ЯДЕРНАЯ ФИЗИКА, 2020, том 83, № 6, с. 1–13

SELF-CONSISTENT CALCULATION OF THE CHARGE RADII IN THE ISOTOPIC CHAIN $^{58-82}$Cu

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The charge radii in a long isotopic chain of copper, including exotic nuclei ^{58}Cu, ^{79}Cu close to doubly-magic ^{56}Ni, ^{78}Ni and nuclei near magic sub-shells $N = 32, 34, 40$ are calculated. The self-consistent theory of finite Fermi systems and the family of density energy functionals proposed by Fayans et al. (DF3, DF3-a) are used. A comparison is made with experiment and similar calculations in self-consistent models using new versions of the Fayans functional with parameters obtained using the extended optimization protocol: Fy (std) and Fy (HFB, ∇r), as well as with calculations in the renormalization group method and with density dependent spin-orbit interaction. The weakening of the even-odd "staggering" in isotopes approaching the semi-magic nucleus of ^{79}Cu found in ISOLDE-CERN experiments is analyzed. The correlation of the isotopic dependences of charge radii and total beta decay energies is shown.

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Isotopic dependence of nuclear radii reflect mesoscopic features of atomic nucleus:

Bulk isotopic dependence – liquid drop model:

$$R_{L.D.} \sim r_0 A^{1/3}$$

where the Wigner–Seitz radius is related to the nuclear saturation density

$$r_0 = [3/4\pi\rho_0]^{1/3}$$

Observed isotopic dependence:

Negative isotopic shifts c.f. L-D model

Specific quantum fluctuations:

Nuclei with odd neutron number are smaller.

Universal odd-even staggering (OES).

Local min/max at the closed shells (kinks);

For Energy Density Functional theory :

- ***Inclusion of charge radii (or charge densities) increases the quality of optimization protocol for EDF.***

- ***A study of odd-odd and odd-A (Z=29) Cu isotopes approaching N=50 may refine the features of the proton-neutron interaction. Namely, a self-consistent coupling between the proton density and neutron pairing field.***

- ***A study of OES gives us an estimate of accuracy of Equal Filling Approximation (EFA) often used for restoring the time-reversal invariance broken in the odd systems.***

Most of the nuclear EDFs used in self-consistent mean-field calculations have been derived from phenomenological effective interactions. A recent proposal: the Skyrme functional combined with the surface and pairing parts from the Fayans functional.

$$\mathcal{E} = \mathcal{E}^{\rm v}(\rho,\tau) + \mathcal{E}^{\rm s}(\rho) + \mathcal{E}^{\rm ls}(\rho,\vec{J}) + \mathcal{E}^{\rm Coul}(\rho) + \mathcal{E}^{\rm pair}(\rho) + \mathcal{E}^{\rm c.m.}(\rho) \quad .$$

	Skyrme	Fayans
volume:	$\mathcal{E}^{\rm v}_{\rm Sk} = \sum_{t=0}^{1}\left[(C^{\rho\rho}_{t0} + C^{\rho\rho}_{t{\rm D}}\rho_0^{\alpha})\rho_t^2 + C^{\rho\tau}_t\rho_t\tau_t\right]$	$\mathcal{E}^{\rm v}_{\rm Fy} = \frac{1}{3}\varepsilon_F\rho_{\rm sat}\left[a^{\rm v}_+\frac{1-h^{\rm v}_{1+}x_0^{\sigma}}{1+h^{\rm v}_{2+}x_0^{\sigma}}x_0^2 + a^{\rm v}_-\frac{1-h^{\rm v}_{1-}x_0}{1+h^{\rm v}_{2-}x_0}x_1^2\right]$
	$C^{\rho\rho}_{t0}, C^{\rho\rho}_{t{\rm D}}, \alpha, C^{\rho\tau}_t \leftrightarrow E/A_{\rm eq}, \rho_{\rm eq}, K, J, L, \frac{m^*}{m}, \kappa_{\rm TRK}$	$a^{\rm v}_{\pm}, h^{\rm v}_{1\pm}, h^{\rm v}_{2\pm} \leftrightarrow E/A_{\rm eq}, \rho_{\rm eq}, K, J, L, h^{\rm v}_{2-}$
surface :	$\mathcal{E}^{\rm s}_{\rm Sk} = \sum_{t=0}^{1} C^{\rho\Delta\rho}_t\rho_t\Delta\rho_t$	$\mathcal{E}^{\rm s}_{\rm Fy} = \frac{1}{3}\varepsilon_F\rho_{\rm sat}\frac{a^{\rm s}_+ r_s^2(\vec{\nabla}x_0)^2}{1+h^{\rm s}_+x_0^{\sigma}+h^{\rm s}_{\nabla}r_s^2(\vec{\nabla}x_0)^2}$
spin-orbit:	$\mathcal{E}^{\rm ls}_{\rm Sk} = \sum_{t=0}^{1} C^{\rho\nabla J}_t\rho_t\boldsymbol{\nabla}\cdot\boldsymbol{J}_t$	$\mathcal{E}^{\rm ls}_{\rm Fy} = \sum_{t=0}^{1} C^{\rho\nabla J}_t\rho_t\boldsymbol{\nabla}\cdot\boldsymbol{J}_t$
pairing:	$\mathcal{E}^{\rm pair}_{\rm Sk} = \frac{1}{4}\sum_{q\in\{p,n\}} V_{{\rm pair},q}\left(1-\frac{\rho_0}{\rho_{\rm pair}}\right)\breve{\rho}_q^2$	$\mathcal{E}^{\rm pair}_{\rm Fy} = \frac{2\varepsilon_F}{3\rho_{\rm sat}}\breve{\rho}_q^2\left[f^{\xi}_{\rm ex} + h^{\xi}_+x^{\gamma}_{\rm pair} + h^{\xi}_{\nabla}r_s^2(\vec{\nabla}x_{\rm pair})^2\right]$

where $x_t = \rho_t/\rho_{\rm sat}$ and $x_{\rm pair} = \breve{\rho}_q/\rho_{\rm sat}$. The γ, $\rho_{\rm sat} = 0.16$ fm^{-3} and $\varepsilon_F = \varepsilon_F(\rho_{\rm sat})$ are given, fixed values. The non-linear surface coefficient is fixed as $h^s_+ = h^v_{2+}$. Coulomb term and c.m. correction are irrelevant here. Note that the parameters for the volume terms are handled in term of nuclear matter parameters $E/A_{\rm eq}$ etc as is indicted in the line below the volume terms.

