Nuclear charge radius predictions with Fayans EDF

Gogny Conference - Nuclear structure and reactions
Dec 10 – 13, 2024, Paris

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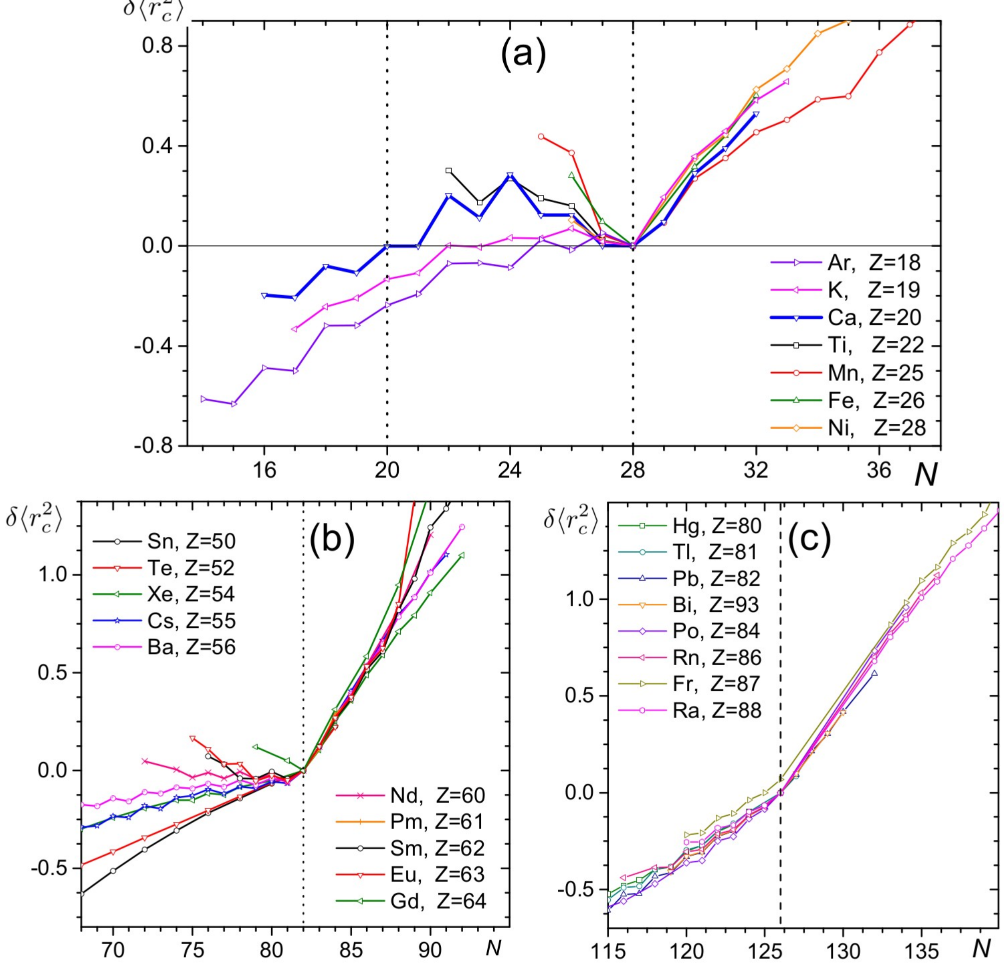
Nuclear charge radius

- 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



Trend of the charge radius at shell closures. From Nuclear Charge Radii, Nuclear Physics Handbook, W. Nörtershäuser, I.D. Moore.

