# Self-Consistent Calculation of Nuclear Charge Radii in K Isotopes

**I. N. Borzov[a, b, ]\*** and **S. V. Tolokonnikov[a, c, ]\*\***

[a] *National Research Centre "Kurchatov Institute," Moscow, Russia*
[b] *Bogoliubov Laboratory of Theoretical Physics, Joint Institute of Nuclear Research, Dubna, Russia*
[c] *Moscow Institute of Physics and Technology (National Research University), Dolgoprudny, Russia*
*\*e-mail: Borzov_IN@nrcki.ru*
*\*\*e-mail: Tolokonnikov S.V@nrcki.ru*

**Abstract**—Fully self-consistent study of the charge radii in Ca region is exemplified by the calculation in the long chains of K isotopes. The neutron-deficient and neutron-rich nuclei with pairing in both neutron and proton sectors, as well as the (semi-) magic nuclei around the closed neutron shells at $N = 20, 28, 32$ are treated within the Energy Density Functional (EDF) approach with the Fayans functional DF3-a. The performance of the DF3-a is analysed in describing the odd-even staggering effects found both in previous and in more recent CERN-ISOLDE experiments for $^{36-52}$K isotopes.

## INTRODUCTION

Nuclear radii carry important information about mesoscopic nature of nuclei and give an insight to nuclear structure helping to pin down nucleon-nucleon interaction. Global behavior of the nuclei dimensions (the radii of their proton and neutron distributions, their matter radii, or their charge radii) as the mass number grows are described by the liquid-drop formula $R = r_0 A^{1/3}$ where $r_0$ is the Wigner–Seits radius for nuclear matter. The experiments show, however a weaker $A$ dependence of the radii with a "negative" (compared to the liquid-drop model) isotopic shift and sizable local fluctuations. This specific quantum phenomenon reflects the evolution of the nuclear shell structure which manifest itself by formation of local minima (maxima) upon the crossing of closed shells and odd–even staggering of charge radii (OES effect).

In the recent years, amount of information about the charge radii of nuclei has grown significantly owing to the development of the collinear resonance ionization spectroscopy (CRIS) [1]. New data on isotopic dependence of charge radii obtained in the ISOLDE-CERN experiments provide a testing ground for the predictions of microscopic self-consistent models for very neutron-rich isotopes.

The calcium region containing the isotopes near a magic proton number $Z = 20$ and neutron closed shells $N = 20, 28, 32, 34$ is important nuclear structure laboratory. A bulk of information on masses, nuclear spins, magnetic and quadrupole moments, as well as charge radii has been obtained for the first time for the isotopes crossing the $N = 28$ shell closure [2–9]. A lot of attention has also been attracted to the isotopes near exotic $N = 32$ neutron closed (sub)shell in the Ca

region and beyond [2–10]. In calcium isotopes, the filling of orbitals near the new neutron magic subshell of $N = 32$ shows up as an anomalous growth of the charge radii. A striking example: the change of the $^{52}$Ca charge radius (with respect to $^{48}$Ca) is $\delta r_{ch}^2$ $(48, 52) = 0.530(5)$ fm$^2$ [7].

We have performed a detailed study of the charge radii in K, Ca, and Sc isotopes which is exemplified by the results for a long isotopic chain of potassium isotopes. The neutron-deficient and neutron-rich nuclei with pairing in both neutron and proton sectors, as well as the (semi-) magic nuclei around the classical closed neutron shells at $N = 20, 28$ and new magic (sub)shell $N = 32$ are treated within the Energy Density Functional (EDF) approach with the Fayans functional DF3-a used in our studies of the Ca and Cu isotopes [11, 12].

An impact of the different forms of paring correlations (volume, surface, surface plus gradient) on the charge radii is analyzed. A comparison with the new options of the Fayans functional, namely Fy(stand) and more recent Fy($\Delta r$, HFB) [13] is done. The performance of the DF3-a is analysed in describing both absolute radii and OES effects found in the previous [4, 6] and more recent CERN-ISOLDE experiments $^{36-52}$K [9] isotopes.

## THEORY BACKGROUND

The charge radii are treated within the self-consistent theory of finite Fermi systems (TFFS) in terms of the energy density functional theory (EDF). This approach makes use of the new versions of the EDF proposed by Fayans and coauthors in [13–17]. The resulting effective nucleon–nucleon ($NN$) forces are

independent of energy, but the dependence of the density functional on the nuclear density $\rho$ is more complex than that in the Skyrme functionals. The surface and pairing components in the FaNDF0 and DF3a EDF versions depend both on the nuclear-density and its gradient [14], which takes effectively into account the coupling to phonon excitations. This allowed us to explain for the first time the OES effect in Ca isotopes including the well-known "inverse parabolic" shape in the isotopic dependence of radii between $^{40}$Ca and $^{48}$Ca, as well as anomalous grows of radii at $N > 28$ [11].

