

Nuclear charge radius predictions from DFT-based models

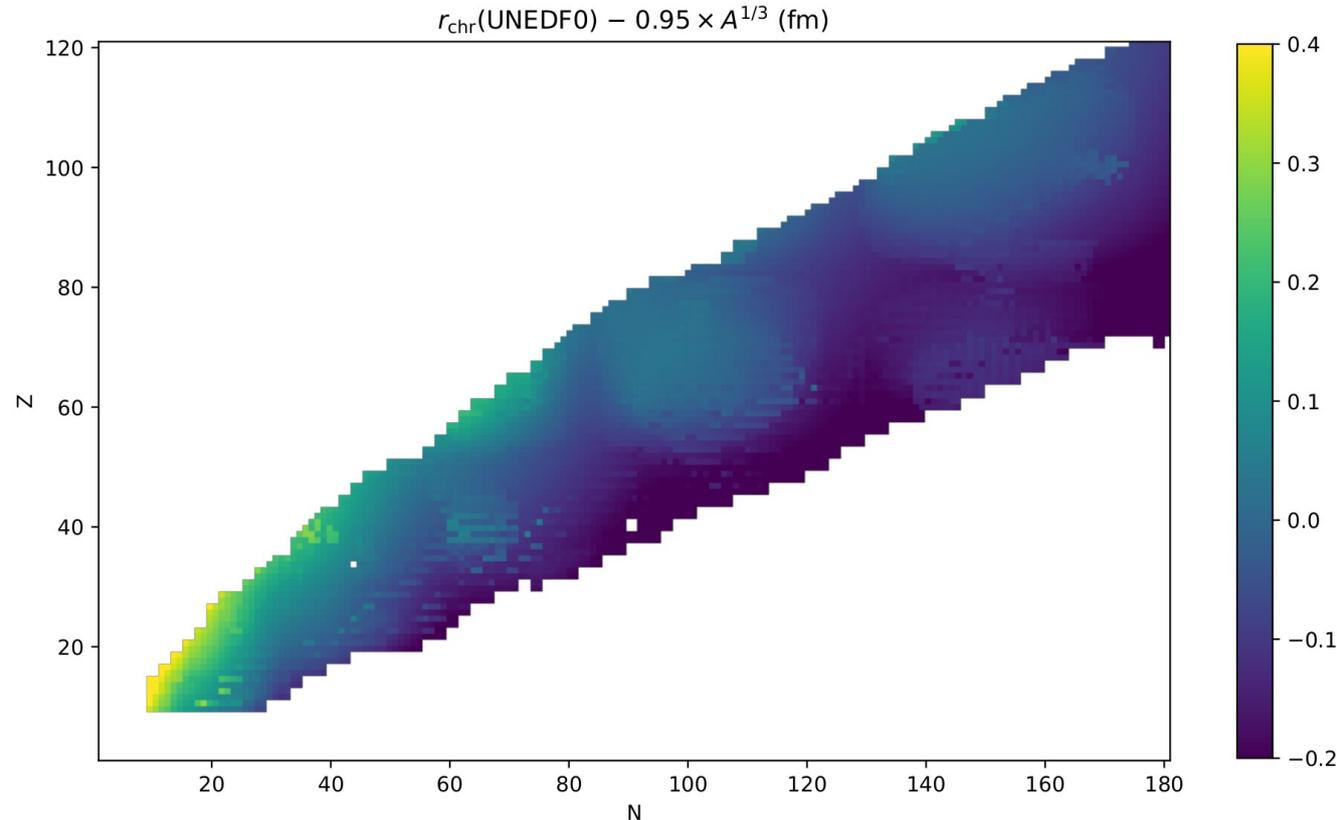
10th International workshop on Quantum Phase Transitions in Nuclei and Many-Body Systems

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Nuclear charge radius

- Nuclear charge radius can provide a lot of information about the nuclear structure
- Although charge radius roughly behaves as $\sim A^{1/3}$, to explain its local variation requires precise nuclear structure calculations
- Various microscopical effects impact on the radius: shell structure, deformation, pairing, presence of continuum, etc.
- A sudden change in the systematics of the radius can signal a transition between, e.g., deformed and spherical systems
- During recent years, a lot of new experimental data has been obtained. This allows to test nuclear structure models more systematically