V.A Khodel, E.E Saperstein Phys.Repts. 92 (1982) , A.B Migdal FFST. 2nd ed. 1983, S.A Fayans JETP Letters 104 (1998)

Pairing EDF - depends on ρ ... and grad(ρ).

$$\varepsilon_{\rm pair}(\mathbf{r}) = \frac{1}{2}\sum_{\tau=n,p} \mathcal{F}^{\xi,\tau}(\rho_+(\mathbf{r}))|\nu_\tau(\mathbf{r})|^2.$$

$$f^{\xi}(x_+(\mathbf{r})) = f^{\xi}_{\rm ex} + h^{\xi}(x_+)^q(\mathbf{r}) + f^{\xi}_{\nabla} r_0^2 \left(\nabla x_+(\mathbf{r})\right)^2 .$$

$x_+ = (\rho_p+\rho_n)/ 2\,\rho_0$, we use futher on : f^S ↑

A recent proposal:

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

A hybrid EDF → *normal part of the Skyrme functional*
+ the surface and pairing parts from the Fayans functional:

Fy (stand) and Fy (Δr) – without and with the gradient pairing.

DF1 *S. A.Fayans, S. V.Tolokonnikov et al. Sov. J. Nucl.Phys. 84, 995* ***(1988)***

DF3 *I.N. Borzov, S.A. Fayans, E. Kromer, D. Zawischa., Z.Phys. A335, 117 (1996).*

S. Fayans, S. Tolokonnikov, E. Trykov, and D. Zawischa,Nucl. Phys. A676, 49 (2000)

****** > 30 years later ******

A "workflow" of collinear laser spectroscopy measurements of radii from CERN analyzed with "recently developed Fayans functional

Fy (Δr; HFB) which is a hybrid one: the Skyrme + paring part from Fayans EDF

- *R. F. Garcia Ruiz ..... P.-G. Reinhard and W. Nazarewicz.... et al., Nature Physics 12, 594 (2016). Unexpectedly large charge radii of neutron-rich calcium isotopes*
- *P.-G. Reinhard and W. Nazarewicz, Phys.* ***Rev. C 95, 064328 (2017).***

  Toward a global description of nuclear charge radii:

  Exploring the Fayans energy density functional
- *K. Minamisono, ... W. Nazarewicz, .., P.-G. Reinhard, E. E. Saperstein, S. V. Tolokonnikov, et.al.* ***Phys. Rev. Lett.117, 252501 (2016).*** *Laser Spectroscopy of Neutron-Rich Fe Isotopes....*

- *A. J. Miller, et.al,PHYS. REV. LETTERS 122, 192502 (2019)*

  Laser Spectroscopy of Neutron-Rich Tin Isotopes....

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W.Nazarewicz et.al , Nature Physics volume 15, 432 (2019).

Laser Spectroscopy of Neutron-Rich Cu Isotopes....

R.P de Groote et al., Nature Physics volume 16*, 620 (2020)*

Mean-squared radius ***(MS)***

$$\langle r_{ch}^2 \rangle = 1/Z \int r^2 \ \rho_{ch}(r) d^3r$$

Differential mean-squared radii ***(DMS)***

$$\delta \langle r_{ch}^2 (A, A') \rangle$$

Related to the observables – isotopic shifts of hyperfine structure in atomic spectra

Root mean-squared radius ***(RMS)***

$$Rch = \sqrt{\langle r_{ch}^2 \rangle}$$

Higher radial moments $\langle r^n \rangle^{1/n}$ ***(RM)***

$$R_n = (< r^n >)^{1/n} = \left(\frac{\int r^n \rho_{ch}(\mathrm{r}) d^3r}{\int \rho_{ch}(\mathrm{r}) d^3r} \right)^{1/n} .$$

See P-G. Reinhardt, W. Nazarewicz, RF. Garcia-Ruiz ArXiv 1911.00699 (2019)

Effective charge density

HFB-like point density

$$\rho_\tau(\mathbf{r}) = \sum_{jls} n_\lambda^\tau \phi_\lambda^\tau(\mathbf{r}).$$

Finite-range effects
and nucleon EM-structure

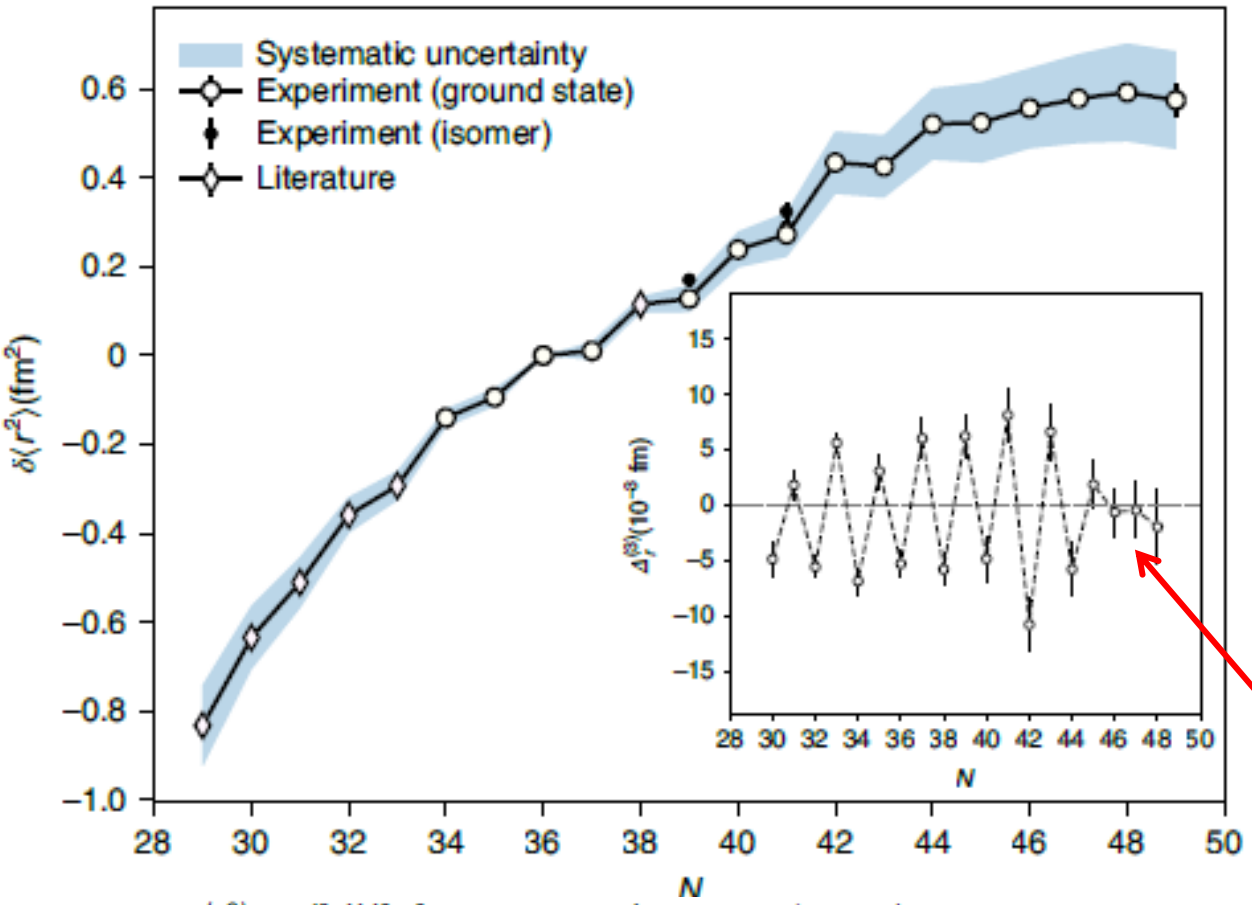
$$\rho_{\rm ch}(\mathbf{r}) = \sum_\tau \int \rho_\tau(\mathbf{r}-\mathbf{r}') F_{E\tau}(\mathbf{r}') d^3r',$$

