Extracting information on nuclear charge distributions from isotope shift studies

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"The interplay between atomic and nuclear physics to study exotic nuclei"
ECT Workshop - Trento

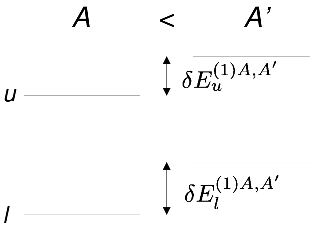
In collaboration with

- Per Jönsson, Malmö University
- Michel Godefroid and Cedric Nazé, Université Libre de Bruxelles
- Gediminas Gaigalas, Vilnius University
- B.G. Carlsson and Asimina Papoulia, Lund University

Outline

- Isotope shifts
- Reformulated field shift and implementation in GRASP2K
- Applications
  - Refined extraction of $\delta\langle r^2\rangle$ values
  - Higher order corrections from realistic charge distrbutions
  - Simultaneous extraction of $\delta\langle r^2\rangle$ and $\delta\langle r^4\rangle$ values
- Conclusions and Outlook

Isotope shifts



$$\delta\nu_{k,\mathrm{IS}}^{A,A'} = \delta E_u^{A,A'} - \delta E_l^{A,A'}$$

$$= \underbrace{\Delta K_{k,\mathrm{MS}} \frac{M' - M}{MM'}}_{\text{Mass Shift}} + \underbrace{\sum_N F_{k,N} \delta \langle r^{2N} \rangle^{A,A'}}_{\text{Field Shift}}$$

Isotope shifts

$$\sum_N F_{k,N}\delta\langle r^{2N}\rangle^{A,A'} = \delta\nu_{k,\mathrm{IS}}^{A,A'} - \Delta K_{k,\mathrm{MS}}\frac{M'-M}{MM'} = \delta\nu_{k,\mathrm{FS}}^{A,A'}$$

The possibility to extract accurate $\delta\langle r^{2N}\rangle^{A,A'}$ ultimately depends on how well we measure experimental $\delta\nu_{k,\mathrm{IS}}^{A,A'}$ and calculate $F_{k,N}, \Delta K_{k,\mathrm{MS}}$.

Reformulated field shift and implementation in GRASP2K

J. Ekman, P. Jönsson, M. Godefroid, C. Nazé and G. Gaigalas,
to be submitted to CPC

Reformulated field shift

The first order level field shift is given by

$$\delta E_{i,\mathrm{FS}}^{(1)A,A'} = -\int_{\mathbf{R}^3} \left[V_N^A(\mathbf{r}) - V_N^{A'}(\mathbf{r}) \right] \rho_i^e(\mathbf{r}) d^3\mathbf{r},$$

where

- $V_A(\mathbf{r})$ and $V_{A'}(\mathbf{r})$ are the electronic potentials due to (different) charge distributions in the two isotopes A and A'.
- $\rho_i^e(\mathbf{r})$ is the electron density distribution within the nuclear volume

Reformulated field shift

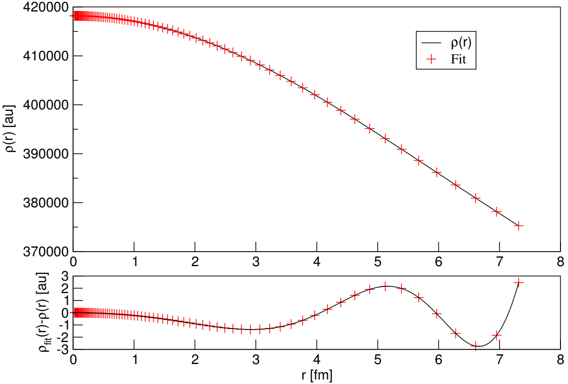
Assuming a homogenous charge distribution (hard sphere) it can be shown that the electron density distribution for level i inside the nuclear volume to a very good approximation can be expanded as [1]:

$$\rho_i^e(\mathbf{r}) \approx b_{i,0} + b_{i,2} r^2 + b_{i,4} r^4 + b_{i,6} r^6.$$

[1] Blundell *et al.*, Journal of Physics B **20**, 3663 (1987)

In fact, the polynomial expansion also holds for more realistic Fermi-type charge distributions:

Reformulated field shift



Electron density for the $1s^2 2s\ \ ^2S$ level in Li-like ^{142}Nd
($\approx$ 7 % fall-off within nuclear volume)

Reformulated field shift

Using the polynomial expansion $\rho_i^e(\mathbf{r}) \approx b_{i,0} + b_{i,2}r^2 + b_{i,4}r^4 + b_{i,6}r^6$ and following the work by Seltzer and Blundell *et al.* the first order frequency field shift can then be written

$$\delta\nu_{k,\mathrm{FS}}^{(1)A,A'} = F_{k,0}\delta\langle r^2\rangle^{A,A'} + F_{k,2}\delta\langle r^4\rangle^{A,A'} + F_{k,4}\delta\langle r^6\rangle^{A,A'} + F_{k,6}\delta\langle r^8\rangle^{A,A'}$$

where

$$F_{k,n} = \frac{4\pi}{(n+2)(n+3)} Z \frac{\Delta b_n}{h}, \quad \Delta b_n = b_{u,n} - b_{l,n}.$$

Seltzer, Phys. Rev. **188**, 1916 (1969)
Blundell *et al.*, Journal of Physics B **20**, 3663 (1987)

GRASP2K implementation

Routines for the derivation of the electronic factors F_N are implemented in GRASP2K through the program RIS4.

Level J Parity Field shift electronic factors and average point discrepancy in fit

Level	J Parity	F0 (GHz/fm^2)	F2 (GHz/fm^4)	F4 (GHz/fm^6)	F6 (GHz/fm^8)	Disc. (per mille)
1	1/2 -	0.1155473544D+06	-0.9457001725D+02	0.3054728900D+00	-0.6051012375D-03	0.0020
1	3/2 -	0.1152739390D+06	-0.9435715260D+02	0.3047762374D+00	-0.6037193610D-03	0.0020

J. Ekman, P. Jönsson, M. Godefroid, C. Nazé and G. Gaigalas,
to be submitted to CPC

Example: Level field shifts in meV Li-like ^{150,142}Nd

Decomposition of the level field shifts of the $^2S_{1/2}$ and $^2P_{1/2,3/2}$ states in Li-like ^{150,142}Nd from a $n = 5$ + Breit calculations.

	$1s^2 2s\ ^2S_{1/2}$	$1s^2 2p\ ^2P_{1/2}$	$1s^2 2p\ ^2P_{3/2}$
$\mathcal{F}_0 \delta \langle r^2 \rangle^{150,142}$	656.78	614.67	613.23
$\mathcal{F}_2 \delta \langle r^4 \rangle^{150,142}$	−33.10	−30.96	−30.89
$\mathcal{F}_4 \delta \langle r^6 \rangle^{150,142}$	5.89	5.50	5.49
$\mathcal{F}_6 \delta \langle r^8 \rangle^{150,142}$	−0.66	−0.62	−0.62
$\delta E_{\mathrm{FS}}^{(1)150,142}$	628.91	588.60	587.21

Example: Frequency field shifts in meV in Li-like ^{150,142}Nd

Decomposition of the frequency field shifts in meV of the $^2P_{1/2} - ^2S_{1/2}$ and $^2P_{3/2} - ^2S_{1/2}$ transitions in Li-like ^{150,142}Nd from a resulting $n = 5$ + Breit calculation.

	$^2P_{1/2} - ^2S_{1/2}$	$^2P_{3/2} - ^2S_{1/2}$
$F_0\delta\langle r^2\rangle^{150,142}$	-42.11	-43.55
$F_2\delta\langle r^4\rangle^{150,142}$	2.13	2.20
$F_4\delta\langle r^6\rangle^{150,142}$	-0.38	-0.39
$F_6\delta\langle r^8\rangle^{150,142}$	0.04	0.04
$\delta\nu_{\mathrm{FS}}^{(1)150,142}$	-40.31	-41.70

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Comparison of different approaches of frequency field shifts calculations of the $^2P_{1/2} - ^2S_{1/2}$ transition in Li-like ^{150,142}Nd as a function of active orbital set.

	Variational	Reformulated	1st. ord. pert.
DF	-40.44	-40.39	-40.39
$n = 2$	-40.43	-40.55	
$n = 3$	-40.44	-40.51	
$n = 4$	-40.45	-40.53	
$n = 5$	-40.45	-40.53	
$n = 5$ + Breit	-40.30	-40.31	

Effect from deformation in Li-like ^{150,142}Nd

From a n=5 + Breit calculation. Values in meV.