A fine tuning of the DF3a functional was performed by employing the systematics composed by H. Grawe and coauthors in [18] on the basis of 105 experimental single-particle energies (including several evaluated ones) and 65 values of spin−orbit splitting (data on the "new" doubly magic nuclei of $^{78}$Ni and $^{100,132}$Sn being incorporated in this systematics). The resulting Fayans functional DF3-a [16] made it possible to describe $\_r^2\_{\text{ch}}\_$ for a number of isotopic chains with a precision of 0.01 to 0.02 fm [17], which is superior to the precision provided by modern versions of the Skyrme functional [19, 20].

The mean-square charge radius of a nucleus is determined in terms of the charge density $\rho_{\text{ch}}(\mathbf{r})$. Precision measurements of cross sections for elastic electron scattering at electron energies of $E_e \approx 500$ MeV enable a model-independent method for extracting charge densities of nuclei.

The radial moments of the charge density distribution $\rho_{\text{ch}}(\mathbf{r})$ are of importance for comparison with the CRIS-CERN measurements using the collinear laser spectroscopy method:

$$R_n = \left(\langle r^n \rangle\right)^{1/n}$$
$$= \left(\int r^n \rho_{\text{ch}}(r) d^3 r \Big/ \int \rho_{\text{ch}}(r) d^3 r\right)^{1/n}. \quad (1)$$

The most used are the mean-square charge radii:

$$\langle r_{\text{ch}}^2 \rangle = Z^{-1} \int r^2 \rho_{\text{ch}}(\mathbf{r}) d^3 r. \quad (2)$$

The isotopic differences of the mean-square (differential mean-square, or dms) radii $\delta\langle r_{\text{ch}}^2(A, A')\rangle$ are directly related to the observable isotopic shifts of the hyperfine structure centroids of atomic level energies.

The calculated mean-square charge radius of a nucleus includes the standard relativistic, spin−orbit and center of mass corrections [21, 22]. The distribution of the nucleon charge could be taken into account in terms of the form factors describing the effects of a spatial extension of the nucleons and their electromagnetic structure [23]. Finally, it has the form:

$$\langle r_{\text{ch}}^2 \rangle = \langle r_p^2 \rangle + \langle \delta r_{\text{ch}}^2 \rangle_p + N/Z\langle \delta r_{\text{ch}}^2 \rangle_n + \langle r_{s-o}^2 \rangle + \langle r_{\text{cm}}^2 \rangle. \quad (3)$$

Here $\langle r_p^2 \rangle$ is the mean-square radius for protons that corresponds to the point-like density $\rho\tau(\mathbf{r}) = \sum jls\, n_{\tau\lambda}\varphi_{\tau\lambda}(\mathbf{r})$, where, $\varphi_{\tau\lambda}$ stands for the single-particle nucleon wave functions in a spherical self-consistent
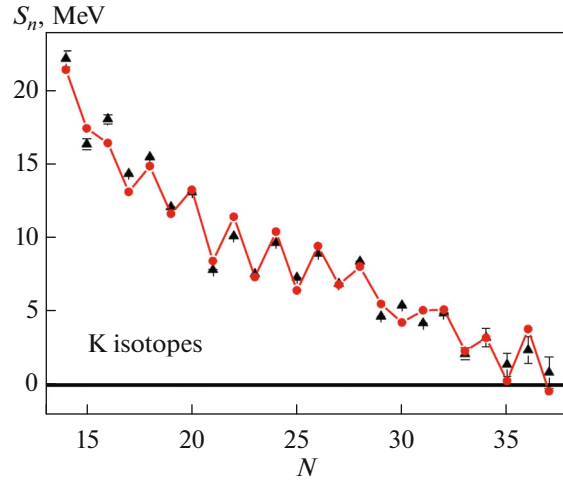


**Fig. 1.** The DF3a calculated $S_{1n}$ values for the K isotopic chain vs. the AME-2016 data [24] (full triangles—experiment).

single-particle potential, where $\lambda = j$, $l = j \pm 1/2$, and $s$ form a standard set of quantum numbers and $\tau = p$, $n$, while $n_{\tau\lambda}$ are nucleon-orbital occupation numbers found in the self-consistent pairing field. More details can be found in our paper [12].