$$\langle r_p^2 \rangle = 0.7080(32) \ \ \text{фм}^2 \qquad \langle r_n^2 \rangle = -0.117(4) \ \text{фм}^2$$

Relativistic effects
c.m. and s-o corrections

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

*Isotopic dependence of the differential MS radii in Cu. R.de Groote, et al. Nat. Phys. **16,** 620–624 (2020).*



of $\delta\langle r^2\rangle$ for $^{63-66,68-78}$Cu (relative to ^{65}Cu) from this work as a function of neutron number *N*, alongside the literature values for $^{58-62,67}$Cu (ref. [9]). The inset shows the OES of the radii defined by equation (1). Error bars are statistical (one standard deviation). In the main plot, these errors are too small to be seen except for ^{78}Cu. The blue shaded area represents the systematic uncertainty due to the atomic parameters.

Statistical errors are small.

Large systematic errors due to atomic "field" and "shift" parameters .

OES in terms of

$\Delta r^{(3)} = 1/2\,(r_{A+1} - 2\,r_A + r_{A-1})$

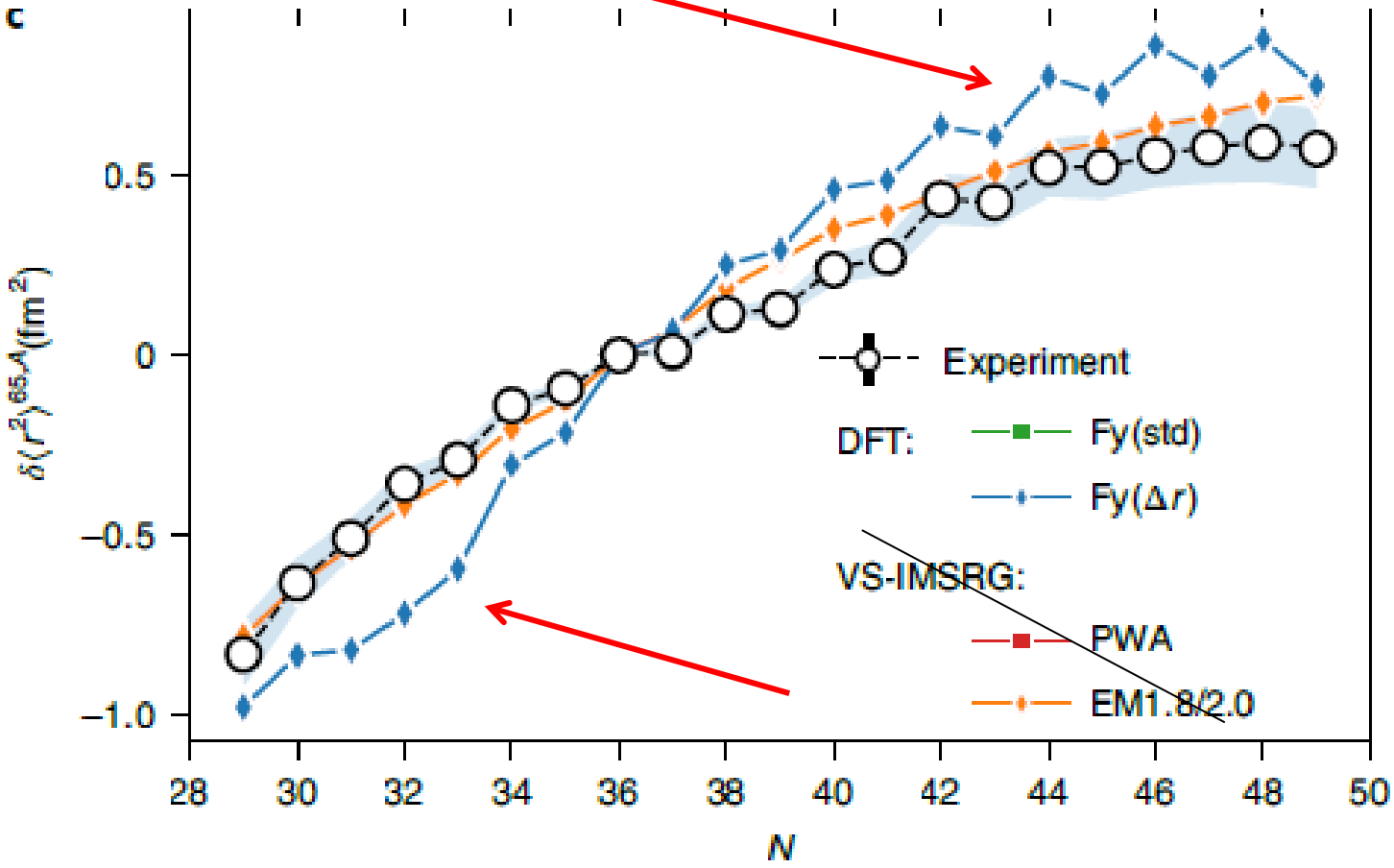
$r \rightarrow rms = \sqrt{\langle r^2\rangle_{Charge}}$

