{(\alpha)} = e^{-\mathrm{i}\omega t} \sum_i e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}_i} \Theta_i^{(\alpha)}$$

with $\Theta_i^{\mathrm{ss}} = 1_i\,, \quad \Theta_i^{\mathrm{vs}} = \boldsymbol{\sigma}_i\,, \quad \Theta_i^{\mathrm{sv}} = \boldsymbol{\tau}_i \quad \mathrm{or} \quad \Theta_i^{\mathrm{vv}} = \boldsymbol{\sigma}_i \boldsymbol{\tau}_i\,.$

- Response of the system at a given density within the RPA approx.

$$\chi^{(\alpha)}(\omega, \mathbf{q}) = \frac{1}{\Omega} \sum_n \left| \langle n | \mathcal{Q}^{(\alpha)} | 0 \rangle \right|^2 \left(\frac{1}{\omega - E_n + \mathrm{i}\,\eta} - \frac{1}{\omega + E_n - \mathrm{i}\,\eta} \right)$$

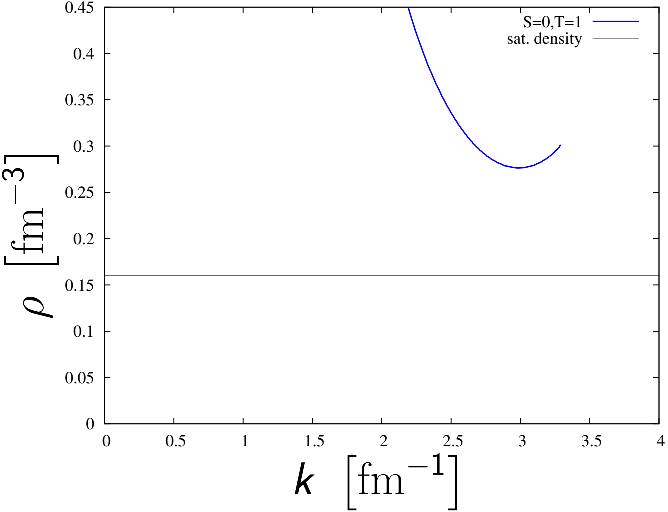
$n \in$ excited states of the system $\Omega =$ normalization volume

- Pole at zero energy for given finite values of $\mathbf{q}$ and ρ_0 $\Rightarrow$ instability

[2] Don't forget to cite this erratum, it helps to increase my H index.

Linear response as a tool for diagnosis

Pole of the response at $E = 0$ $\equiv$ instability



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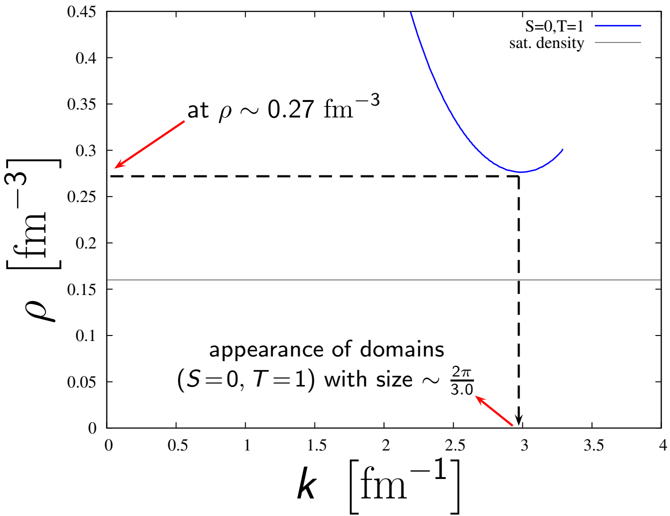
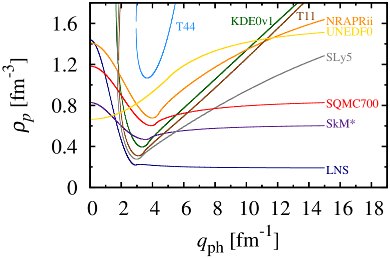


Attempt to build a stability criterion

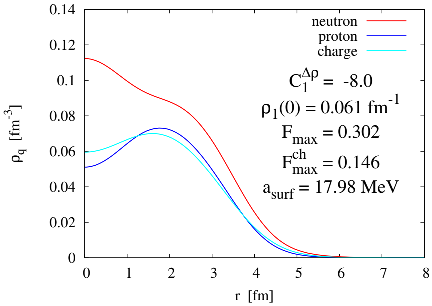
V. Hellemans, A. Pastore, T. Duguet, K.B., D. Davesne, J. Meyer, M. Bender, P. -H. Heenen,
PRC 88, 064323