Fayans energy density functional

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

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

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

where free parameters are indicated with red color

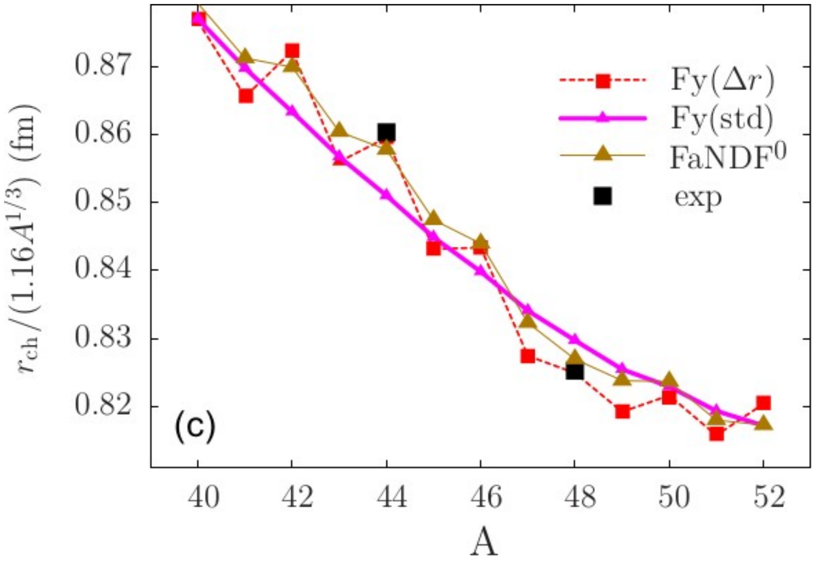
- Recent Fayans functionals add gradient term on pairing energy density

$$\mathcal{E}^{\mathrm{pair}}_{\mathrm{Fy},q} = \frac{2\varepsilon_F}{3\rho_{\mathrm{sat}}}\breve{\rho}_q^2\left[f^{\xi}_{\mathrm{ex}} + h^{\xi}_{+}x^{\gamma}_{\mathrm{pair}} + h^{\xi}_{\nabla}r_s^2(\nabla x_{\mathrm{pair}})^2\right]$$

- This term probably helps to reproduce observed strong odd-even charge radius staggering in Ca isotopic chain

- In many other isotopic chains, Fy(Δr) and Fy(Δr,HFB) seem to predict too strong odd-even staggering of charge radius
- Fayans EDF used to interpret many recent measurements of nuclear charge radius

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



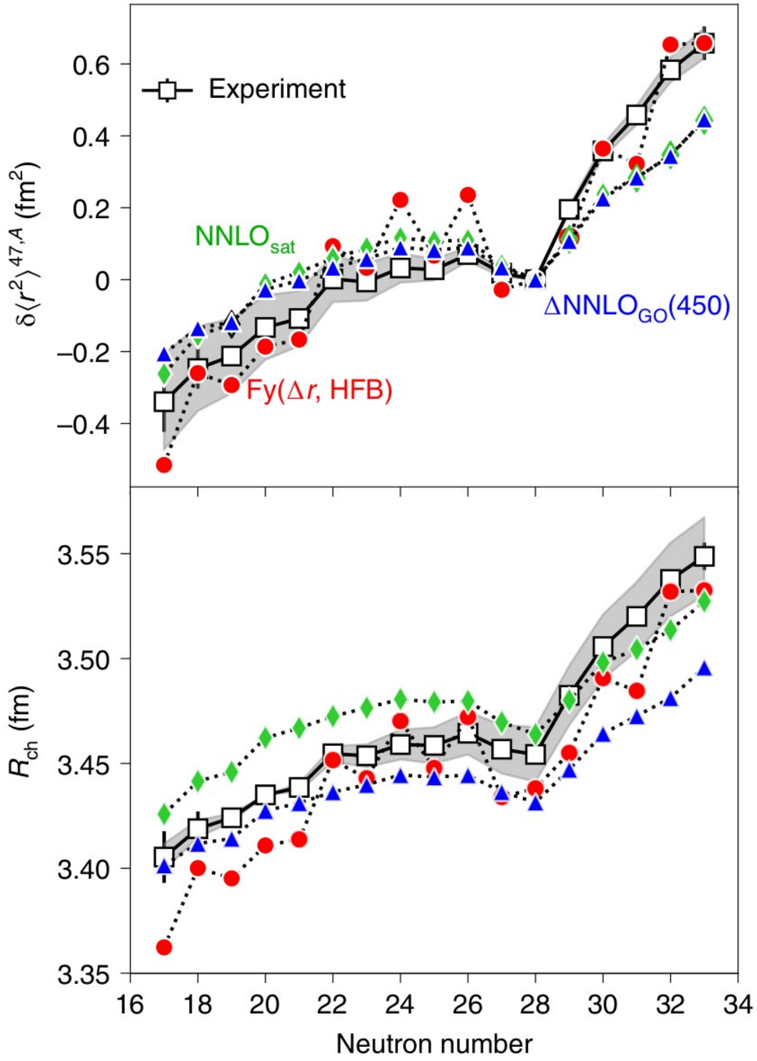
K isotopic chain

- 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(Δr,HFB) EDF, and with ab-initio coupled-cluster calculations with $NNLO_{sat}$ and $\Delta NNLO_{GO}$

