On the use of charge distribution in nuclei to constrain effective interactions

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December 13th, 2024

5th Gogny conference – Paris 2024, December 10-13

Outline

Mean-field models

- Stationary Schrödinger equation for A particles

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

- 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?

Sets of data and algorithm

Non-relativistic functionals, see for example:

- Fayans functionals:

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

- Regularized interactions:

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

- Skyrme functionals:

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

  UNEDF2: M. Kortelainen *et al.*, PRC 89, 054314 (2014).

  BSkG2: W. Ryssens, G. Scamps, S. Goriely, M. Bender, EPJA 59, 96 (2023).

  and many more...

- Gogny interactions:

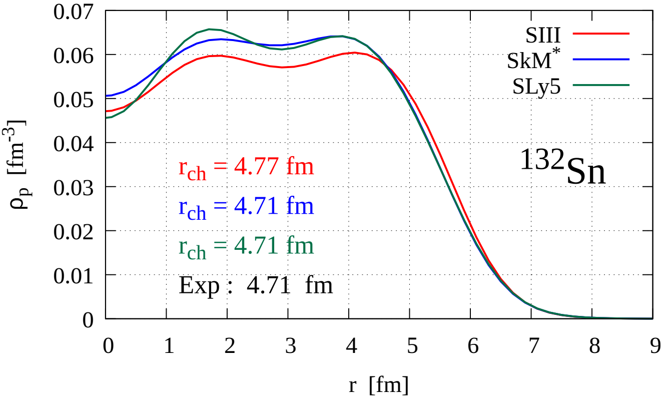
  D1S: J.F. Berger, M. Girod and D.Gogny, Comp. Phys. Comm. 63, 365 (1991).

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

- M3Y interactions:

  G. Bertsch, J. Borysowicz, H. McManus, and W. Love, Nucl. Phys. A 284, 399 (1997).

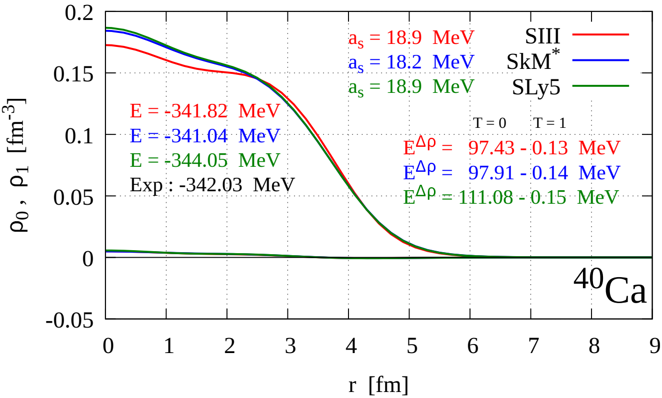
Charge distribution in ^{132}Sn with Skyrme functionals



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

Isoscalar and isovector distributions in ^{40}Ca



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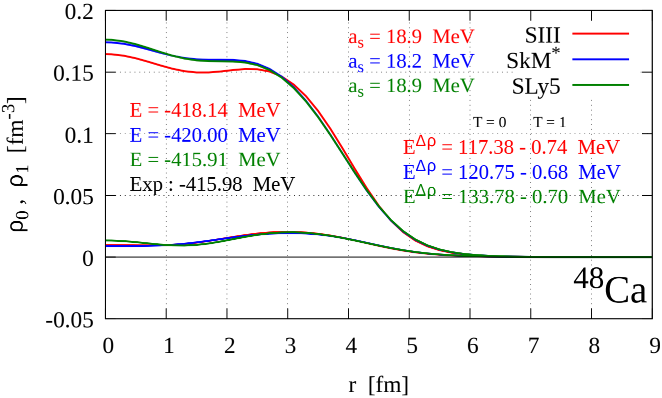
Isoscalar and isovector distributions in ^{48}Ca