Fayans energy density functional

- Compared to Skyrme EDF, Fayans EDF has a more complicated structure. A unique feature is density dependence and gradient term in denominator parts. Volume and surface part of the Fayans EDF are

$$\mathcal{E}_{\text{Fy}}^{\text{v}} = \frac{1}{3} \varepsilon_F \rho_{\text{sat}} \left[a_+^{\text{v}} \frac{1 - h_{1+}^{\text{v}} x_0^\sigma}{1 + h_{2+}^{\text{v}} x_0^\sigma} x_0^2 + a_-^{\text{v}} \frac{1 - h_{1-}^{\text{v}} x_0}{1 + h_{2-}^{\text{v}} x_0} x_1^2 \right]$$

where free parameters are indicated with red color

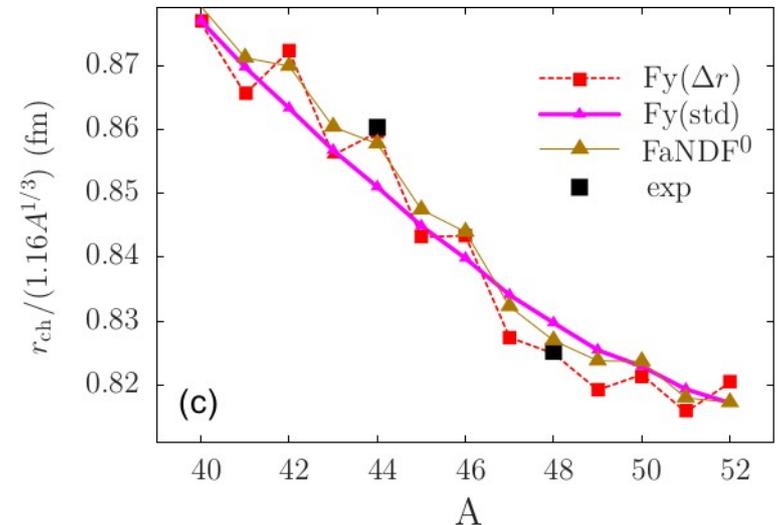
$$\mathcal{E}_{\text{Fy}}^{\text{s}} = \frac{1}{3} \varepsilon_F \rho_{\text{sat}} \frac{a_+^{\text{s}} r_s^2 (\nabla x_0)^2}{1 + h_+^{\text{s}} x_0^\sigma + h_\nabla^{\text{s}} r_s^2 (\nabla x_0)^2}$$

- Recent Fayans functionals add gradient term on pairing energy density

$$\mathcal{E}_{\text{Fy},q}^{\text{pair}} = \frac{2\varepsilon_F}{3\rho_{\text{sat}}} \tilde{\rho}_q^2 \left[f_{\text{ex}}^\xi + h_+^\xi x_{\text{pair}}^\gamma + h_\nabla^\xi r_s^2 (\nabla x_{\text{pair}})^2 \right]$$

- This term probably helps to reproduce observed strong odd-even charge radius staggering in Ca isotopic chain
- In many other isotopic chains, $\text{Fy}(\Delta r)$ and $\text{Fy}(\Delta r, \text{HFB})$ seem to predict too strong odd-even staggering of charge radius