- Fy(Δr,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(Δr,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 $N = 32$

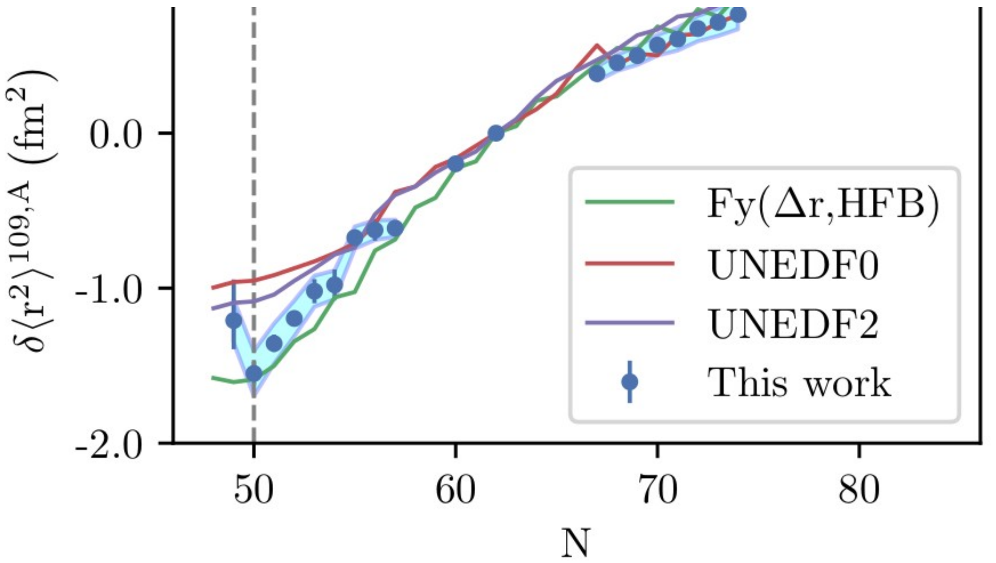


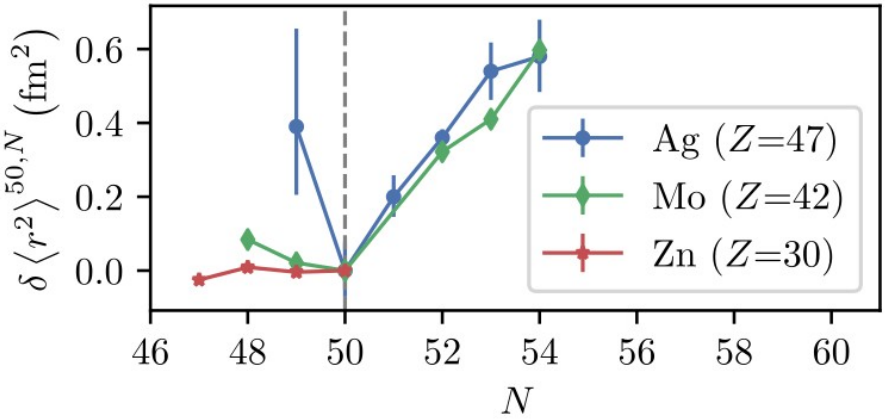
Right: Isotopic shifts and charge radii in potassium
Á. Koszorús et al, Nature Phys. 17, 439 (2021)

Ag isotopic chain

- Ag, and Pd, isotopic shifts were measured at JYFL acc. lab, Jyväskylä
- Generally, Fy(Δr,HFB) seems to follow experimental results more closely than UNEDF0 or UNEDF2 EDFs
- Odd-even effect with Fy(Δr,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