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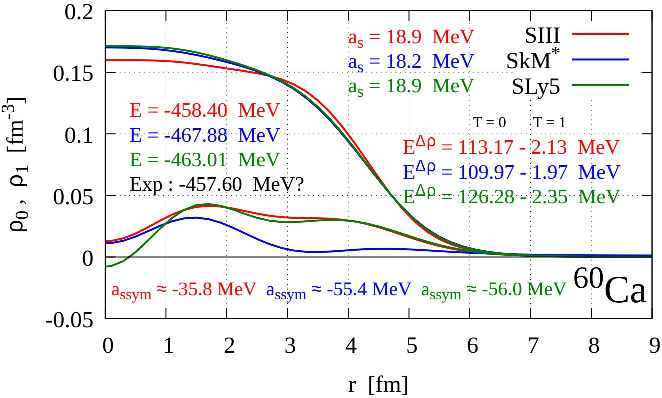
Isoscalar and isovector distributions in ^{60}Ca



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

Finite-size effects $\neq$ Surface effects

Finite size instabilities

Large 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 Gogny functionals.

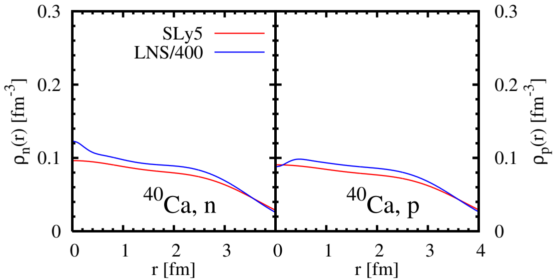
M. Martini, A. De Pace, K.B. EPJA 55, 150 (2019).

- Constraints on charge distributions might be used to avoid *isovector* finite-size instabilities?

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

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

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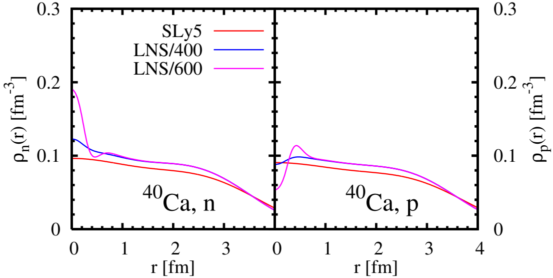

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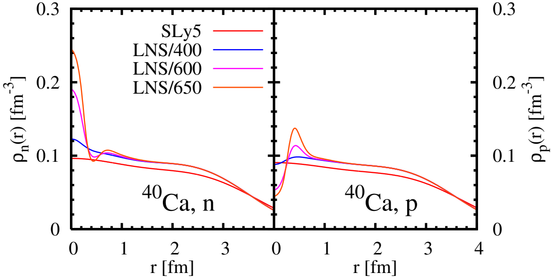

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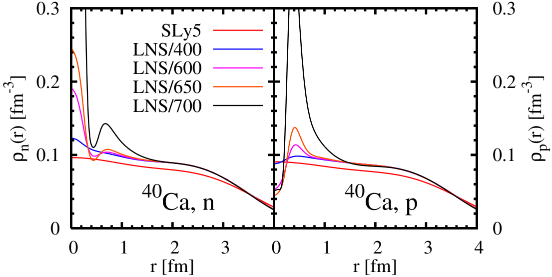

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Linear response method in infinite nuclear matter

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

- 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 **q** and $\rho_0 \Rightarrow$ instability

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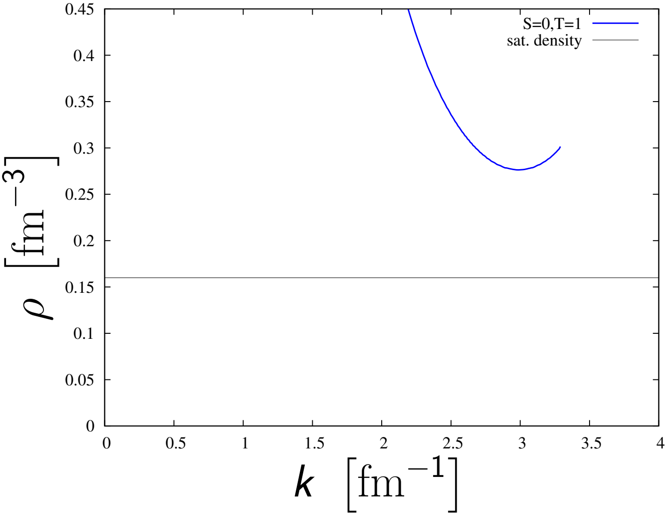
[2] Don't forget to cite this erratum, it helps to increase my H index.