	$\delta\langle r^2\rangle$ [fm^2]	$\delta\langle r^4\rangle$ [fm^4]	$\delta\langle r^6\rangle$ [fm^6]	$\delta\langle r^8\rangle$ [fm^8]
^{150}Nd (sph.)	1.29094	79.4628	4 375.68	248 818
^{150}Nd ($\beta_{20} = 0.28$)	1.29094	94.5064	6 016.55	386 461

	$^2P_{1/2} - ^2S_{1/2}$ (sph.)	$^2P_{1/2} - ^2S_{1/2}$ ($\beta_{20} = 0.28$)	Difference
$F_0\delta\langle r^2\rangle^{150,142}$	-42.11	-42.11	0.00
$F_2\delta\langle r^4\rangle^{150,142}$	2.13	2.54	0.40
$F_4\delta\langle r^6\rangle^{150,142}$	-0.38	-0.52	-0.14
$F_6\delta\langle r^8\rangle^{150,142}$	0.04	0.07	0.02
$\delta\nu_{\mathrm{FS}}^{(1)150,142}$	-40.31	-40.02	0.29

Effect from deformation: +0.29 meV, in good agreement with

Kozhedub et al., Phys. Rev. A. **77**, 032501 (2008)

Zubova et al., Phys. Rev. A. **90**, 062512 (2014)

Applications: Refined extraction of $\delta\langle r^2 \rangle$ values

Refined extraction of $\delta\langle r^2\rangle$ values

Rearranging, the reformulated field shift

$$\delta\nu_{k,\mathrm{FS}}^{(1)A,A'} = F_{k,0}\delta\langle r^2\rangle^{A,A'} + F_{k,2}\delta\langle r^4\rangle^{A,A'} + F_{k,4}\delta\langle r^6\rangle^{A,A'} + F_{k,6}\delta\langle r^8\rangle^{A,A'}$$

can be written as

$$\delta\nu_{k,\mathrm{FS}}^{(1)A,A'} = F_{k,0}\lambda_k^{A,A'}$$

where the so-called nuclear parameter $\lambda_k^{A,A'}$ is given by

$$\lambda_k^{A,A'} = \delta\langle r^2\rangle^{A,A'} + \frac{F_{k,2}}{F_{k,0}}\delta\langle r^4\rangle^{A,A'} + \frac{F_{k,4}}{F_{k,0}}\delta\langle r^6\rangle^{A,A'} + \frac{F_{k,6}}{F_{k,0}}\delta\langle r^8\rangle^{A,A'}$$

Refined extraction of $\delta\langle r^2\rangle$ values

In the following $\delta\langle r^2\rangle$ values are extracted from the nuclear parameter

$$\lambda_k^{A,A'} = \delta\langle r^2\rangle^{A,A'} + \frac{F_{k,2}}{F_{k,0}}\delta\langle r^4\rangle^{A,A'} + \frac{F_{k,4}}{F_{k,0}}\delta\langle r^6\rangle^{A,A'} + \frac{F_{k,6}}{F_{k,0}}\delta\langle r^8\rangle^{A,A'}$$

for the ${}^2P_{1/2} - {}^2S_{1/2}$ transition in Li-like systemts using different Fermi charge distribution parameters for the two isotopes A and A'

$$\rho(r,\theta) = \frac{1}{1+\exp(\frac{r-c(\theta)}{a})}, \qquad c(\theta) = c_0\left[1+\beta_{20}Y_{20}(\theta)\right]$$

The skin diffusiness is often characterised by the parameter $t = 4\ln(3)a$.