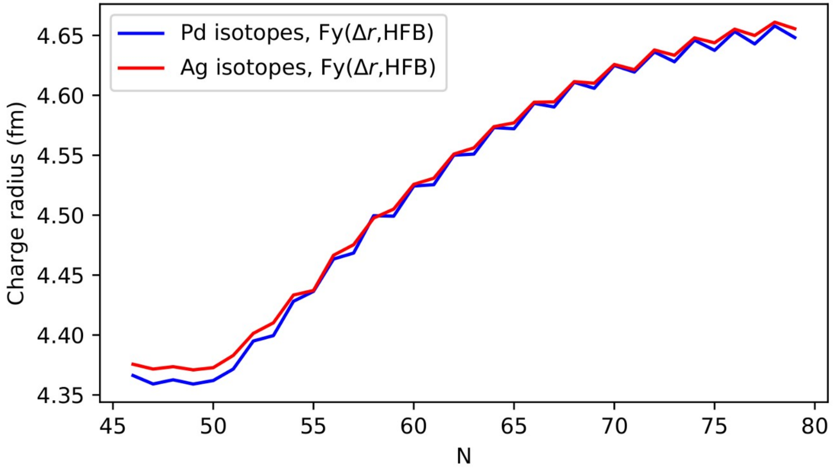
Ag isotopic shifts, M. Reponen et al, Nature Comm 12, 4596 (2021)