## RESULTS AND DISCUSSION

First, the neutron-separation energies are of importance, as the pairing-functional parameters of the DF3a were determined from optimal description of $S_{1n}$ and $S_{2n}$ experimental data in a wide region of nuclei. The one-neutron separation energies in potassium isotopes are shown in Fig. 1. The deviation from the experimental data on $S_n$ [24] is at a level of 1 MeV for all potassium isotopes in question, with the exception of $^{24,25,49}$K, where the deviations are up to 900 keV, respectively.

The results of our calculation of the root-mean-square radii $R_{\text{ch}}$ are displayed in Fig. 2 for potassium isotopes in comparison with available data [4, 6, 9]. Though the OES effect in the calculation is significant for $N < 28$, it is within large systematic errors. They are due to the $R_{\text{ch}}$ extraction from the measured isotopic shifts and related mostly to the choice of the so-called specific mass shift $K_{\text{SMS}}$. It is true for both neutron-deficient isotopes up to $N = Z = 19$ and for isotopes approaching to the neutron closed shell $N = 28$. In the region above the $N = 28$, the calculations show an underestimate of the data which is a universal feature in Ca region [10]. It has been also found in our calculations for Ti−Fe chains made with the functionals DF3-a, FANDF0, UNEDEF in [11].

In Fig. 3, our calculation is given in a form of differential mean-square radii $\delta r^2$ ($N = 28$, $A = 47$; $A'$). The reason is that in these quantities, the above mentioned systematical errors are effectively cancelled in the region of $N = 28$. The calculated $\delta r^2$ ($N = 28$, $A = 47$; $A'$) reveal a good description of the OES effect found in the experiments [5]. Notice, that the analo-
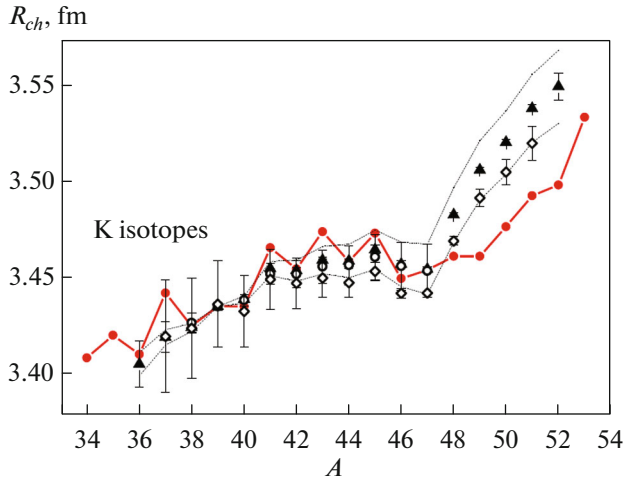
**Fig. 2.** Absolute root- mean-square charge radii $R_{ch}$ calculated from the DF3-a density functional (red circles) for potassium isotopes along with the experimental ones: open circles [4], open triangles [5], full triangles [9] versus the mass number. The dashed lines correspond to the systematic errors derived in [9].



**Fig. 3.** Differential mean square charge radii $\delta r^2$ ($N = 28$; $N'$) of the potassium isotopes relative to the reference $N = 28$, $A = 47$ isotope. Calculations from the DF3a functional with different radial dependence of paring interaction: volume ($1$—in blue), surface ($2$—in green) and surface-gradient one ($3$—in red). The comparison with the $\delta r^2$ ($N = 28; N'$)-values measured in [9] is given. The full triangles correspond to the statistical errors, dashed lines to the systematic errors derived in [9].

gous calculations with the modified Fayans functional Fy(HFB, $\Delta$) [13] have shown much stronger OES effect at $N < 28$ (see Fig. 3 in [9]).

In the potassium isotopes with an odd proton located above the fully occupied $\pi 1p1/2$ shell, the filling of the $\nu 2p3/2$ neutron shell may cause the of the ground-state spin inversion due to strong monopole neutron–proton interaction between the $\pi 2s1/2$ and $\nu 2p3/2$ orbits. The measurements of magnetic moments and ground state spins in K isotopes [5] revealed the ground-state spin inversion $3/2+ \rightarrow 1/2+$ for the mass number s of $A = 47–49$.