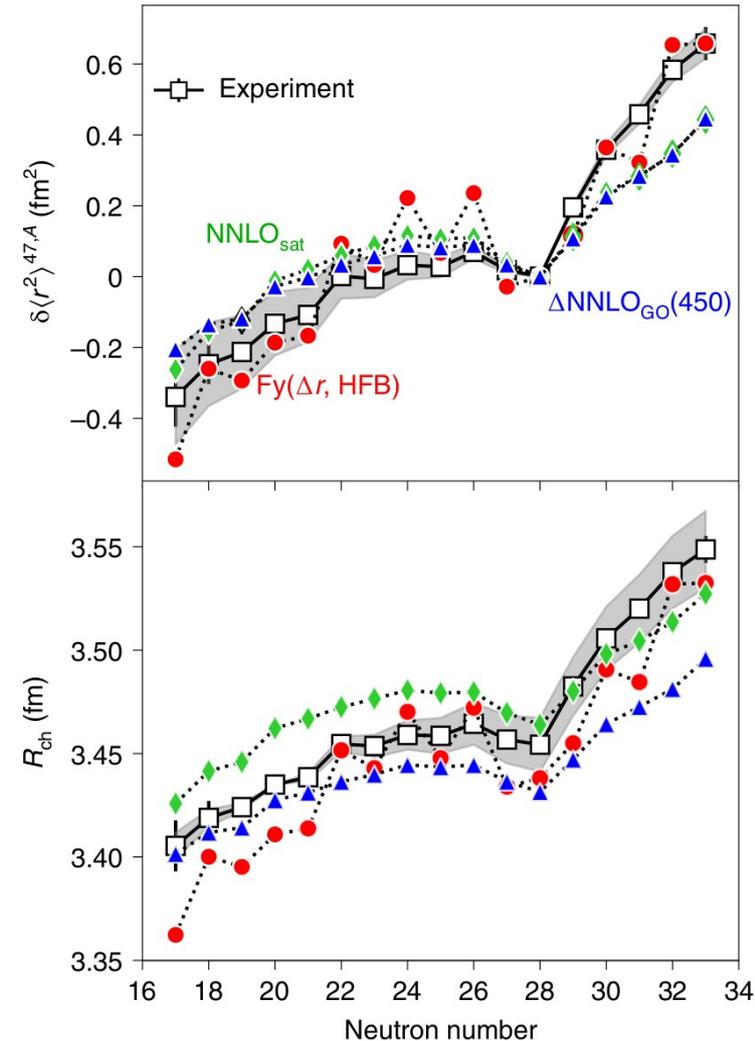
Charge radius along Ca isotopic chain. Figs from P.-G. Reinhart, et.al, Phys Rev C 95, 064328 (2017)



K isotopic chain

- The charge radius of potassium isotopes were recently measured at ISODLE with laser spectroscopy
- Theoretical calculations were carried out in DFT framework, by using $Fy(\Delta r, HFB)$ EDF, and with ab-initio coupled-cluster calculations with $NNLO_{sat}$ and $\Delta NNLO_{GO}$
- $Fy(\Delta r, HFB)$ reproduces the kink and trend after $N = 28$ well. However, it shows too strong odd-even effect. (Too strong odd-even effect was also present in some earlier $Fy(\Delta r, HFB)$ results too)
- Ab-initio results show more realistic odd-even effect, but the trend after $N = 28$ is not so well reproduced
- The charge radii show no signature of a magic shell gap at $N = 32$