Linear response as a tool for diagnosis

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



Linear response as a tool for diagnosis

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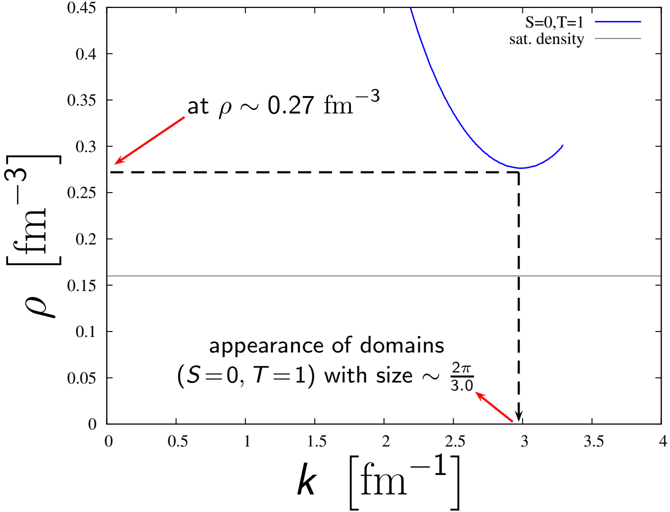


at $\rho \sim 0.27\ \mathrm{fm}^{-3}$

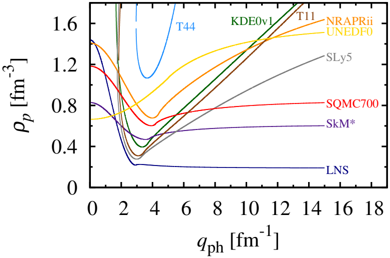
appearance of domains
$(S=0, T=1)$ with size $\sim \frac{2\pi}{3.0}$

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.

Instability and densities oscillations with Skyrme EDFs

Skyrme functional (time-even part)

- Parameters: t_0, x_0, t_1, x_1, t_2, x_2, t_3, x_3, α, W_{so}.
- Functional:

$$E = T + \int \mathcal{E}\,\mathrm{d}^3 r$$

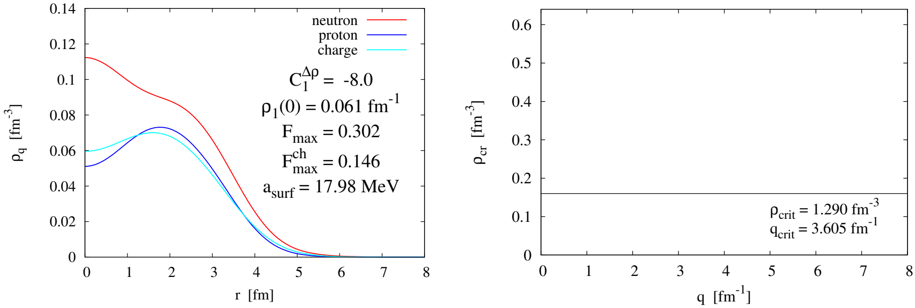
with (for time-even nuclei)

$$\begin{aligned}\mathcal{E} =& C_0^{\rho}[\rho_0]\rho_0^2 + C_0^{\tau}\rho_0\tau_0 - C_0^{\Delta\rho}\left(\boldsymbol{\nabla}\rho_0\right)^2 + C_0^{J}\mathbf{J}_0^2 + C_0^{\nabla\cdot J}\rho_0\boldsymbol{\nabla}\cdot\mathbf{J}_0 \\ &+ C_1^{\rho}[\rho_0]\rho_1^2 + C_1^{\tau}\rho_1\tau_1 - C_1^{\Delta\rho}\left(\boldsymbol{\nabla}\rho_1\right)^2 + C_1^{J}\mathbf{J}_1^2 + C_1^{\nabla\cdot J}\rho_1\boldsymbol{\nabla}\cdot\mathbf{J}_1\end{aligned}$$