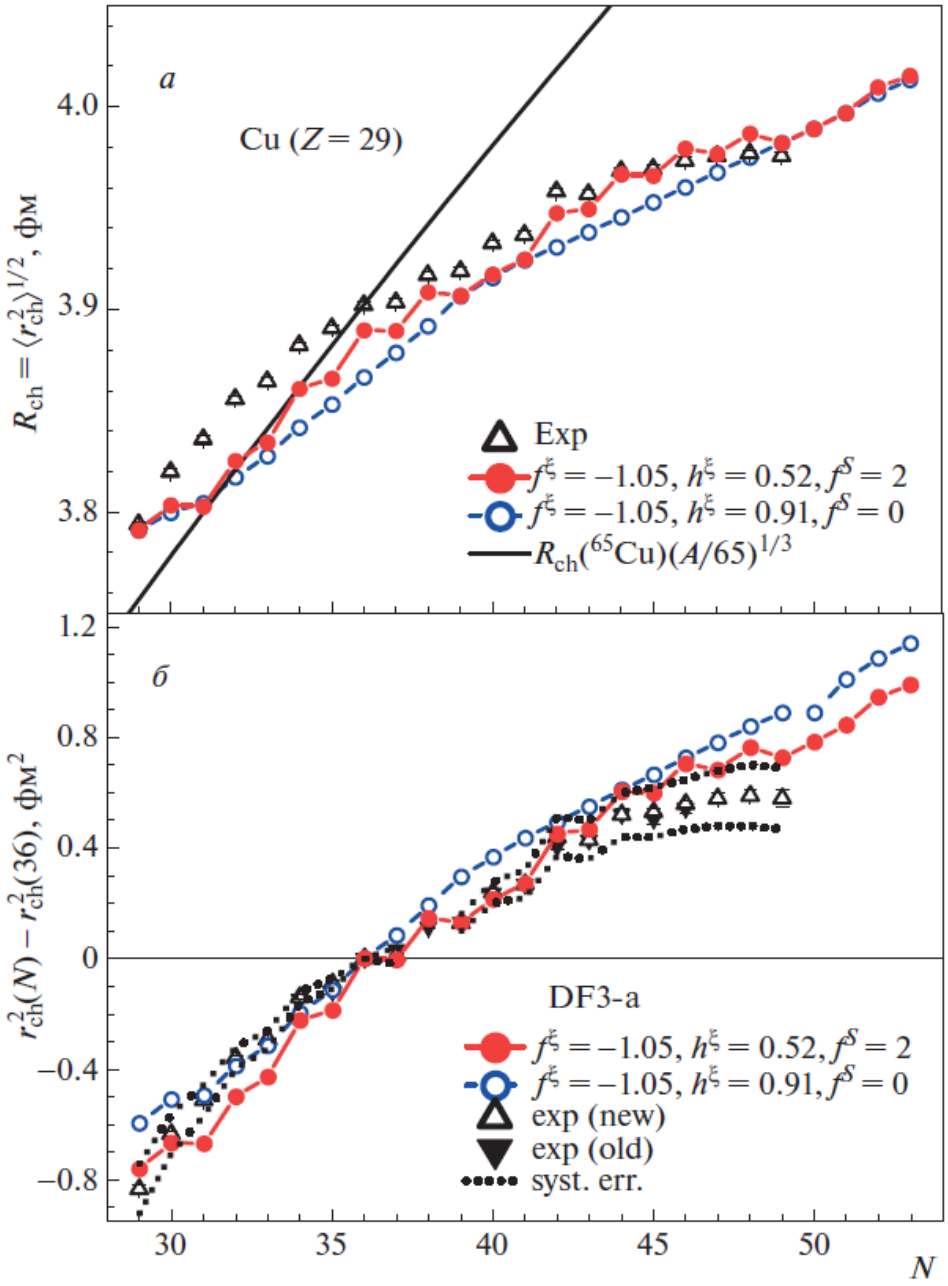
OES quenching at N →50

Notice !
Fy(HFB) calculation is far out of uncertainty margins

DMS δ<r2> (65, A) Fy (std), Fy(Δr)

R.P de Groote et al., *Nature Physics* ***volume 16****, 620 (2020)*



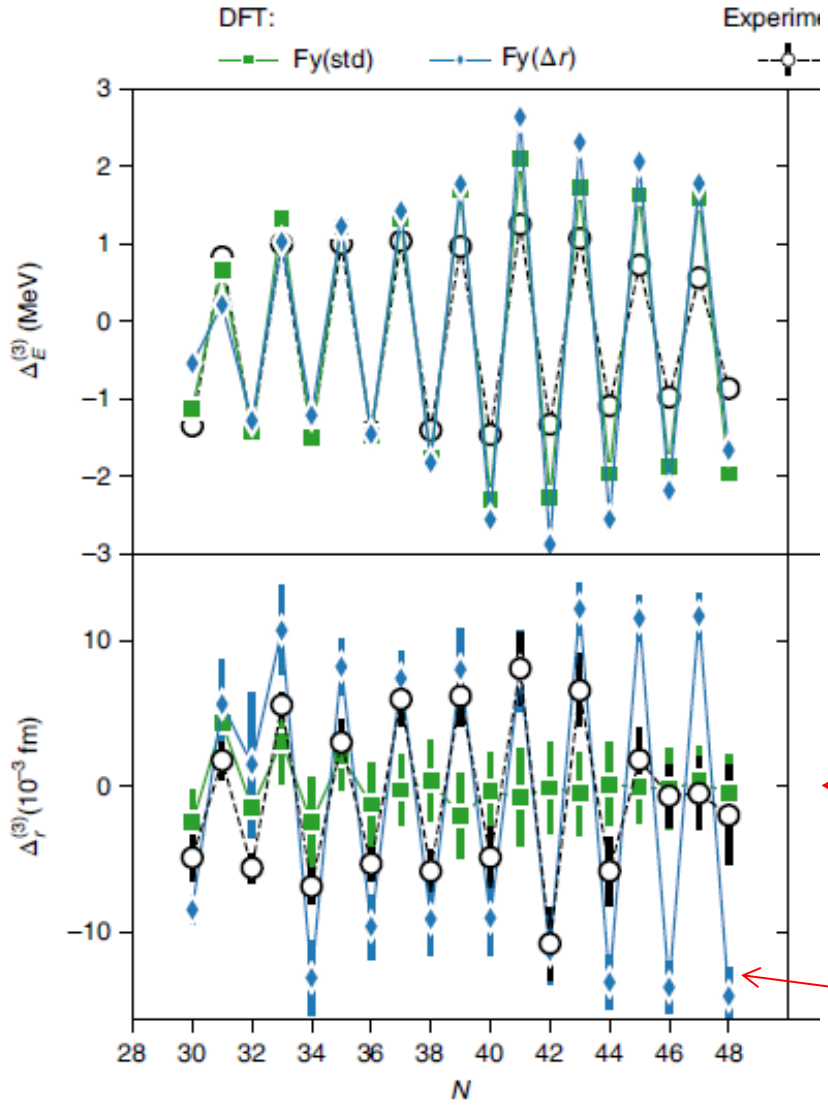


Df3a calculation is closer to uncertainty margins

Df3a calculation predicts a flat (with no OES) idependence of Rch… at N>50

As in Fy-case Df3a calculation shows no OES if $f^{s}=0$ (no gradient pairing)

R.de Groote, et al.
Nat. Phys. **16,** 620–624 (2020).