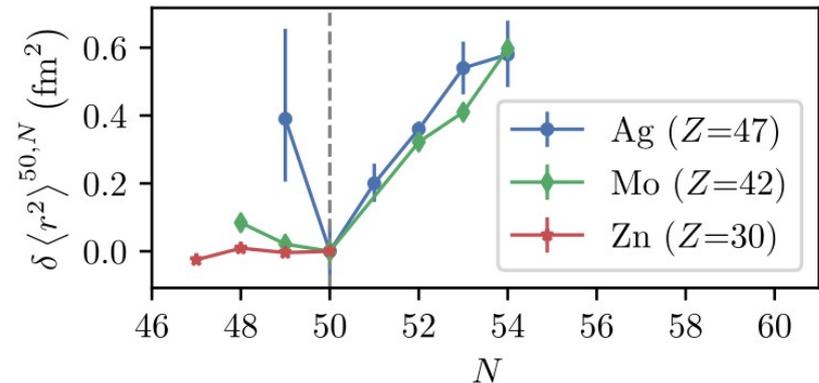
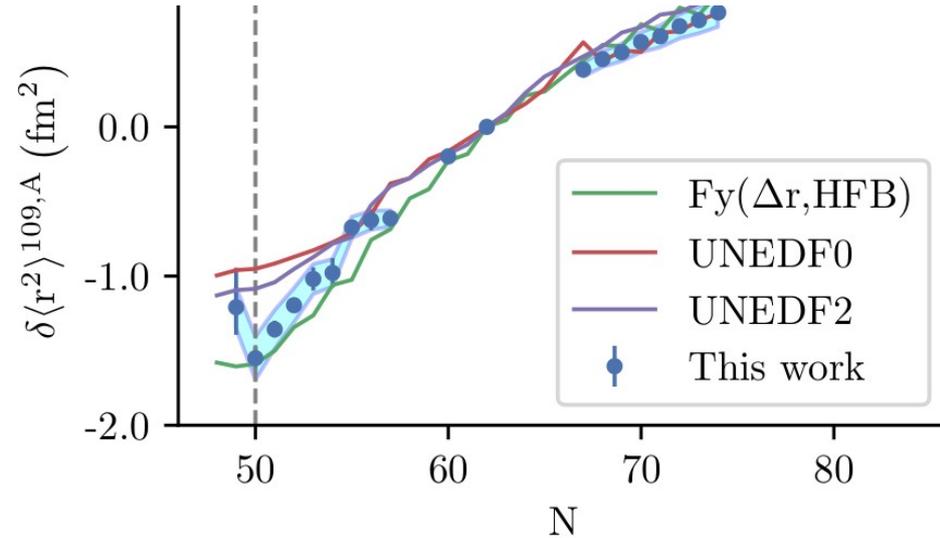
Right: Isotopic shifts and charge radii in potassium
Á. Koszorús et al, Nature Phys. 17, 439 (2021)