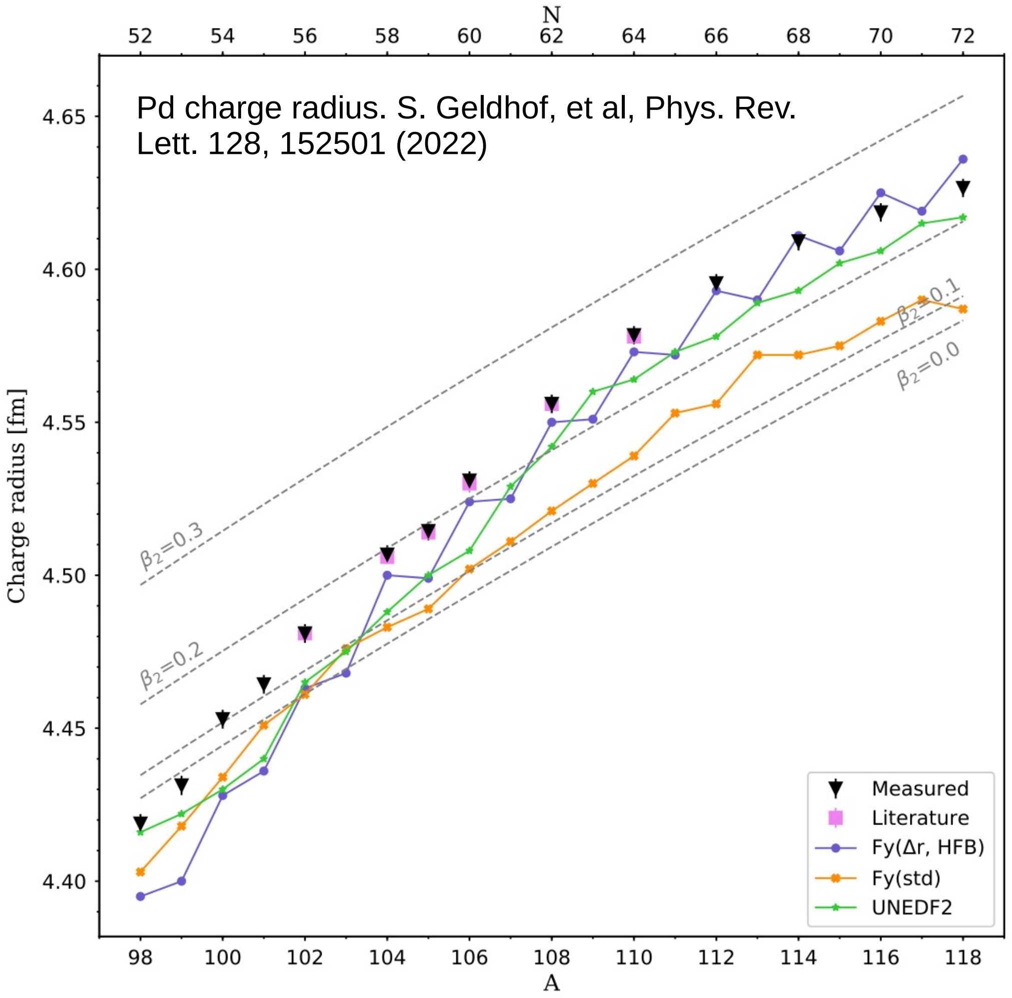




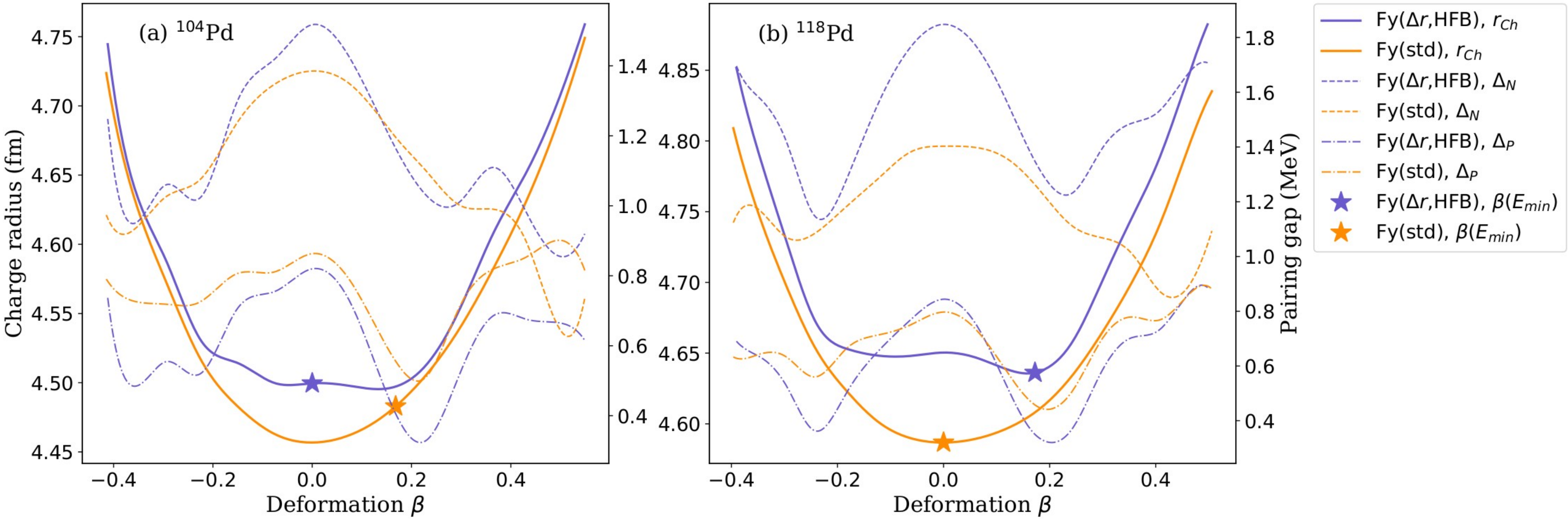
Pd isotopic chain

- Again, Fy(Δr,HFB) seems to follow experimental results most closely, especially in heavier isotopes.
- Calculated Fy(Δr,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 Fy(Δr,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 the 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 whole 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