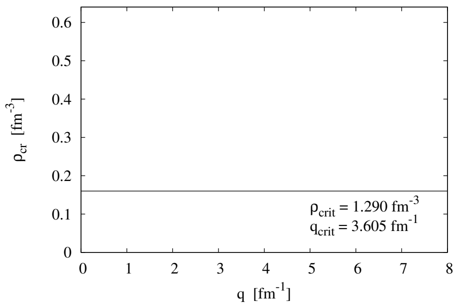
Study in the scalar-isoscalar channel ($S = 0, T = 1$) based on 9 functionals based on totally different fitting procedures



- Lowest density $\rho_{\rm min}$ for which the response has a pole must be
$$\rho_{\rm min} > 1.2 \times \rho_{\rm sat}$$
- But: **not based** on observables and **very difficult** to use with finite-range interactions.

^{34}Si with SLy interactions with constrained $C_1^{\Delta\rho}$





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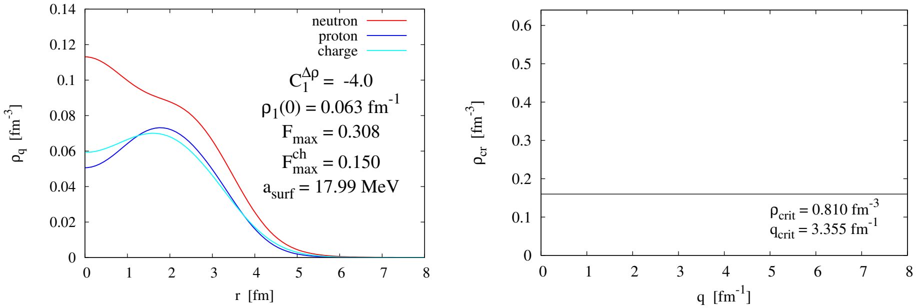

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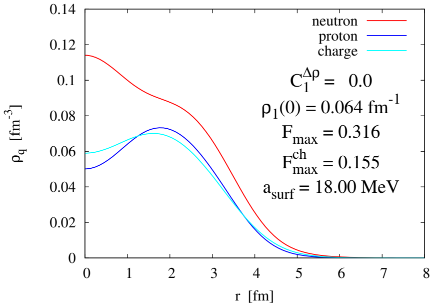

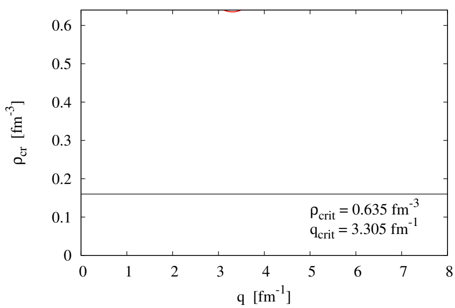

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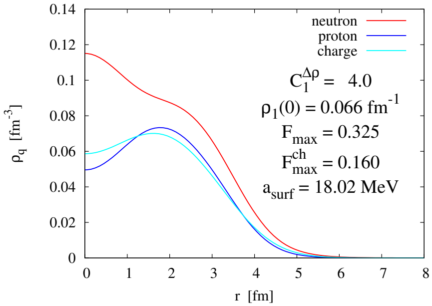

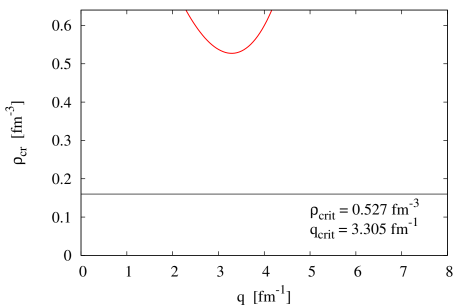

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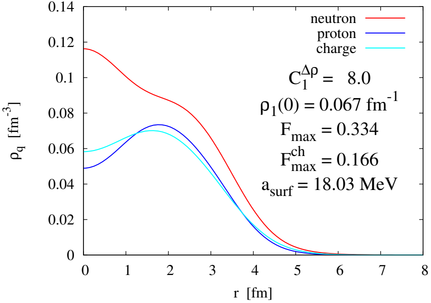