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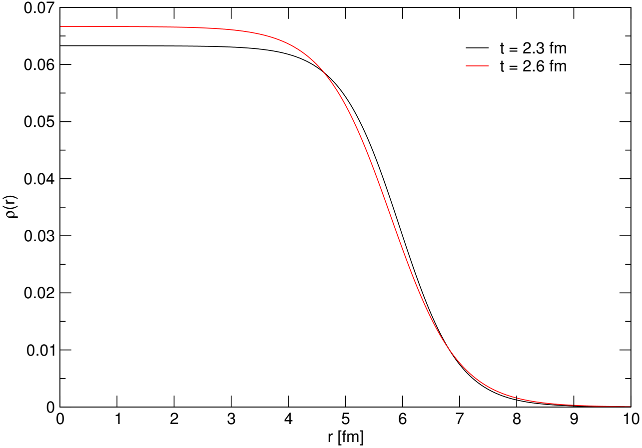
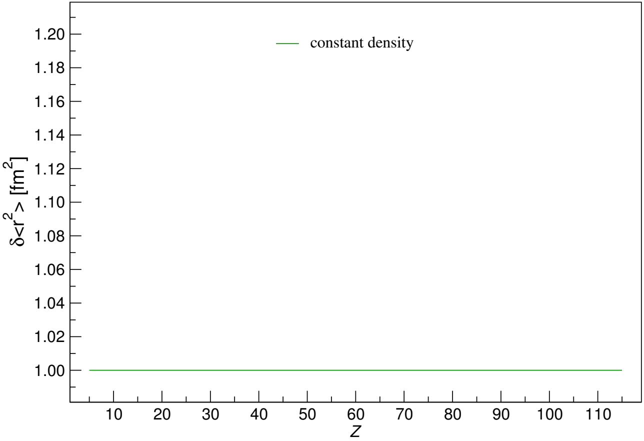
Refined extraction of $\delta\langle r^2\rangle$ values



Fermi model charge distributions with $\langle r^2\rangle^{1/2} = 5.0$ fm and different skin diffusiness parameters t.

Refined extraction of $\delta\langle r^2\rangle$ values

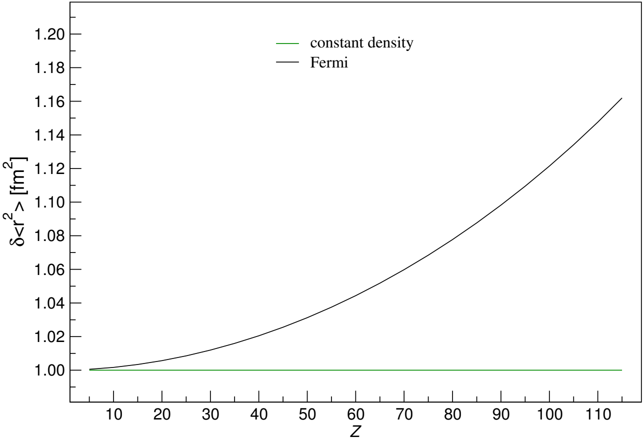
Constant density approximation: $\delta\langle r^2\rangle = \lambda$



$$\lambda_k^{A,A'} = 1.00 \text{ fm}^2 \text{ and } \langle r^2\rangle^A > \langle r^2\rangle^{A'}$$

Refined extraction of $\delta\langle r^2\rangle$ values

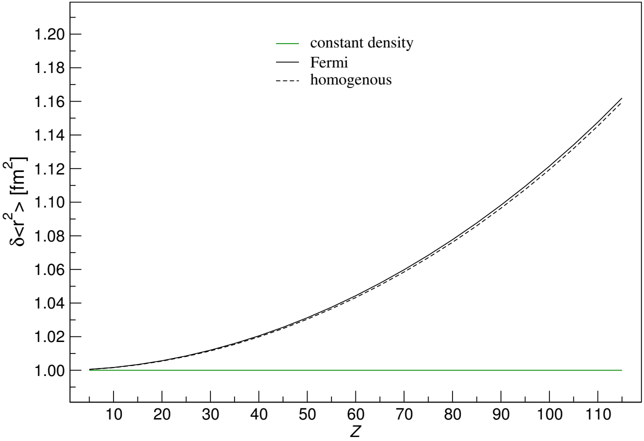
Spherical Fermi distributions with $t = 2.3$ fm for both isotopes



$$\lambda_k^{A,A'} = 1.00 \text{ fm}^2 \text{ and } \langle r^2\rangle^A > \langle r^2\rangle^{A'}$$