Ag isotopic chain

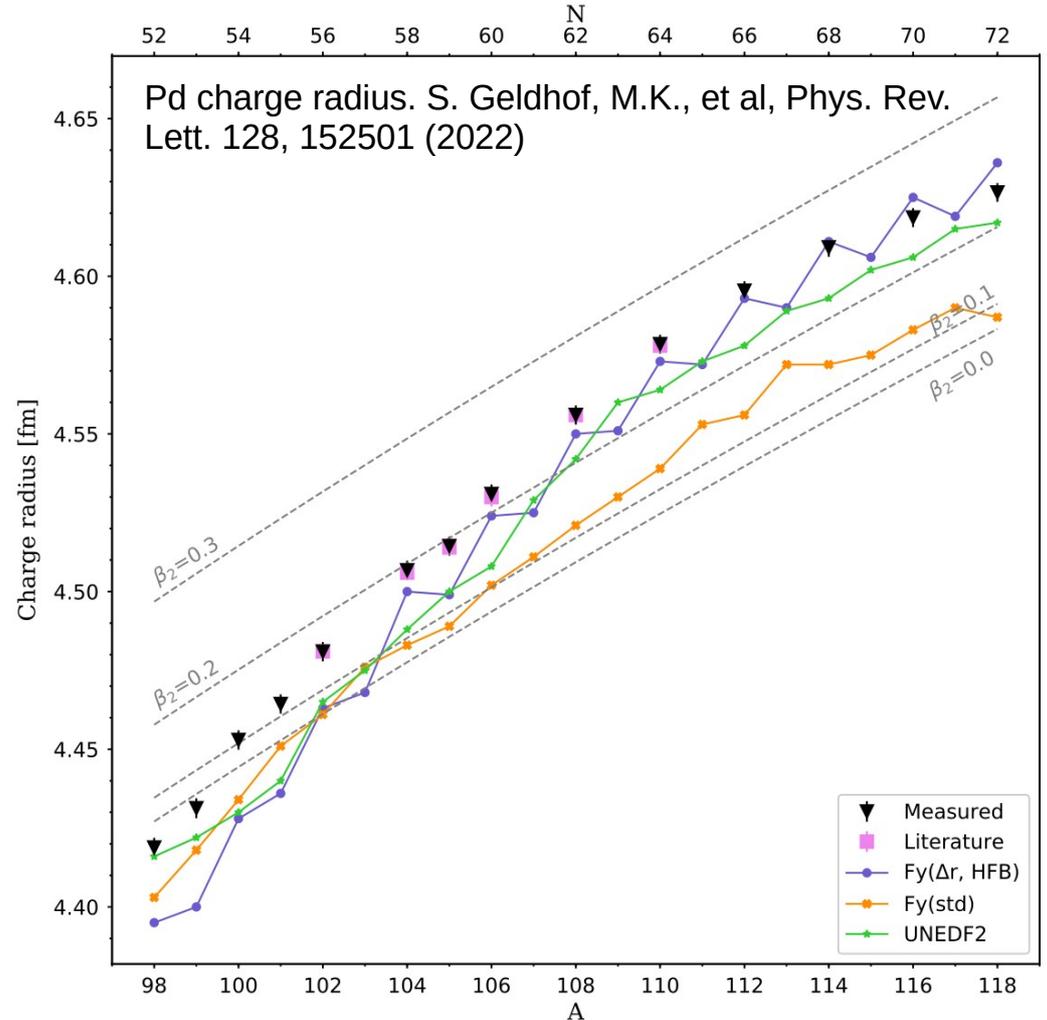
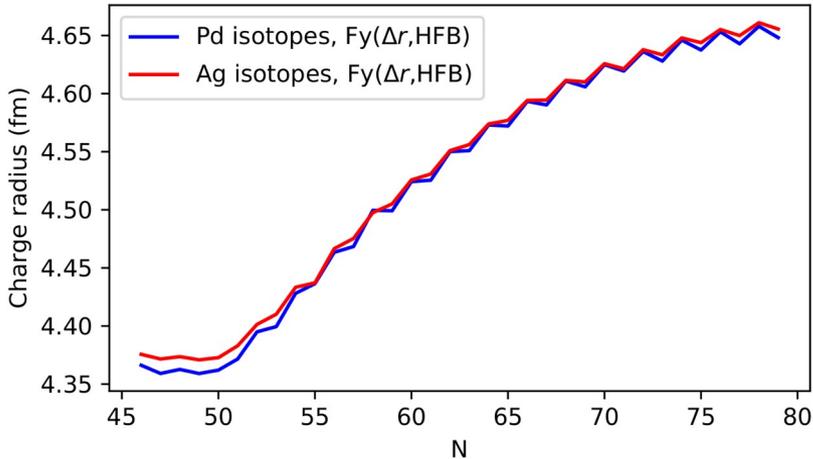
- Ag, and Pd, isotopic shifts were measured at JYFL acc. lab, Jyväskylä
- Generally, $Fy(\Delta r, \text{HFB})$ seems to follow experimental results more closely than UNEDF0 or UNEDF2 EDFs
- Odd-even effect with $Fy(\Delta r, \text{HFB})$ is too strong
- The measured charge radius of ^{96}Ag ($N=49$) is surprisingly large.
- With e.g. Mo or Zn isotopic chains, crossing of the $N=50$ shell gap does not lead such a large increase of the radius
- Such a large increase in ^{96}Ag radius can not be probably explained by any reasonable single-reference EDF model

Ag isotopic shifts, M. Reponen et al, Nature Comm 12, 4596 (2021)