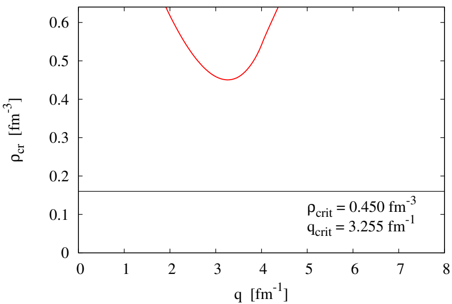

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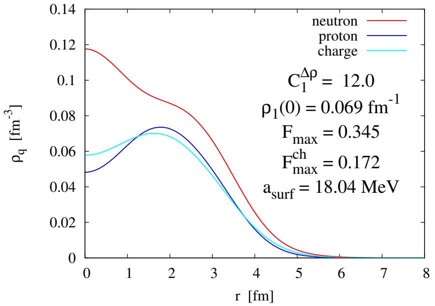

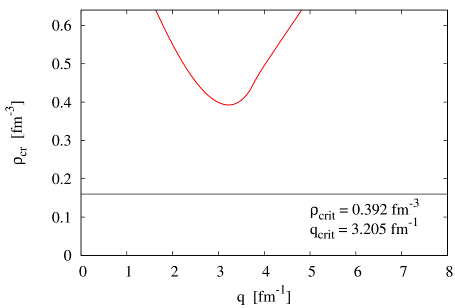

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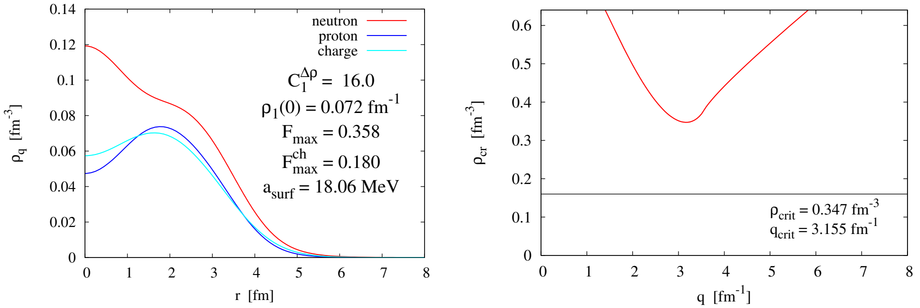

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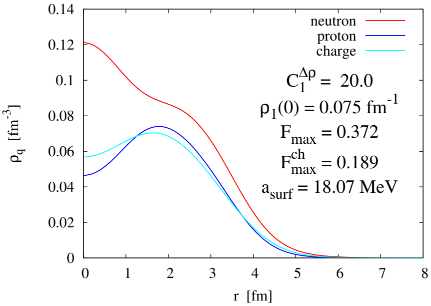

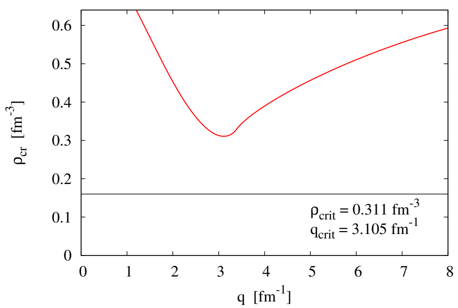

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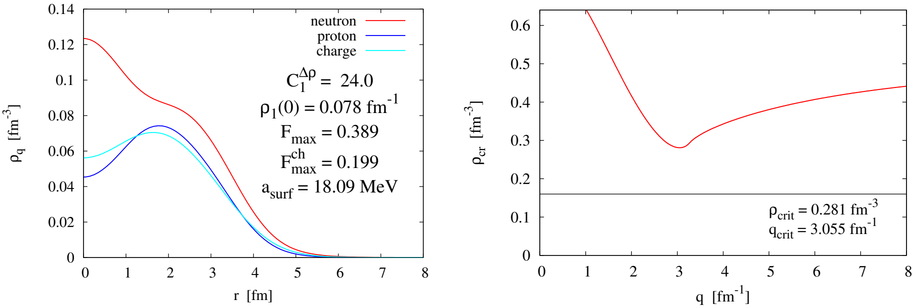