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

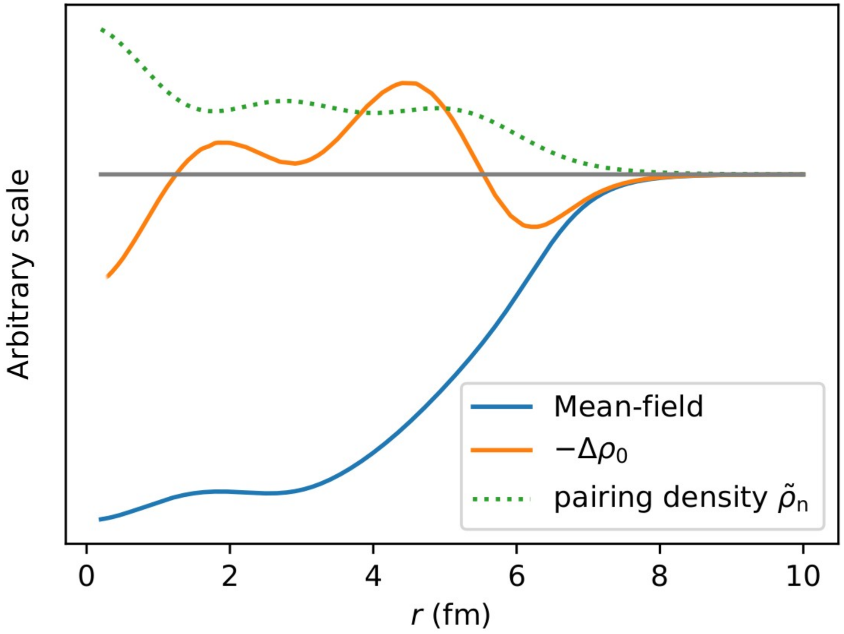
- This gives following contribution to the mean-field

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

- Larger pairing correlations means larger pairing density $\tilde{\rho}$, 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 $\tilde{\rho}$ 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

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

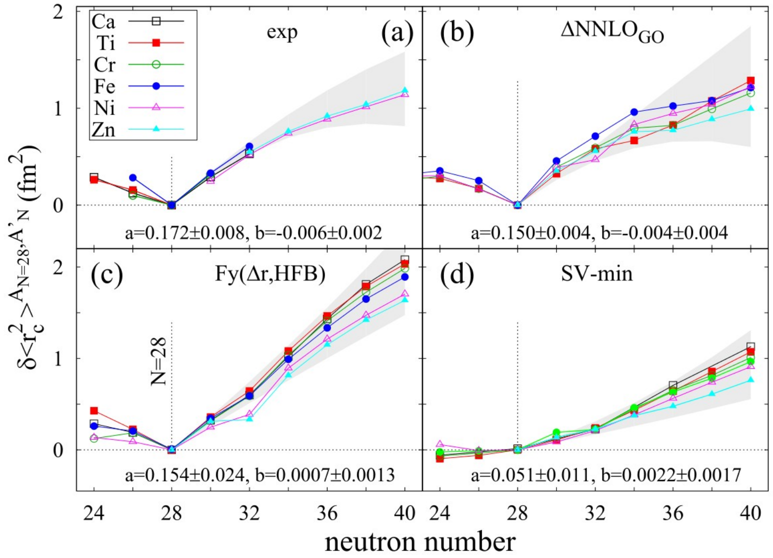
where *a* and *b* depend on used model, and *N* = 28 isotopes are used as reference point

- This behavior occurs with DFT models and also with ab-initio calculations

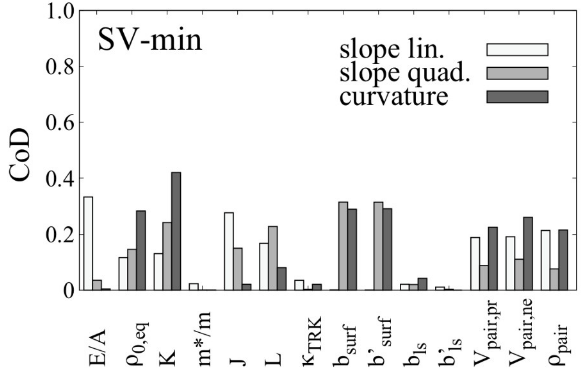
- Experimental data, where available, also follows this same pattern

- 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)

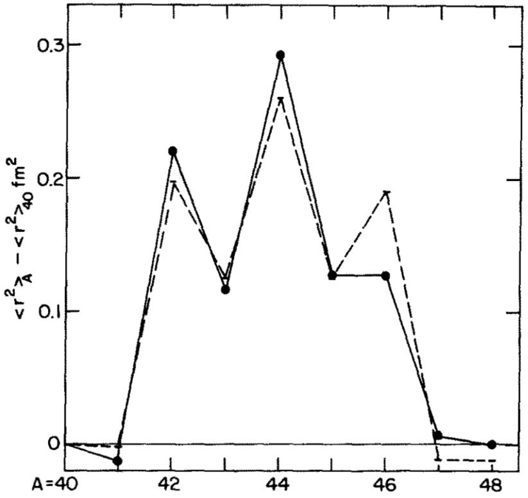


Coefficients of determination



Arc-like trend in the charge radius

I. Talmi, Nuclear Physics A423 (1984) 189



- The Fy(Δr,HFB) results show an arc-like isotopic trend of charge radius, between magic numbers, as well as strong odd-even effect