OES in E_B
is qualitatively reproduced
(both with and without gradient pairing)

$$\Delta_r^{(3)} = \frac{1}{2}\left(r_{A+1} - 2r_A + r_{A-1}\right)$$

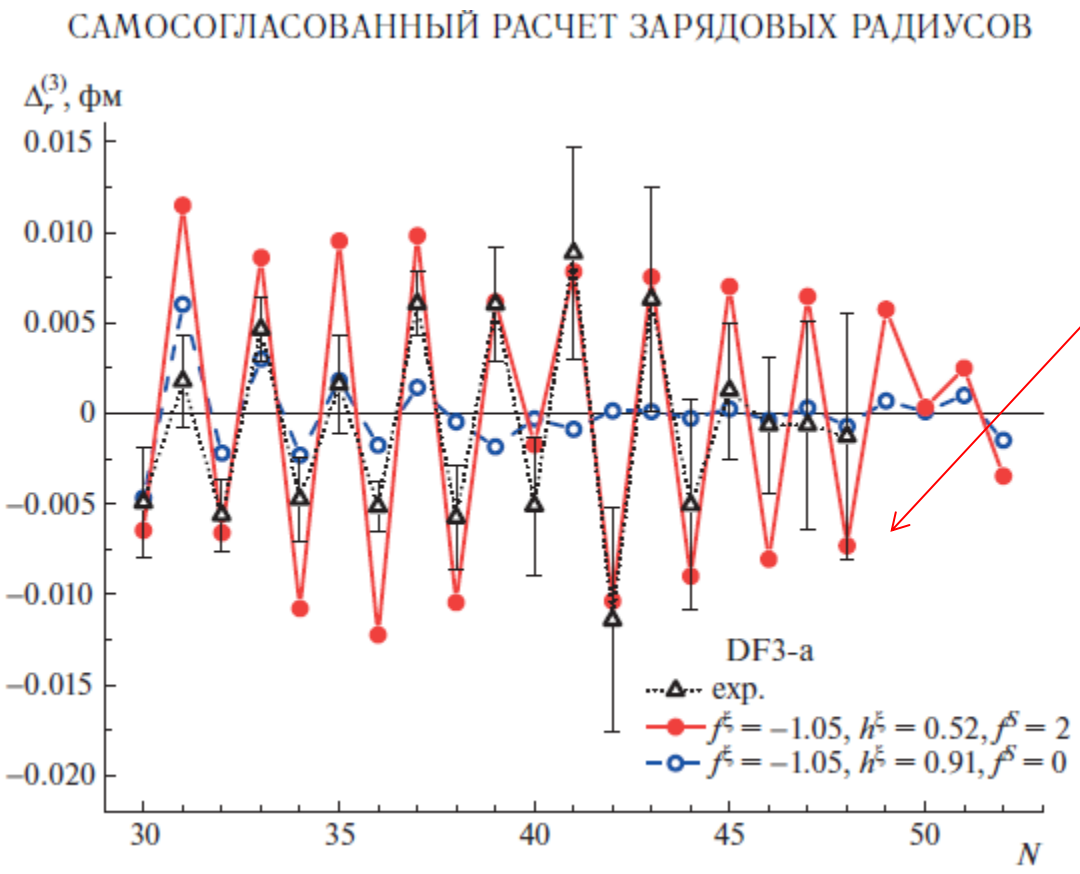
green squares
Fy(std) – no gradient pairing;
OES is absent .

blue
Fy(Δr) – with gradient pairing;
OES is too strong.
No quenching of $\Delta^{(3)}(r)$ at all !

Here the strength of the gradient pairing was assumed to be the same, as in Ca chain

DF3a calculation.

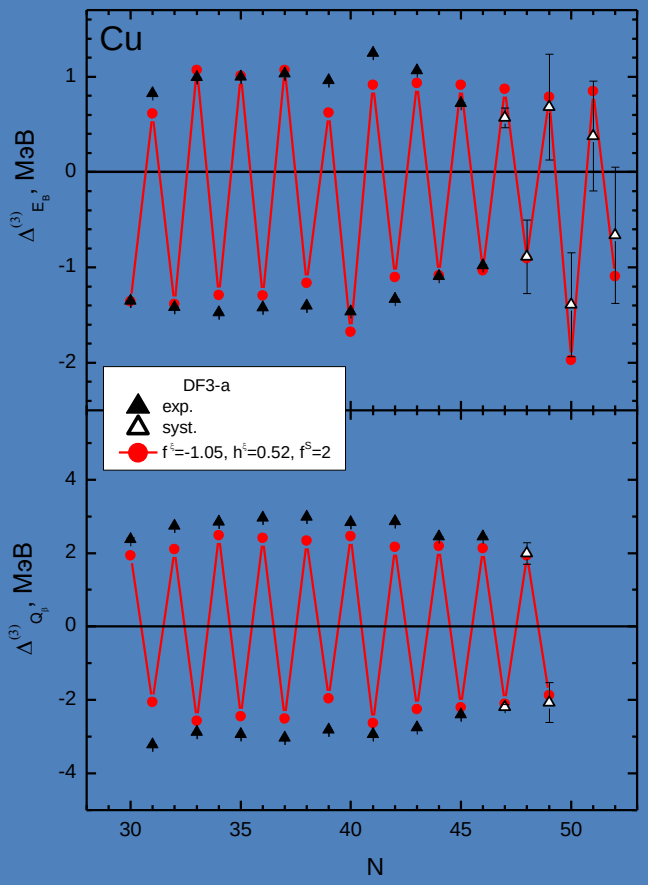
$$\Delta(3,R) = R_{A+1} - 2R_A + R_{A-1}$$



Notice !
The DF3 calculation is closer to the exp. margins than the Fy(HFB)

Weakend (by 17%) gradient pairing
$f^S \sim 1.65$
describes exp.data
on smoothing of $\Delta^{(3)}(r)$