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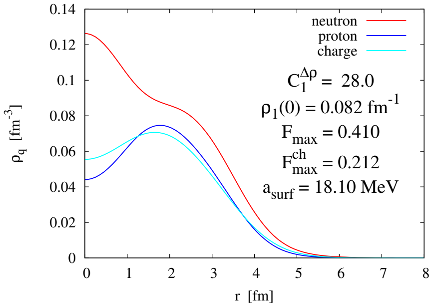

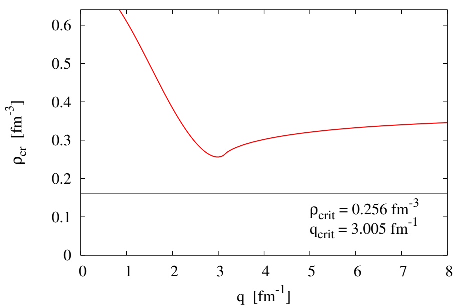

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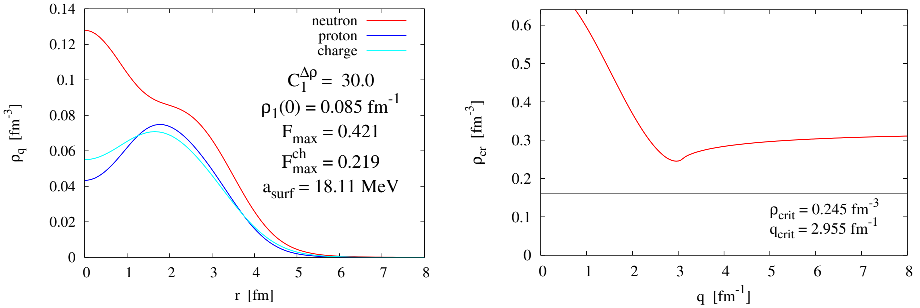
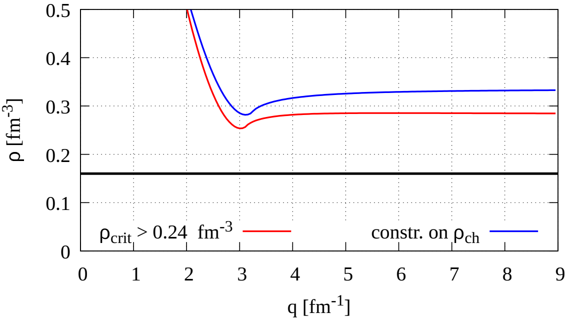


Use of charge distributions to constrain the functional parameters

Skyrme SLy functional constrained with

- $\rho_{\rm crit} > 0.24~{\rm fm}^{-3} > 1.2 \times \rho_{\rm sat}$,
- charge densities in ^{40}Ca, ^{90}Zr and ^{208}Pb.

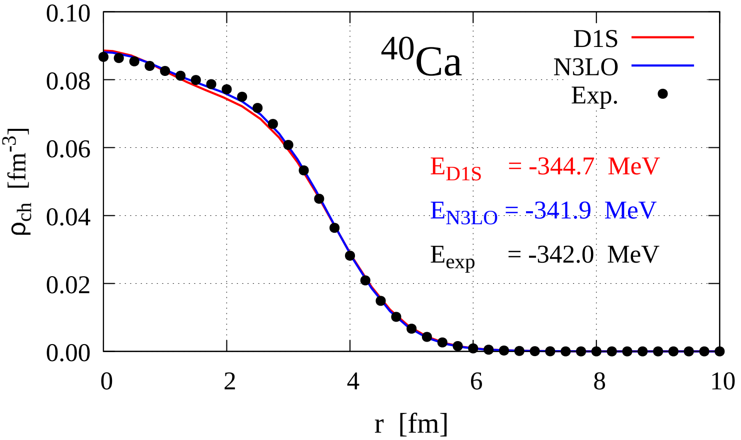


The criterion $\rho_{\rm min} > 1.2 \times \rho_{\rm sat}$ may **not be conservative enough**.