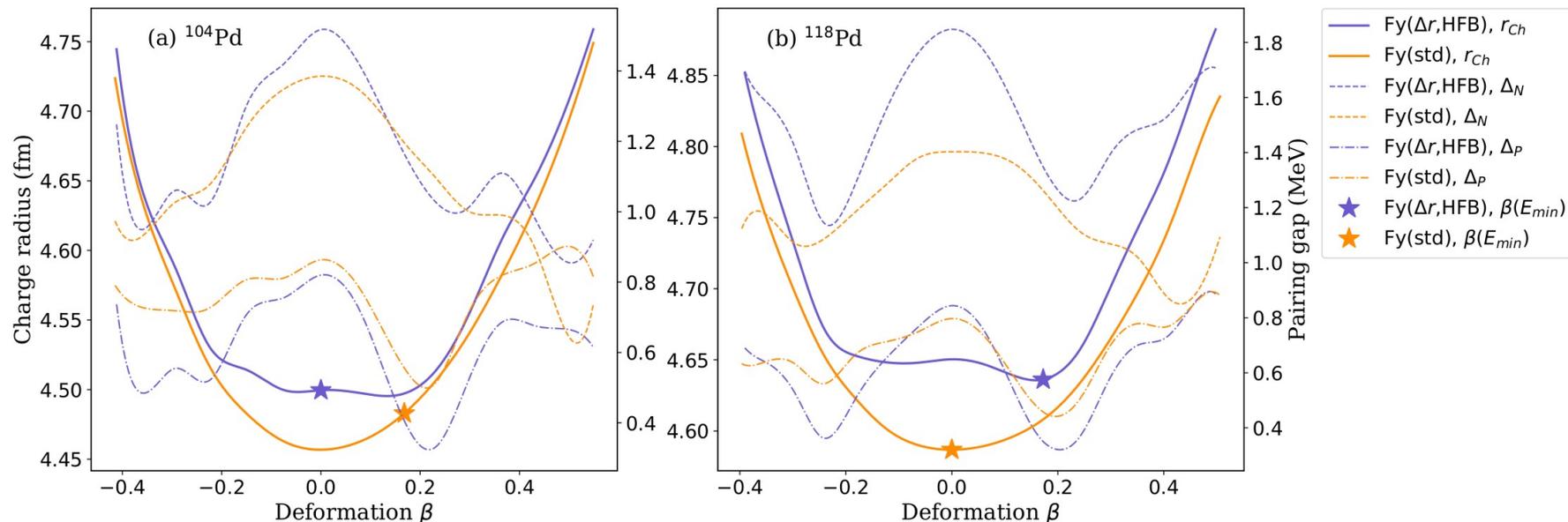


Pd isotopic chain

- Again, $F_y(\Delta r, \text{HFB})$ seems to follow experimental results most closely, especially in heavier isotopes.
- Calculated $F_y(\Delta r, \text{HFB})$ pattern of radii in Pd is very similar to Ag isotopic chain. This is probably a limitation of the single-reference EDF approach
- Odd-even effect with $F_y(\Delta r, \text{HFB})$ is too strong



Pd isotopic chain and Fayans functional



- Pd isotopic chain can be used to test interplay between deformation, pairing and charge radius
- Usually r_{rms} behaves approximately parabolically as a function of quadrupole deformation, like Fy(std) results above
- At small deformation, Fy(Δr , HFB) produces a rather constant radius as a function deformation
- Close to spherical shape, pairing correlations increase. With the strong coupling between surface term and pairing density this lead to increase of r_{rms} .
- Similar behavior seen throughout the isotopic chain

Coupling between surface term and pairing correlations

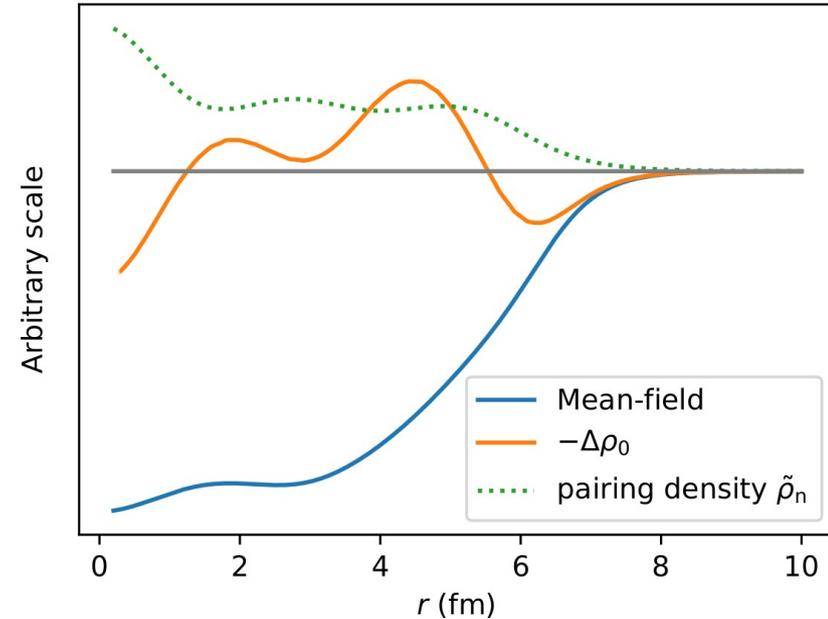
- The coupling between surface term and pairing in Fayans EDF stems from the pairing EDF term