It could be expected that such spin-inversion followed by re-inversion may have an impact on the properties of ground and excited states of nuclei. Interestingly, in this region, the experimental charge radii show the trend (within the large systematical errors) towards some weakening of EOS oscillations. In our calculations the ground-state spin for $A = 47$ agrees with the experimental value $J^\pi = 1/2^-$. The resulting charge radii from the calculation where the ground-state spin for $A = 49$ was fixed as $2\pi s1/2$ differ slightly from the results of the calculation with the spin of $\pi 1d3/2$ corresponding to the minimum of the total energy in our calculation. At the same time, the calculations performed earlier within the DF3-a + CQRPA formalism extended in order to allow for spin inversion show that, for K isotopes agreement with experimental beta-decay lifetimes and with the experimental delayed neutron emission rates ($Pxn$) [25] is better in the case of fixing the odd proton in the $\pi 2s1/2$ quasiparticle state than in the $\pi dp3/2$ state.

In Fig. 3, depicted are the differential mean square charge radii differential radii $\delta r^2$ ($N = 28$, $A = 47$; $A'$) of the potassium isotopes relative the reference $N = 28$, $A = 47$ isotope calculated with different radial
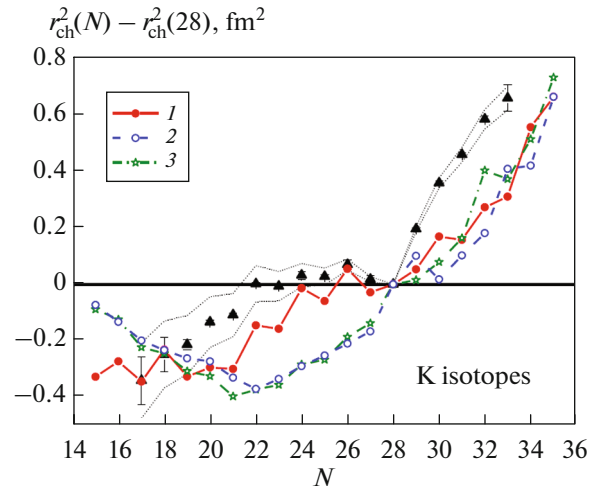
dependence of paring interaction: pure volume, pure surface and "mixed" surface-gradient one. From a comparison with the experimental data [6] it can be concluded that the odd-even staggering seen in the experimental radii can be explained only assuming the complicated gradient form of the EDF paring part.

An underestimate of the charge radii at $N > 28$ has an universal origin stemming from non-regular contribution due to the quasiparticle-phonon coupling. This effect is treated in our framework not *ad hoc* but selfconsistently. It has been found to successfully explain anomalous increase of the experimental charge radii at $N > 28$ in Ca isotopes [10].

## CONCLUSIONS

The fully self-consistent calculations of the charge radii within the framework of the modified Fayans Density Functional (DF3a) have been performed in Ca region (for K to Sc isotopes). The results are exemplified by the detailed study for the long chain of the potassium isotopes including the neutron shell closures at $N = 20$, 28, 32,34. The present calculations reveal a good description of the OES effect compared to the one found in experimental isotopic dependence of the differential charge radii $\delta r^2$ ($N = 28$, $A = 47$; $N'$) [6].

The staggering of the experimental radii in our framework can be explained only assuming the complicated surface + gradient form of the paring part of the EDF suggested in [14]. In addition to a large-scale parametric fitting of the modified Fayans EDF suggested in [13], a new physics related to the density gra-

dient terms of higher power in its surface and pairing parts may be of importance.

An underestimate of the charge radii in K isotopes at $N > 28$, it is mostly related to A-dependent contribution of the quasiparticle-phonon coupling. This effect treated self-consistently has been found previously to successfully explain the charge radii at $N > 28$ in Ca isotopes [10]. More detailed calculations with allowance for deformations on the basis of the DF3 + HFBTHO approach [26] are required for drawing more reliable conclusions. Since pairing is weakened in the vicinity of $N = 28$, an interplay of deformation effects with contribution of the quasiparticle–phonon interaction may be essential in the region of $N > 28$.

## CONFLICT OF INTEREST

## OPEN ACCESS

## REFERENCES

1. T. E. Cocolios, H. Al Suradi, J. Billowes, et al., Nucl. Instrum. Methods Phys. Res., Sect. B **317**, 565 (2013).

2. D. Steppenbeck, S. Takeuchi, N. Aoi, et al., "Evidence for a new nuclear 'magic number' from the level structure of $^{54}$Ca," Nature **502**, 207−210 (2013).

3. F. Wienholtz, D. Beck, K. Blaum, et al., "Masses of exotic calcium isotopes pin down nuclear force," Nature **498**, 346−349 (2013).

4. I. Angeli and K. P. Marinova, "Table of experimental nuclear ground state charge radii: An update. January, 2013," At. Data Nucl. Data Tables **99**, 69−95 (2013).