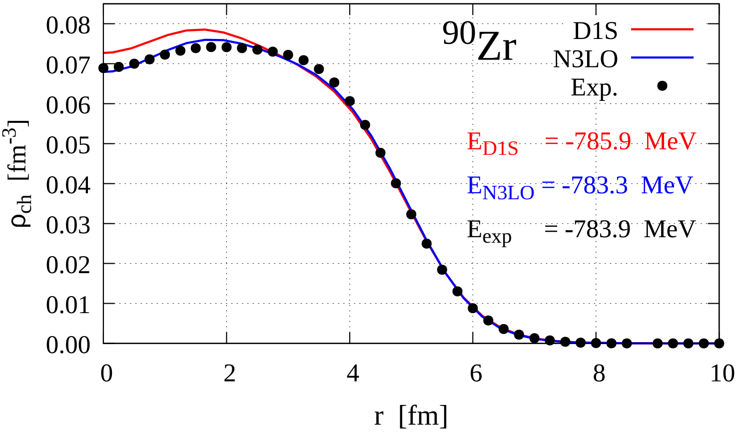
Regularized functional constained with charge distributions

- Ajustement $\sim$ regularized functional from JPG 47, 105101 (2020).
- Constraints on charge distributions in ^{40}Ca, ^{90}Zr and ^{208}Pb.
- Preliminary results!