Refined extraction of $\delta\langle r^2\rangle$ values

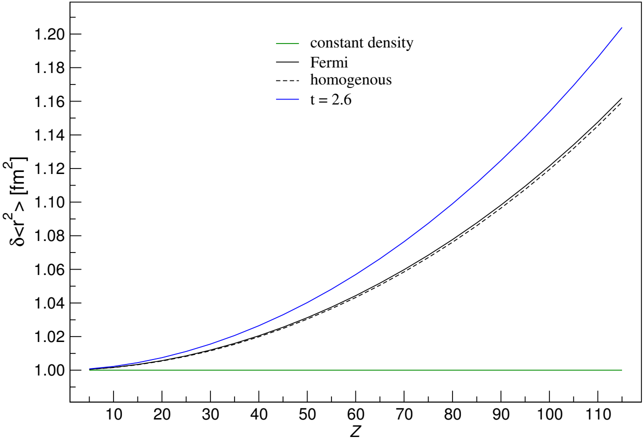
Homogenous distributions ($t = 0.0$ fm) for both isotopes



$$\lambda_k^{A,A'} = 1.00 \text{ fm}^2 \text{ and } \langle r^2\rangle^A > \langle r^2\rangle^{A'}$$

Refined extraction of $\delta\langle r^2\rangle$ values

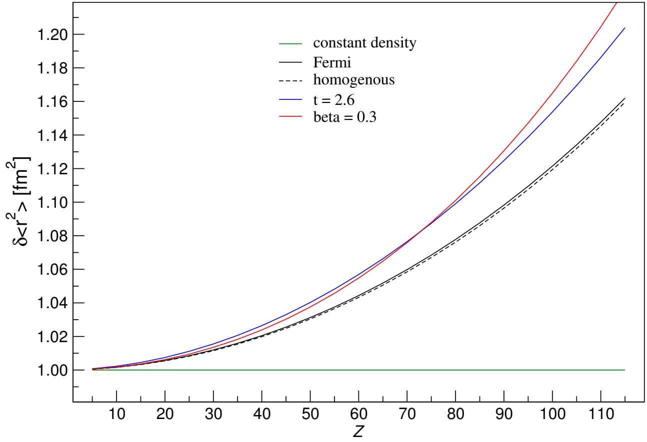
Spherical Fermi distributions with $t_A = 2.6$ and $t_{A'} = 2.3$ fm



$$\lambda_k^{A,A'} = 1.00 \text{ fm}^2 \text{ and } \langle r^2\rangle^A > \langle r^2\rangle^{A'}$$

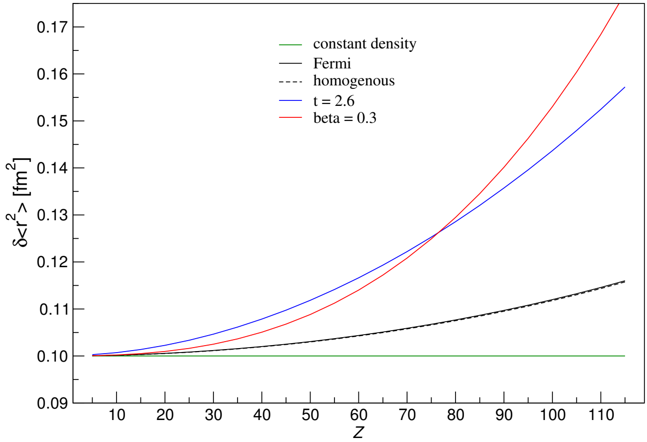
Refined extraction of $\delta\langle r^2\rangle$ values

Fermi distributions with $\beta_{2,A} = 0.3$ and $\beta_{2,A'} = 0.0$



$$\lambda_k^{A,A'} = 1.00 \text{ fm}^2 \text{ and } \langle r^2\rangle^A > \langle r^2\rangle^{A'}$$

Refined extraction of $\delta\langle r^2\rangle$ values



$$\lambda_k^{A,A'} = 0.10 \text{ fm}^2 \text{ and } \langle r^2\rangle^A > \langle r^2\rangle^{A'}$$