- Dangerous term easy to identify for the isovector instabilities

$$-C_1^{\Delta\rho}\left(\boldsymbol{\nabla}\rho_1\right)^2$$

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



Depletion Factor $F_{\max} = \frac{\rho_{\max} - \rho(0)}{\rho_{\max}}$,   *Cf.* M. Grasso *et al.*, PRC 79, 034318 (2009)

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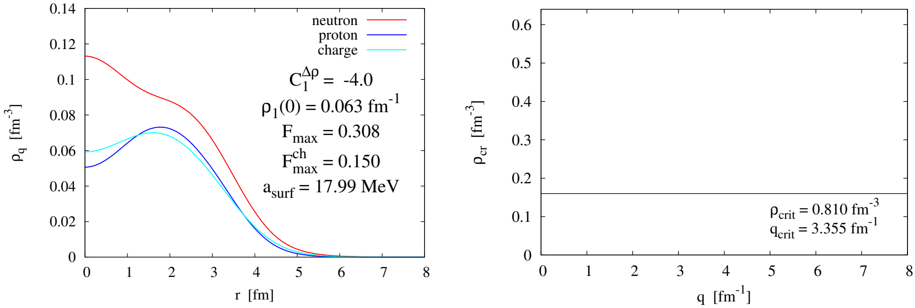

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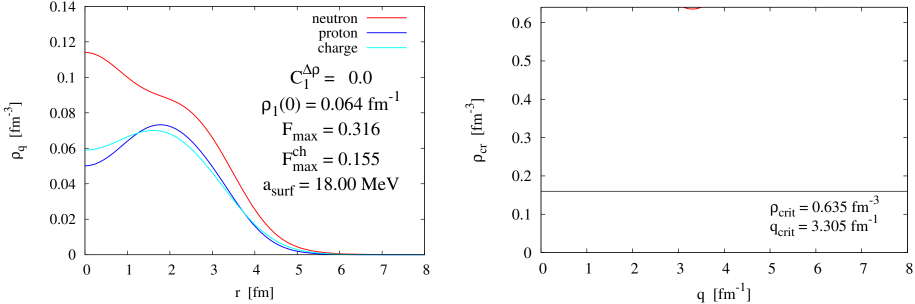

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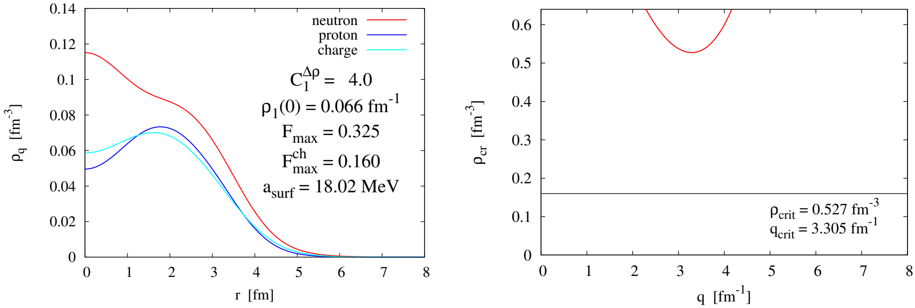

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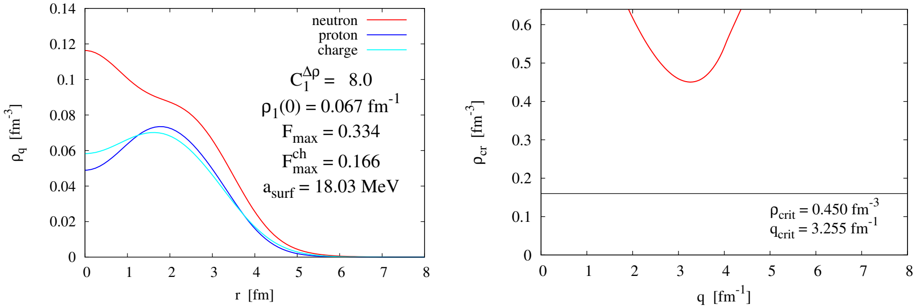