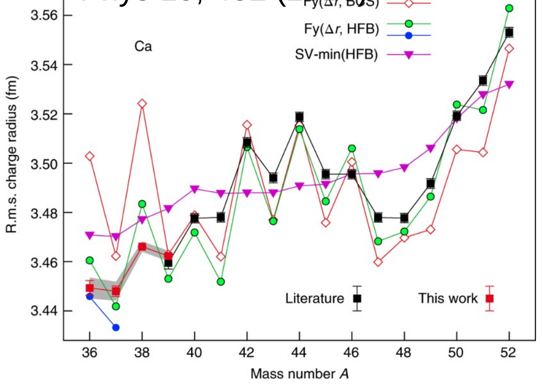
- Similar patter has been discussed in some earlier works. For example, in [Talmi, NPA423], a simple phenomenological model where core polarization by valence neutrons produces similar kind of behavior for the radius:

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

- This was due to core polarization by valence neutrons, when considering states with lowest seniority

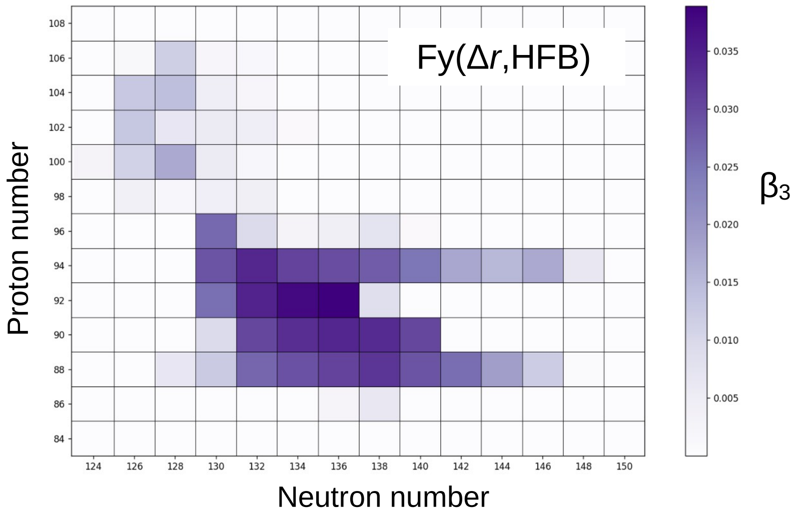
- In DFT approach, however, the picture is not as clear, since the behavior of the radius, and its isotopic trend, is affected by many model parameters and competing EDF terms during the self-consistent loop

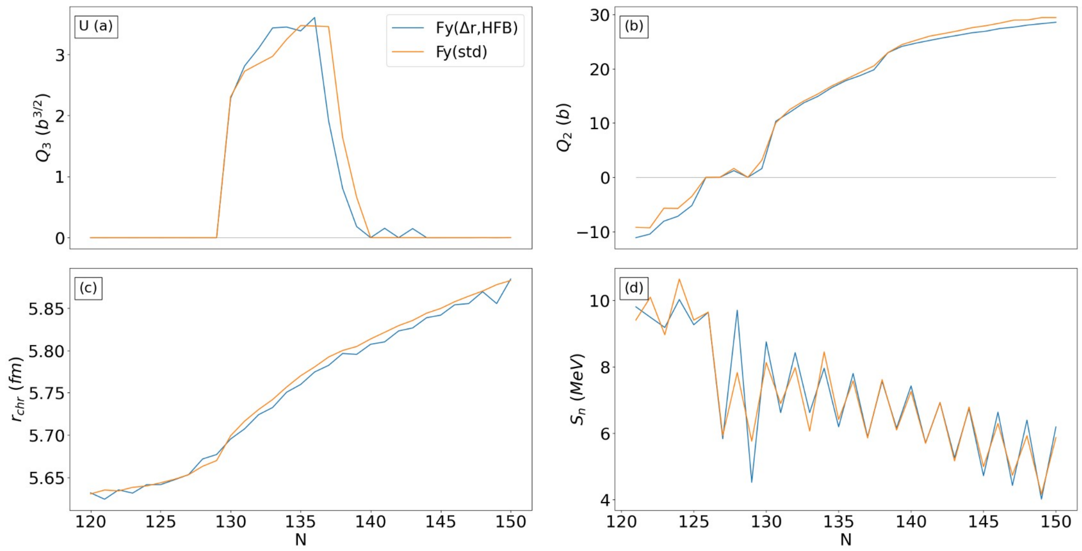
A.J. Miller et al, Nature Phys 15, 432 (2019)