$$E \sim \tilde{\rho}^2 (\nabla \rho_0)^2$$

- This gives following contribution to the mean-field

$$U(r) \sim -\tilde{\rho}^2 \Delta \rho_0$$

- Larger pairing correlations means larger pairing density $\bar{\rho}$, which then lowers the mean-field $U(r)$ at nuclear surface, resulting to density producing a larger r_{rms} .
- In odd or odd-odd nuclei, pairing correlation are weaker. This results to smaller $\bar{\rho}$ and therefore also smaller r_{rms} . Hence the notable odd-even effect.
- This coupling also provides mechanism to increase r_{rms} in mid-shell isotopes, whereas in magic nuclei phase-transition to unpaired state switches this term off



Charge radius in Ca – Zn isotopic chains

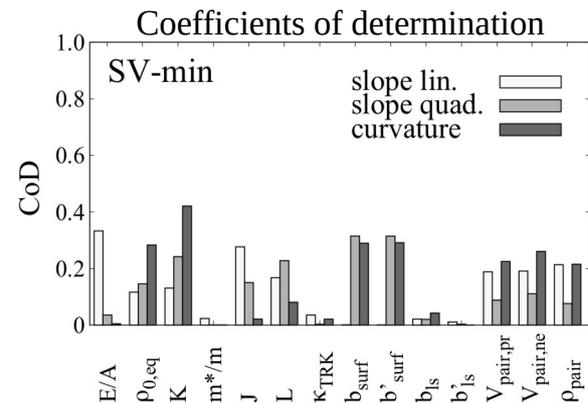
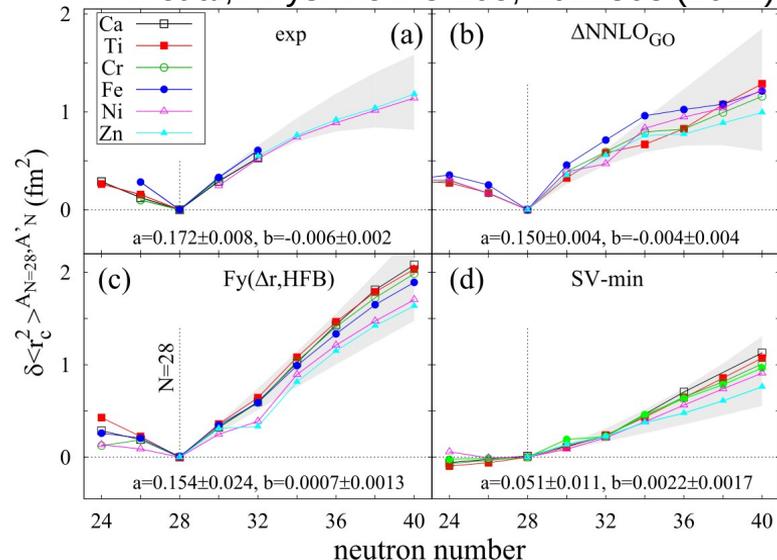
- Calculated charge radii differentials in even-even isotopic chains between Ca and Zn seem to follow remarkable similar pattern
- For each model, the results can be rather well fitted on a curve

$$\delta \langle r_c^2 \rangle_{A_m, A_m+n} = an + bn^2$$

where a and b depend on used model, and $N=28$ isotopes are used as reference point