Total binding E_B and beta decay energies Q_β with DF3a



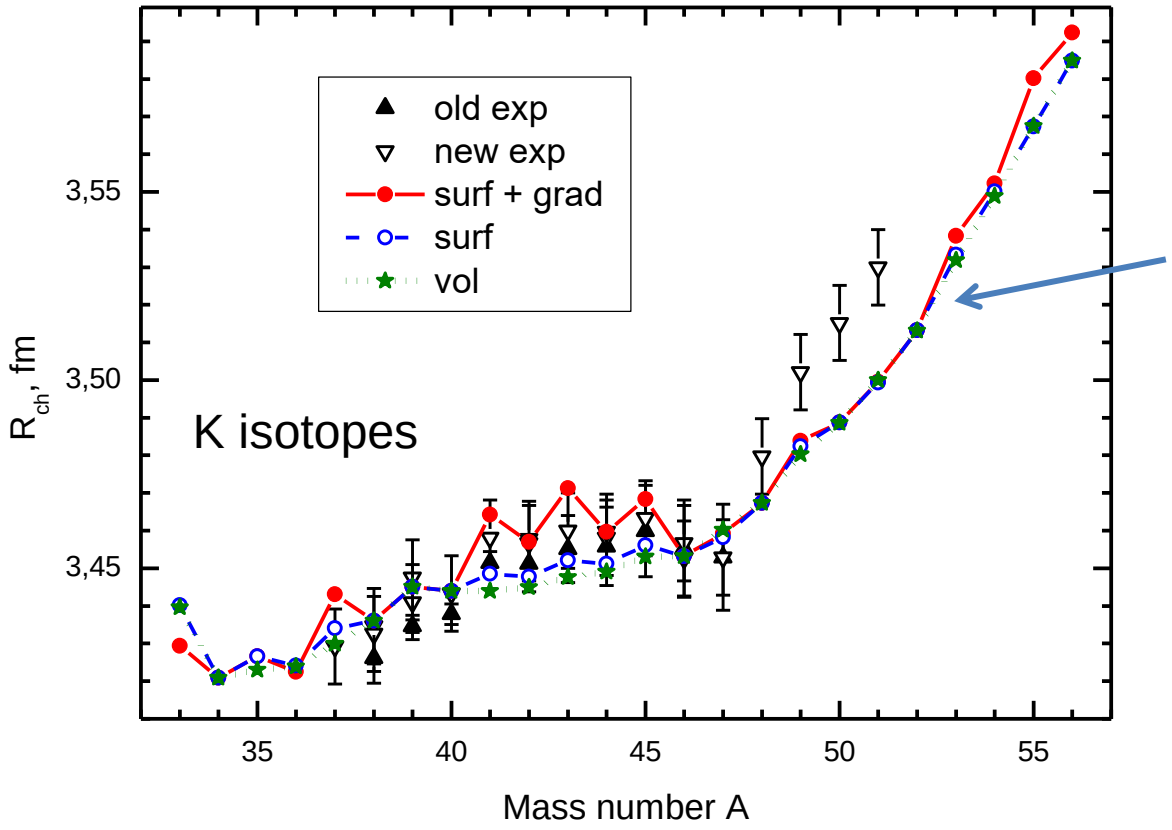
Quenching of the OES for E_B and Q-beta-values is well reproduced

Strong quenching of OES in the Q-beta-values occurs at at N>Nmag .

It has been discussed for Z~50, N~82 in:
I.N.Borzov, J.Cuenca-Garcia, K. Langanke,G. Martinez-Pinedo,F. Montes. Beta-decay of Z<50 nuclei near N=82 closed neutron shell. Nucl.Phys.A814,159, 2008.

Open questions …

Different forms of pairing. Phonon's contribution.



With no phonons

Fy

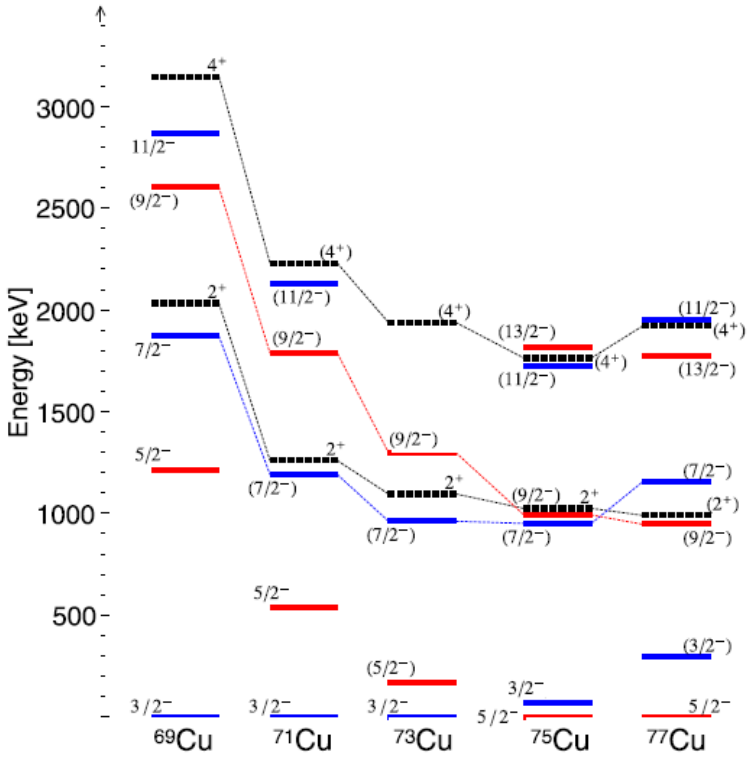
"In principle, through its density dependence, ***the functional alone should be able to reproduce g.s. properties****. Adding correlations "ad-hoc" can lead to uncontrolled cancellations".*

Phonons in our scheme were added in a self-consistent way:
JETP Letters 102 (2017)

Spin-inversion in Cu chain at A>75

PHYSICAL REVIEW C **102**, 034314 (2020)