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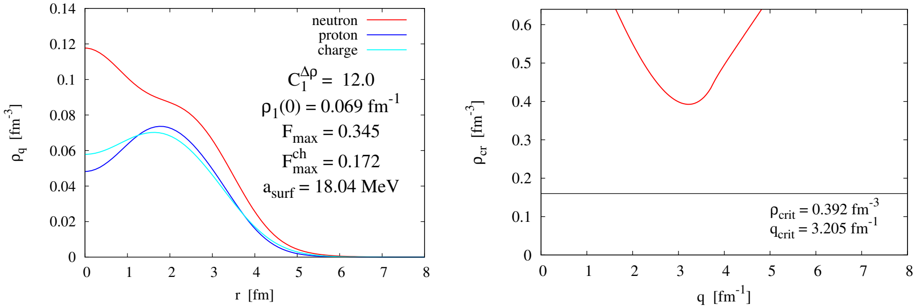

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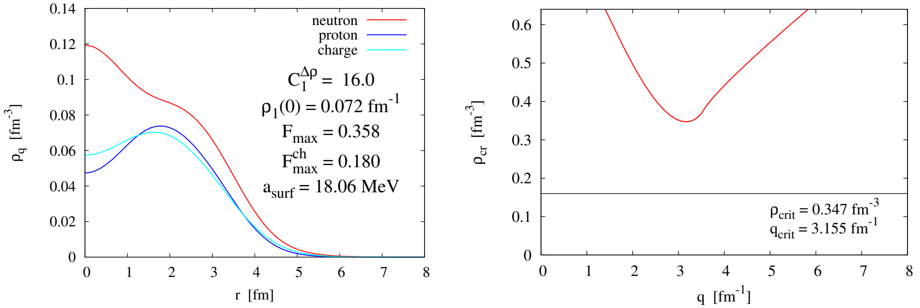

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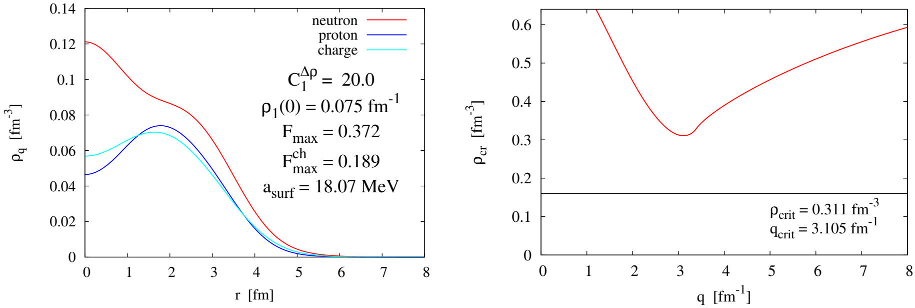

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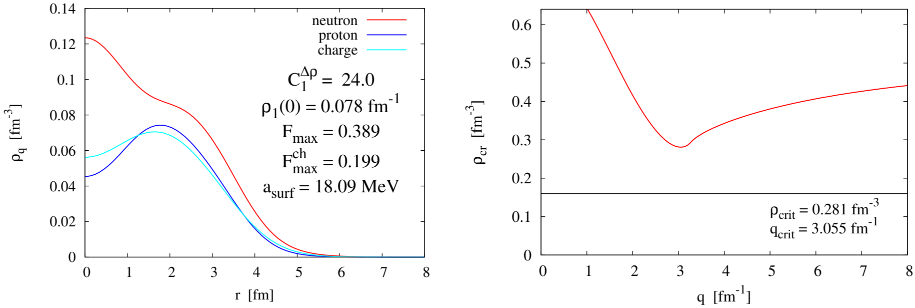

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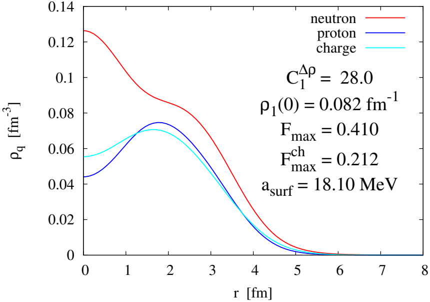