- This behavior occurs with DFT models and also with ab-initio calculations
- Experimental data, where available, also follows this same pattern
- Statistical analysis of SV-min Skyrme EDF parameters indicates that a and b coefficients are not determined strongly by any single model parameter

Charge radii differentials in Ca – Zn isotopes
M. K. et al, Phys. Rev. C 105, L021303 (2022)



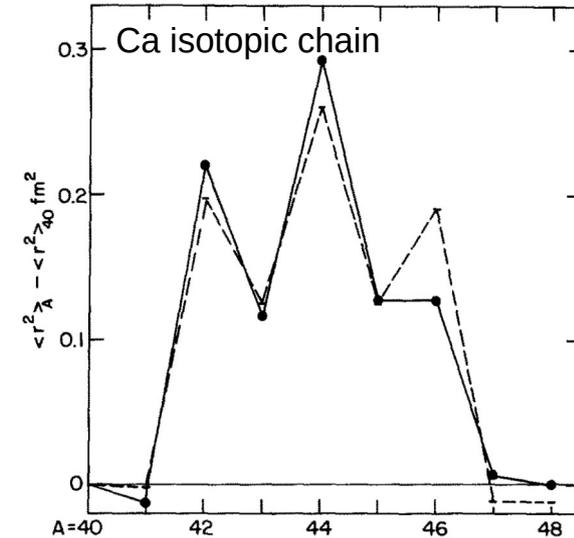
Arc-like trend in the charge radius

I. Talmi, Nuclear Physics A423 (1984) 189

- The $F_y(\Delta r, \text{HFB})$ results show an arc-like isotopic trend of charge radius, between magic numbers, as well as strong odd-even effect
- For Ca – Zn isotopic chains, $\Delta \text{NNLO}_{\text{GO}}$ also follows arc-like trend
- Similar pattern has been discussed in some earlier works. For example, in [Talmi, NPA423 (1984)], a simple phenomenological model produces similar kind of behavior for the radius:

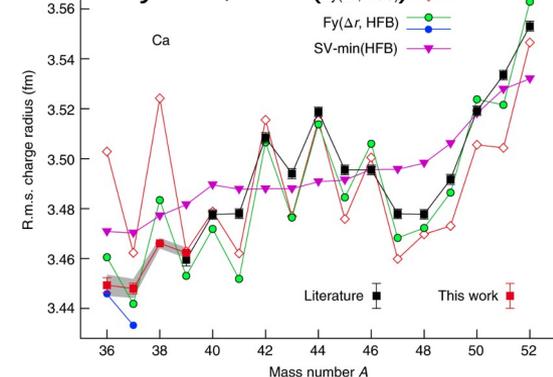
$$\langle 0 | \sum r_i^2 | 0 \rangle = \langle \sum r_i^2 \rangle_0 + nC + \frac{1}{2}n(n-1)A + [\frac{1}{2}n]B.$$

- This was due to core polarization by valence neutrons, when considering states with lowest seniority
- In DFT approach, however, the picture is not as clear, since the behavior of the radius, and its isotopic trend, is affected by many model parameters



A.J. Miller et al, Nature

Phys 15, 432 (2019)



Conclusions and outlook

- Recent charge radii measurements have provided data to test nuclear structure models systematically in many isotopic chain
- Fayans EDF, especially $F_y(\Delta r, \text{HFB})$ parametrization, seems to follow more closely local variation of r_{rms} , when compared to Skyrme-like EDFs
- Compared typical Skyrme-like EDFs the Fayans EDF has potential to better reproduce arc-like isotopic trend
- On the downside, $F_y(\Delta r, \text{HFB})$ has too strong odd-even effect. In addition, its parameter adjustment was only done with spherical nuclei, so its predictive power in deformed nuclei may suffer
- Calculated charge radii in Ca – Zn isotopic chains follow very regular pattern. It would be interesting to see if this pattern holds with more experimental data.
- Adjustment of Fayans EDF parameters with deformed nuclei could improve its predictive power.
- On parallel, ongoing development of EDF intended for the beyond mean-field calculations