5. J. Papuga, M. L. Bessel, K. Kreim, et al., "Spins and magnetic moments of $^{49}$K and $^{51}$K: Establishing the $1/2^+$ and $3/2^+$ level ordering beyond $N = 28$," Phys. Rev. Lett. **110**, 172503-5 (2013).

6. K. Kreim, M. L. Bissell, J. Papuga, et al., "Nuclear charge radii of potassium isotopes beyond $N = 28$," Phys. Lett. B **731**, 97−102 (2014).

7. R. F. Garcia Ruiz, M. L. Bissell, K. Blaum, et al., Nat. Phys. **12**, 594 (2016).

8. A. J. Miller, K. Minamitsono, A. Klose, et al., "Proton superfluidity and charge radii in proton-rich calcium isotopes," Nat. Phys. **15**, 432 (2019).

9. A. Koszorus, X. F. Yang, W. G. Jiang, et al., "Charge radii of exotic potassium isotopes challenge nuclear theory and the magic character of $N = 32$," Nat. Phys. **17**, 439−443 (2021).

10. E. E. Saperstein, I. N. Borzov, and S. V. Tolokonnikov, "On the anomalous $A$ dependence of the charge radii of heavy calcium isotopes," JETP Lett. **104**, 218−223 (2016).

11. K. Minamitsono, D. M. Rossi, R. Beerwerth, et al., "Charge radii of neutron-deficient $^{52,53}$Fe produced by projectile fragmentation," Phys. Rev. Lett. **117**, 252501 (2017).

12. I. N. Borzov and S. V. Tolokonnikov, "Self-consistent calculation of the charge radii in the $^{58-82}$Cu isotopic chain," Phys. At. Nucl. **83**, 795−807 (2020).

13. S. A. Fayans, "Towards a universal nuclear density functional," JETP Lett. **68**, 169 (1998).

14. P. G. Reinhard and W. Nazarewicz, "Toward a global description of nuclear charge radii: Exploring the Fayans energy density functional," Phys. Rev. C **95**, 064328 (2017).

15. I. N. Borzov, S. A. Fayans, A. Krömer, and D. Zawischa, "Ground state properties and β-decay half-lives near $^{132}$Sn in a self-consistent theory," Z. Phys. A **355**, 117 (1996).

16. E. E. Saperstein and S. V. Tolokonnikov, "Self-consistent theory of finite Fermi systems and radii of nuclei," Phys. At. Nucl. **74**, 1277 (2011).

17. E. E. Saperstein and S. V. Tolokonnikov, "Self-consistent theory of finite Fermi systems and Skyrme−Hartree−Fock method," Phys. At. Nucl. **79**, 1030−1066 (2016).

18. H. Grawe, K.-H. Langanke, and G. Martínez-Pinedo, "Nuclear structure and astrophysics," Rep. Prog. Phys. **70**, 1525 (2007).

19. E. Chabanat, P. Bonche, P. Haensel, J. Meyer, and F. Schaeffer, "A Skyrme parametrization from subnuclear to neutron star densities. 2. Nuclei far from stabilities," Nucl. Phys. A **635**, 231 (1998).

20. S. Goriely, N. Chamel, and J. M. Pearson, "Skyrme−Hartree−Fock−Bogoliubov nuclear mass formulas: Crossing the 0.6 MeV threshold with microscopically deduced pairing," Phys. Rev. Lett. **102**, 152503 (2009).

21. W. Bertozzi, J. Frair, J. Heisenberg, and J. W. Negele, "Contributions of neutrons to elastic electron scattering from nuclei," Phys. Lett. B **41**, 408 (1972).

22. H. Chandra and G. Sauer, "Relativistic corrections to the elastic electron scattering from $^{208}$Pb," Phys. Rev. **13**, 245 (1976).

23. J. L. Friar, J. Martorell, and D. W. L. Sprung, "Nuclear sizes and the isotope shift," Phys. Rev. A **56**, 4579 (1997).

24. Meng Wang, G. Audi, F. G. Kondev, W. J. Huang, S. Naimi, and Xing Xu, "The AME2016 atomic mass evaluation," Chinese Phys. C **41** 030003 (2017).

25. I. N. Borzov, "Delayed multineutron emission in the region of heavy calcium isotopes," Phys. At. Nucl. **81**, 680−694 (2018).

26. S. V. Tolokonnikov, I. N. Borzov, V. Kortelainen, Yu. S. Lutostansky, and E. E. Saperstein, "First applications of Fayans functional to deformed nuclei," J. Phys. G **42**, 075102 (2015).