Octupole deformation properties of Fayans EDF

- We have recently investigated octupole deformation properties of Fayans EDF in actinide region
- The Fy(Δr,HFB) and Fy(std) predictions for octupole deformation are rather similar (except for Rn, where Fy(Δr,HFB) predicts much smaller octupole deformation)
- Octupole deformation concentrates in similar region as with Skyrme EDFs
- Fy(Δr,HFB) predicts here too a notable odd-even effect in charge radius
- Work done by Gauthier Danneaux





Figs. by Gauthier Danneaux

Conclusions and outlook

- Recent charge radius measurements have provided data to test nuclear structure models systematically in many isotopic chain
- Fayans EDF, especially Fy(Δr,HFB) parametrization, seems to follow (usually) 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, Fy(Δr,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

- Charge radii in Ca – Zn isotopic chains follow very regular pattern, also with DFT and ab-initio calculations. It would be interesting to see if this pattern holds with more experimental data.

- Octupole deformation properties with Fayans EDFs in actinide region similar to Skyrme EDFs

- Recent work by P.-G. Reinhard et al (J. Phys. G 51 105101 (2024)) showed that isovector dependency in pairing channel can improve description on various observables
- Adjustment of Fayans EDF parameters with deformed nuclei could improve its predictive power.

Acknowledgments

Charge radii of exotic potassium isotopes challenge nuclear theory and the magic character of $N = 32$

Á. Koszorús[1,17], X. F. Yang[1,2], W. G. Jiang[3,4,5], S. J. Novario[3,4], S. W. Bai[2], J. Billowes[6], C. L. Binnersley[6], M. L. Bissell[6], T. E. Cocolios[1], B. S. Cooper[6], R. P. de Groote[7,8], A. Ekström[5], K. T. Flanagan[6,9], C. Forssén[5], S. Franchoo[10], R. F. Garcia Ruiz[11,12], F. P. Gustafsson[1], G. Hagen[4], G. R. Jansen[4], A. Kanellakopoulos[1], M. Kortelainen[7,8], W. Nazarewicz[13], G. Neyens[1,12], T. Papenbrock[3,4], P.-G. Reinhard[14], C. M. Ricketts[6], B. K. Sahoo[15], A. R. Vernon[1,6] and S. G. Wilkins[16]

Evidence of a sudden increase in the nuclear size of proton-rich silver-96

M. Reponen[1], R. P. de Groote[1], L. Al Ayoubi[1,2], O. Beliuskina[1], M. L. Bissell[3], P. Campbell[3], L. Cañete[4], B. Cheal[5], K. Chrysalidis[6], C. Delafosse[1,2], A. de Roubin[1,7], C. S. Devlin[5], T. Eronen[1], R. F. Garcia Ruiz[8], S. Geldhof[1,9], W. Gins[1], M. Hukkanen[1,7], P. Imgram[10], A. Kankainen[1], M. Kortelainen[1], Á. Koszorús[5], S. Kujanpää[1], R. Mathieson[5], D. A. Nesterenko[1], I. Pohjalainen[1,11], M. Vilén[1,6], A. Zadvornaya[1] & I. D. Moore[1]

Impact of Nuclear Deformation and Pairing on the Charge Radii of Palladium Isotopes

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Universal trend of charge radii of even-even Ca–Zn nuclei

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Thank you!