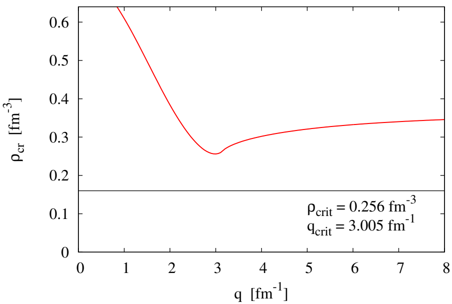

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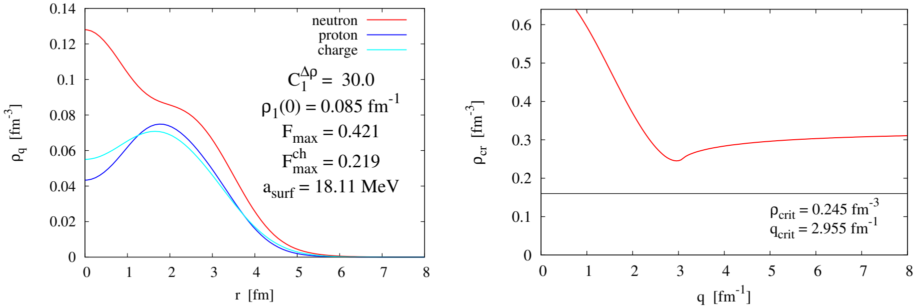

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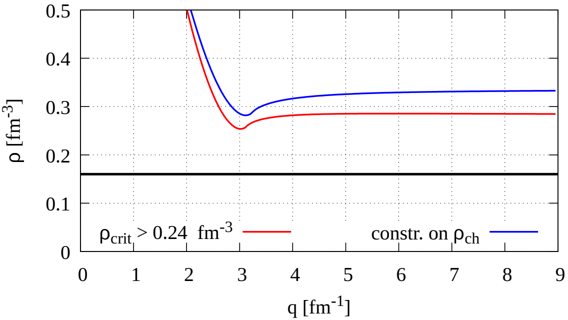
Use of charge distributions to fit the EDFs parameters

Skyrme SLy functional constrained with

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



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

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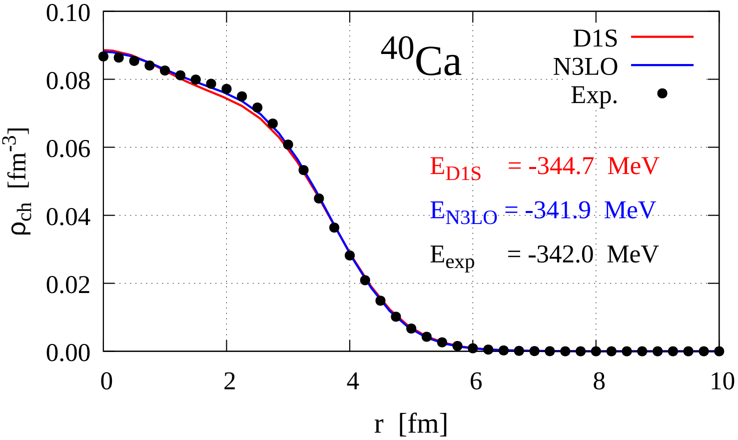
[3] $\rho_{\mathrm{crit}} > 0.24\ \mathrm{fm}^{-3}$ as for SLy5*, *Cf.* A. Pastore *et al.*, arXiv:1210.7937

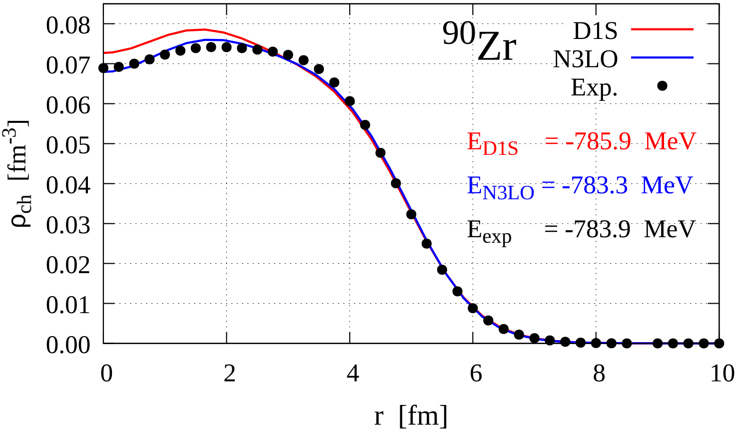
Regularized functional constained with charge distributions