F. L. BELLO GARROTE *et al.*

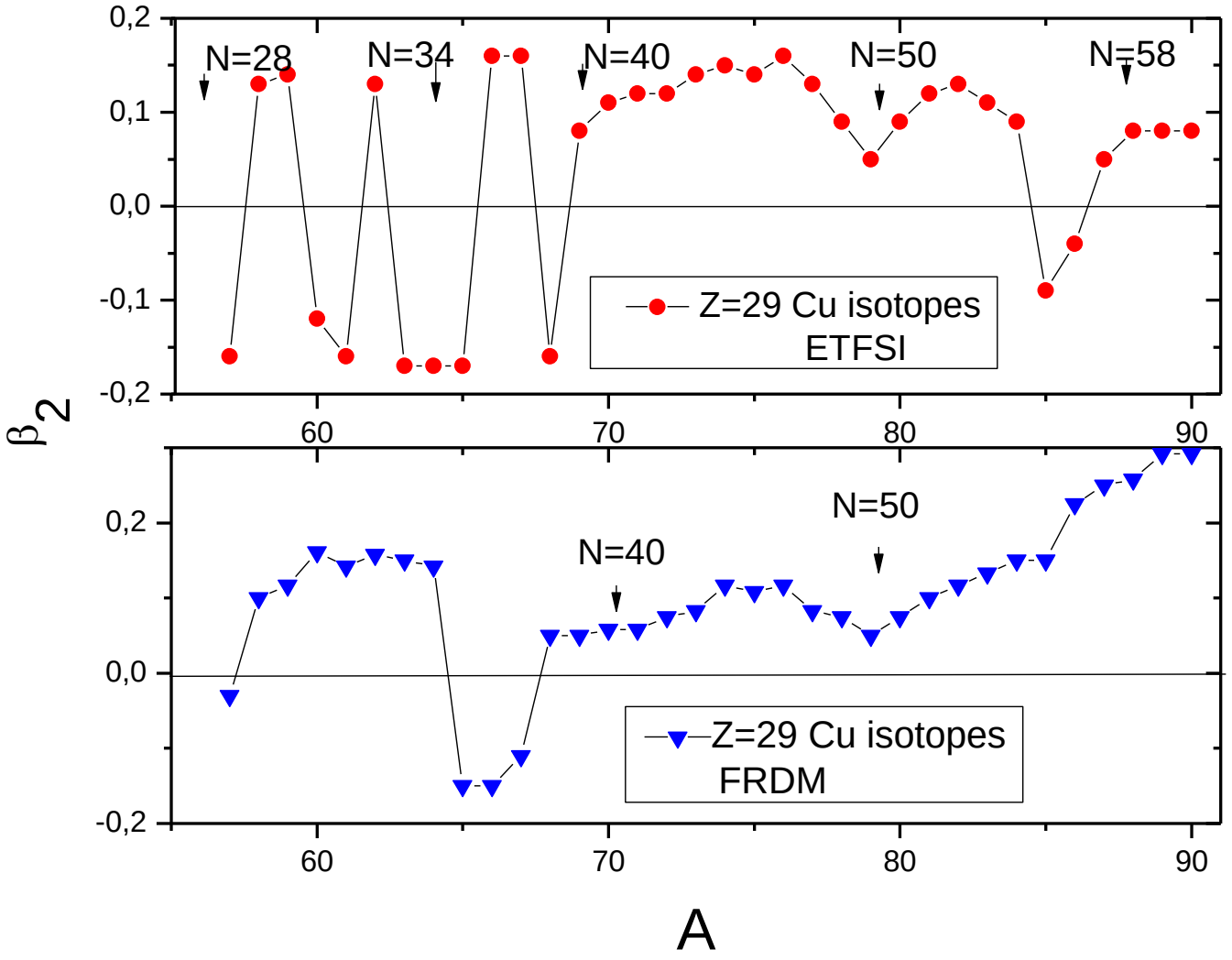


The OES of the radii is quite pronounced near N = 40, but our new data points reveal a reduction of the OES towards N = 50, starting at 74Cu. This is likely to be attributed to the change in the ground-state proton configuration.
Indeed, as reflected in the ground-state spins and moments13,14, up to 73Cu, the odd proton resides predominantly in the πp3⁄2 orbital,
while from 74Cu onwards it occupies the πf5⁄2 shell.

An impact of spin-inversion on radii have not been confirmed in the present (spherical) calculations.

We are studying a deformed scheme.

Deformation



Conclusions

Comparison with the "hybrid" calculations

(Fy = Skyrme+ Fayans pairing part) :

- *DF3a functional even with **strong gradient pairing kept the same as in Fe to Sn** gives a better description of OES in Cu radii both in neutron-deficient region and near N=50 shell. (Some evidence for a weaker pairing.)*

- *A very good description of saturation density and OES in E_B and Q_β.*

- *Flat A-dependence of Rch occurs at N>50*

***

Deformed calculations in Yb+ iso-chain "with an eye" to Rch non-linearity problem. Hypotetical "e-n interaction" beyond the SM or contribution of the HRM → $\langle r^n \rangle^{1/n}$?...

Acknowlegments

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V.G. Nesterenko, N.V. Antonenko for discussions

Ni isotopes : matter and charge radii

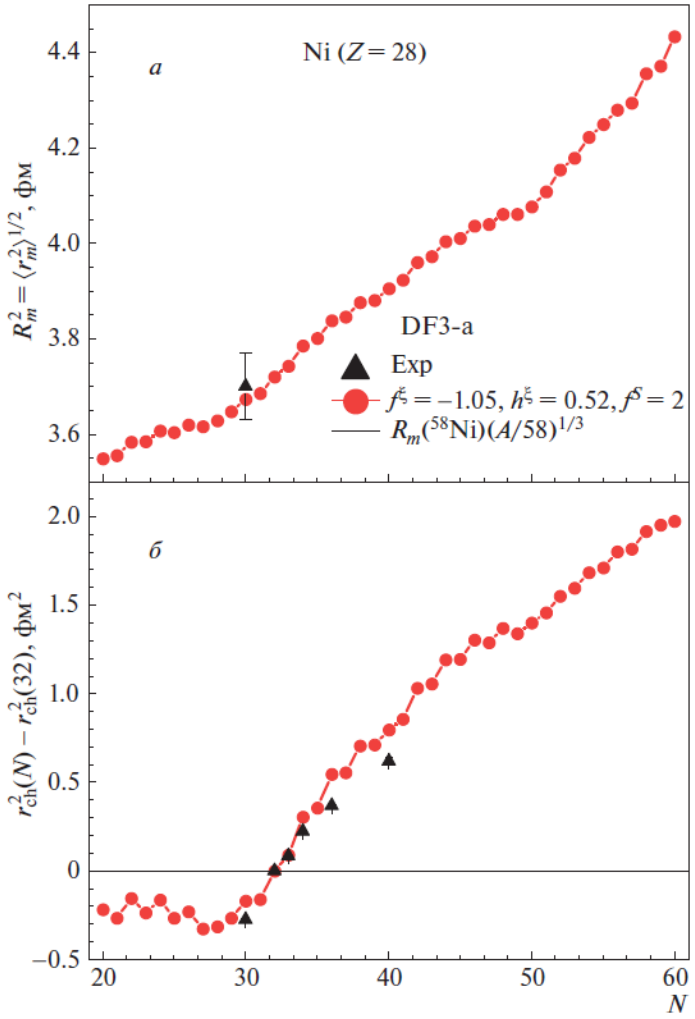
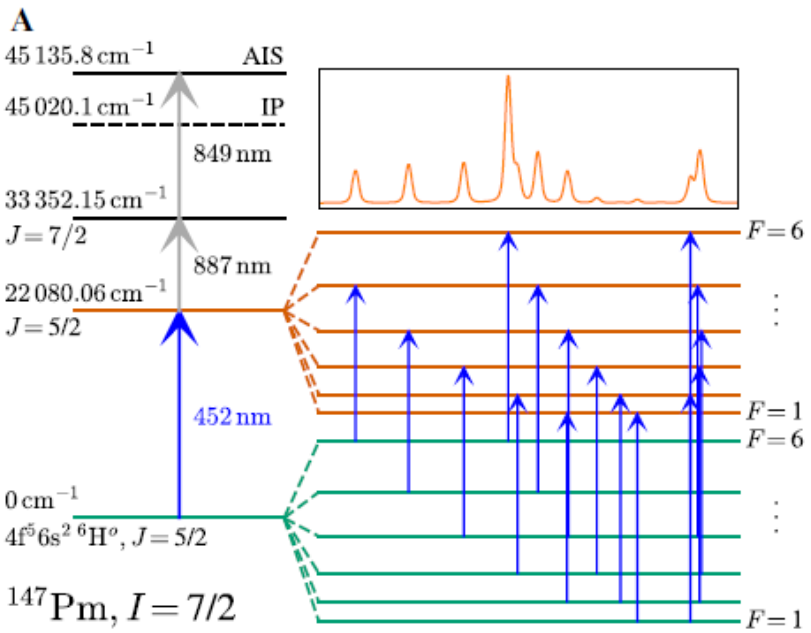


Рис. 5. *а* — Рассчитанные с DF3-a и экспериментальные [41] среднеквадратичные радиусы распределения материи для изотопов Ni в зависимости от числа нейтронов; *б* — рассчитанные с DF3-a и экспериментальные [41] дифференциальные (относительно $N = 32$) средние квадраты зарядовых радиусов для изотопов Ni в зависимости от числа нейтронов.