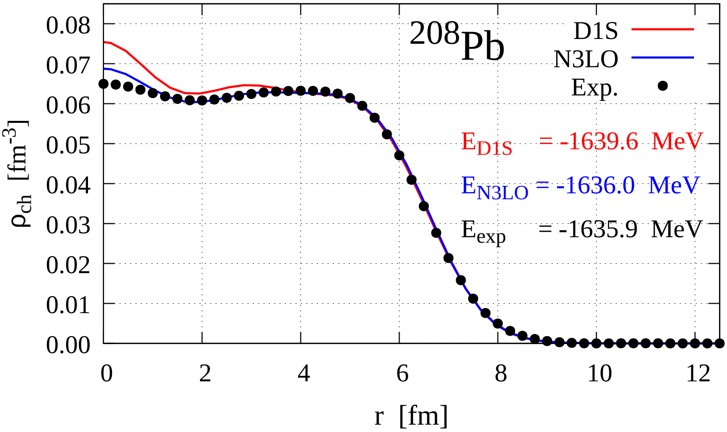
Nuclei use in the fit: ^{40}Ca



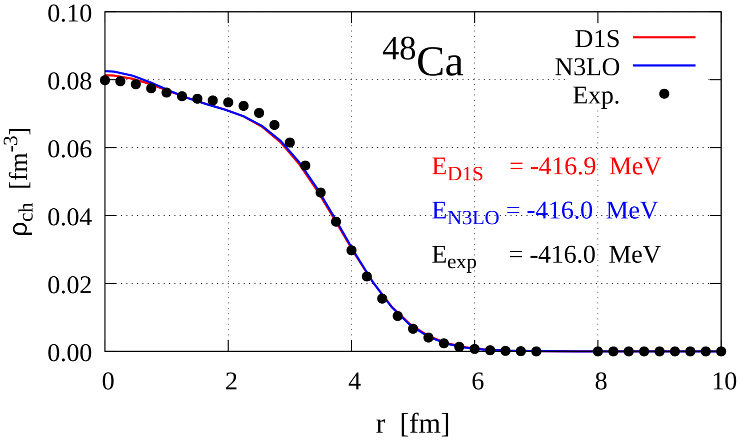
Nuclei use in the fit: ^{90}Zr



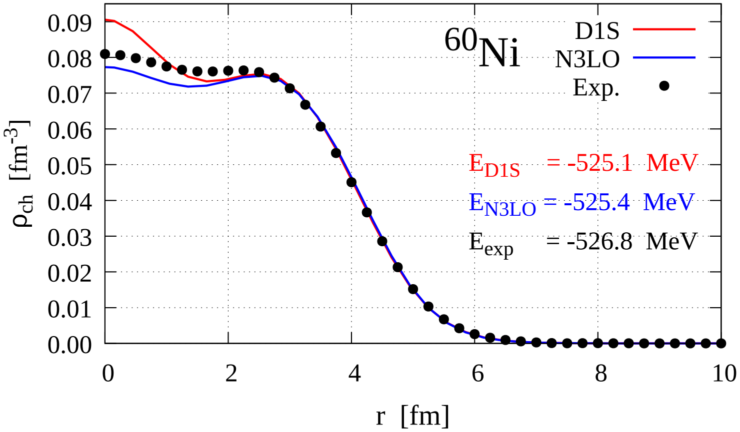
Nuclei use in the fit: ^{208}Pb



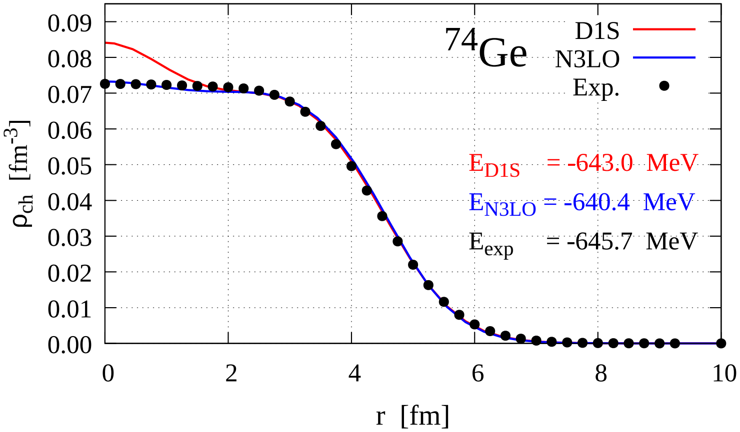
Nuclei not use in the fit: ^{48}Ca



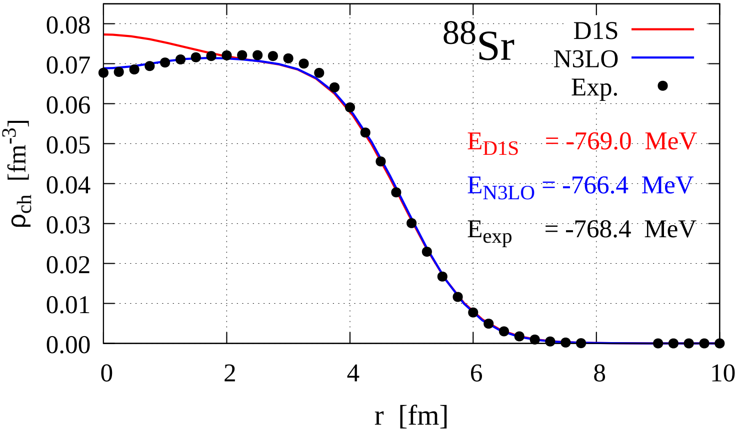
Nuclei not use in the fit: ^{60}Ni



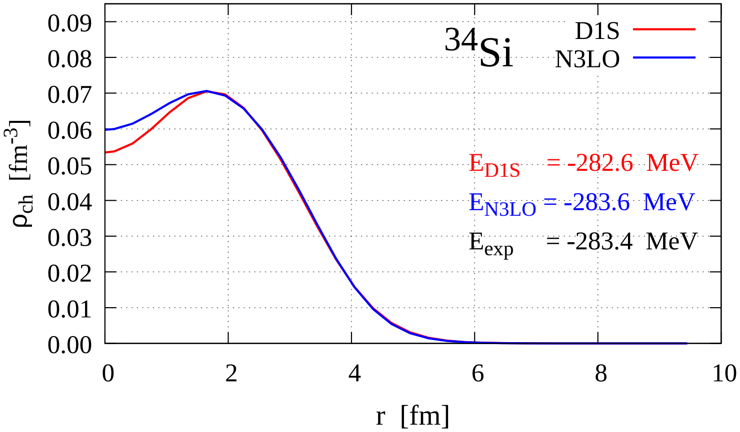
Nuclei not use in the fit: ^{74}Ge



Nuclei not use in the fit: ^{88}Sr



Semi-bubble Nuclei ^{34}Si?



Conclusions and outlooks

- Charge distributions contain information that may be useful to constrain functionals.
- They give and objective criterion to avoid finite-size (isovector) instabilities
- Consequences for binding energies, radii, deformation, spectroscopy... work in progress.
- Charge distributions from
  H. de Vries, C.W. de Jager and D. de Vries, ADNDT 36 (1987) 495.
  very useful compilation... but
  - 37 years old;
  - not always consistent with recent measurements of charge radii;
  - sometimes contains several sets of data for the same nucleus;
  - ...

Thanks to my colleagues involved in this (preliminary) work

- IP2I Lyon:
  M. Bender, Ph. da Costa, D. Davesne, V. Guillon, J. Meyer.
- University of York: J. Dobaczewski.
- CEA / DES, Cadarache: A. Pastore.
- University of Jyväskylä: G. Danneaux, M. Kortelainen, H. Rui.