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

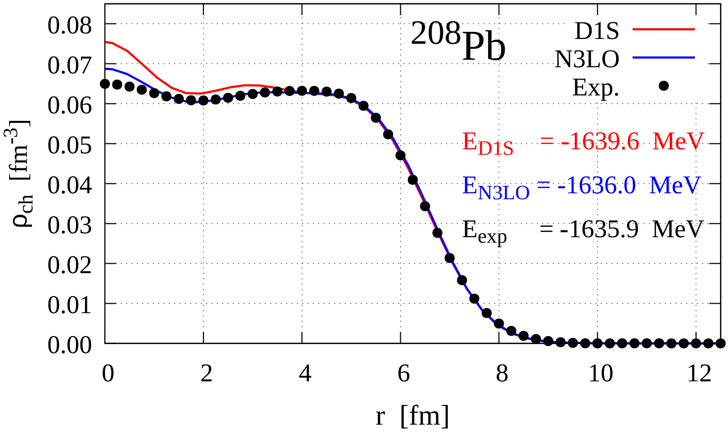
Nuclei use in the fit: ^{40}Ca



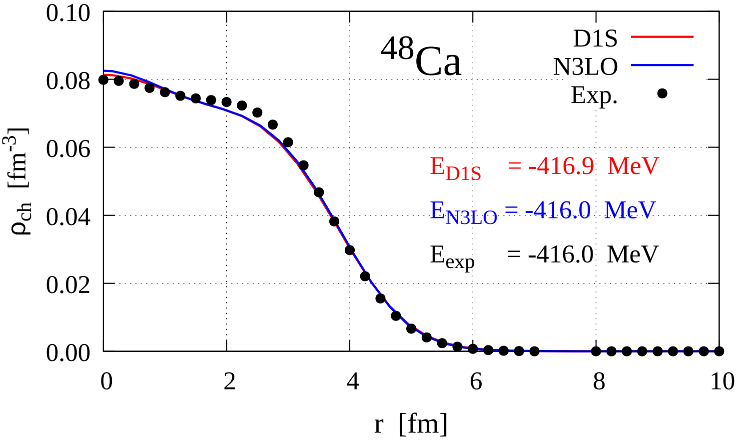
Nuclei use in the fit: ^{90}Zr



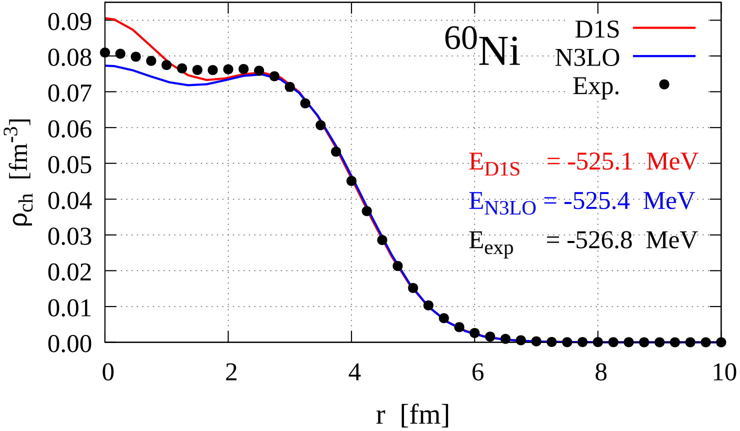
Nuclei use in the fit: ^{208}Pb



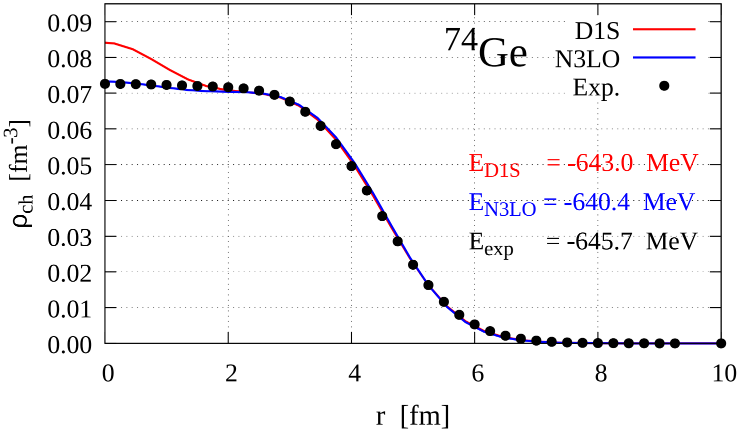
Nuclei not use in the fit: ^{48}Ca