Prometium hyperfine structure



Eur. Phys. J. A (2020) 56:69

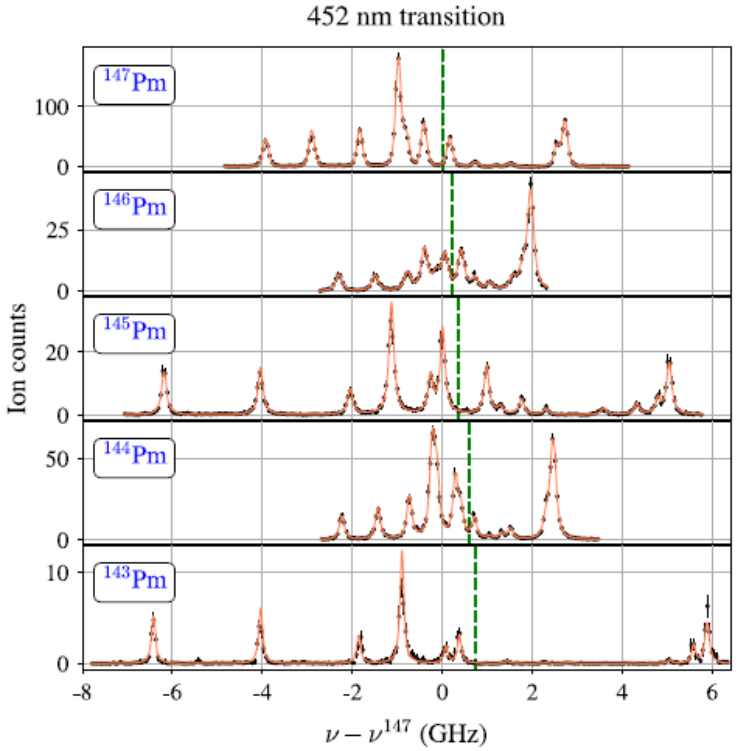


Fig. 5 Measured hyperfine spectra in the ground state transitions of scheme (**A**) at 452 nm (left) and of scheme (**B**) at 468 nm (right). The centroid frequency of the ^{147}Pm hyperfine structure is taken as refer-

Isotopic shift and radii

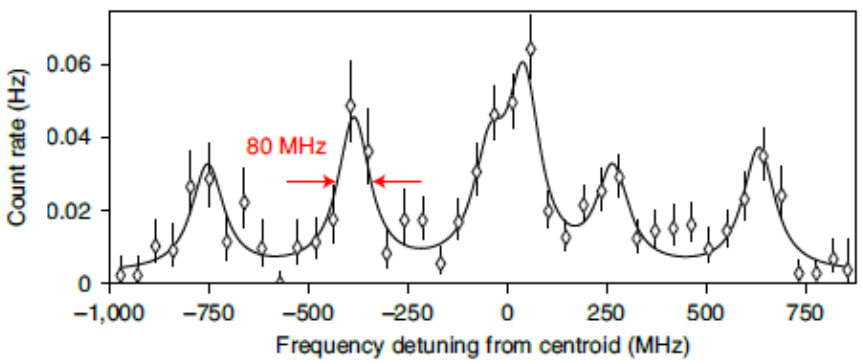


Fig. 1 | Overview of the experimental results. Top: ion rate obtained during the laser scan of ^{78}Cu as a function of resonant laser frequency relative to the hyperfine structure centroid. Error bars show the statistical uncertainty (one standard deviation). The solid line shows the best-fitting set of Voigt profiles centred at the resonance locations (see Methods). Bottom: values of $\delta\langle r^2\rangle$ for $^{63-66,68-78}$Cu (relative to ^{65}Cu) from this work as a function of neutron number N, alongside the literature values for $^{58-62,67}$Cu (ref. [9]).

$$\delta\nu^{65,A'} = M\frac{m_{A'} - m_{65}}{m_{65}m_{A'}} + F\delta\langle r^2\rangle^{65,A'}$$

Table 1 | Summary of the isotope shifts obtained in this work

A	I	IS (MHz)	$\delta\langle r^2\rangle^{65,A'}$ (fm²)	$\delta\langle r^2\rangle^{65,A'}_{\mathrm{lit}}$ (fm²)
63	3/2	+1,055.4(2.6)	−0.140(7)[20]	−0.148(1)[17]
64	1	+508(5)	−0.09(1)[2]	−0.118(3)[13]
65	3/2	0	0(0)[0]	0(0)[0]
66	1	−529(5)	+0.01(1)[2]	+0.033(5)[12]
67	3/2	–	–	+0.115(5)[18]
68	1	−1,498(5)	+0.13(1)[3]	+0.132(5)[31]
68	6	−1,479(4)	+0.17(1)[3]	+0.191(4)[31]
69	3/2	−1,937(5)	+0.24(1)[4]	+0.237(3)[34]
70	6	−2,375(7)	+0.27(2)[5]	+0.270(3)[44]
70	3	−2,390(7)	+0.29(2)[5]	+0.287(11)[44]
70	1	−2,397(6)	+0.32(2)[5]	+0.323(11)[44]
71	3/2	−2,787(4)	+0.44(2)[7]	+0.407(11)[44]
72	2	−3,240(7)	+0.43(2)[7]	+0.429(5)[55]
73	3/2	−3,634(5)	+0.52(2)[8]	+0.523(15)[58]
74	2	−4,057(5)	+0.53(1)[9]	+0.505(18)[72]
75	5/2	−4,455(4)	+0.56(1)[9]	+0.546(21)[80]
76	3	−4,848(5)	+0.58(2)[10]	–
77	5/2	−5,234(5)	+0.59(2)[11]	–
78	(6)	−5,623(10)	+0.58(3)[11]	–

The second column displays the nuclear spin I of the isotopes. For ^{78}Cu, no firm spin assignment has been made, which is why the value is listed in brackets. The isotope shifts (IS) obtained in this work are compared to the available literature[9]. Statistical and systematic atomic uncertainties are enclosed within parentheses and square brackets, respectively.