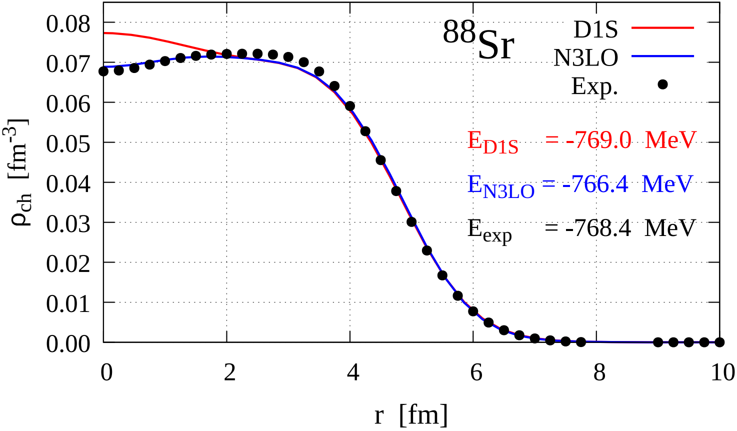
Nuclei not use in the fit: ^{60}Ni



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

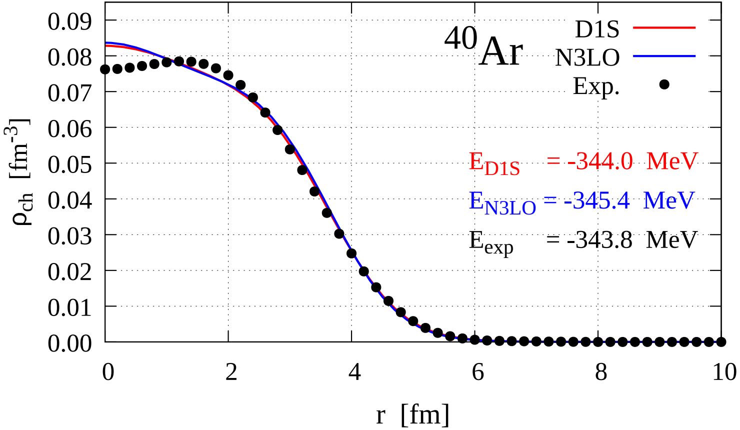


Nuclei not use in the fit: ^{88}Sr

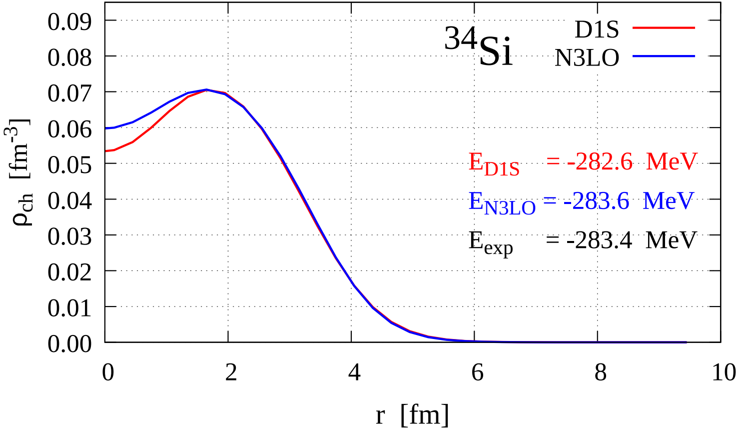


Nuclei not use in the fit: ^{40}Ar

Don't worry, it does not always work...



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.