Applications: Higher order corrections from realistic charge distrbutions

A. Papoulia, Master thesis, Lund University, 2015

B.G Carlsson, J. Ekman and A. Papoulia, in preparation

Higher order corrections from realistic charge distributions

Frequency field shifts are obtained using nuclear radial moments from

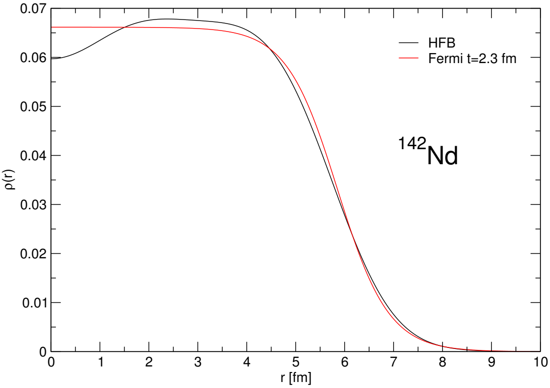
- Nuclear Hartree-Fock-Bogoliubov calculations (HFB)
- Two-parameter Fermi model with $t = 2.3$ fm (Fermi)

a "correction" term is obtained as

$$\delta\nu_{k,\mathrm{corr}}^{(1)A,A'} = \delta\nu_{k,\mathrm{HFB}}^{(1)A,A'} - \delta\nu_{k,\mathrm{Fermi}}^{(1)A,A'}$$

where $\delta\langle r^2\rangle_{\mathrm{Fermi}}^{A,A'} = \delta\langle r^2\rangle_{\mathrm{HFB}}^{A,A'}$

Higher order corrections from realistic charge distributions



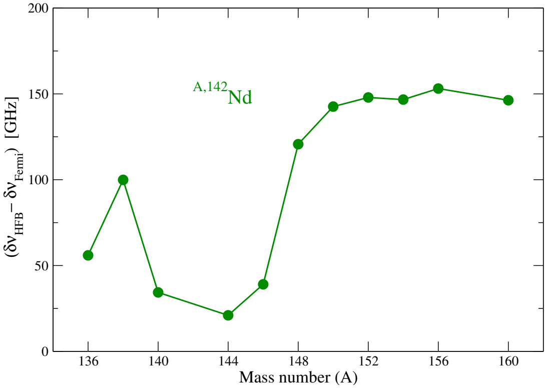
$$\sqrt{\delta\langle r^2\rangle^{A,A'}_{\mathrm{Fermi}}} = \sqrt{\delta\langle r^2\rangle^{A,A'}_{\mathrm{HFB}}} = 4.935 \text{ fm}$$

Higher order corrections from realistic charge distributions

The nuclear Hartree-Fock-Bogoliubov calculations (HFB) are perfomed using the Skyrme interaction with the UDF1 parameter set and the following software:

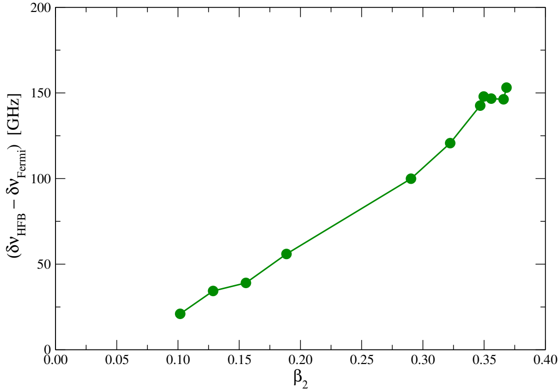
- HOSPHE (v2.00) for spherical nuclei
  B.G. Carlsson et al., Comput. Phys. Commun., 181, 1641 (2010)
- HFBTHO (2.00d) for axially symmetric deformed nuclei
  M.V. Stoitsov et al., Comput. Phys. Commun., 184, 1592 (2013)

Higher order corrections from realistic charge distributions



Higher order corrections, $\delta\nu^{(1)A,142}_{k,\mathrm{corr}}$, from realistic charge distributions for the $^2P_{1/2} - ^2S_{1/2}$ transition in Li-like Nd.

Higher order corrections from realistic charge distributions



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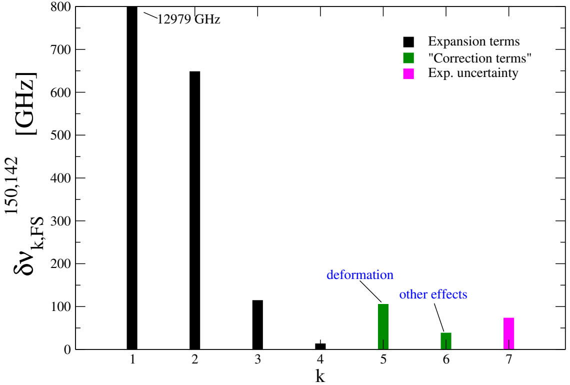
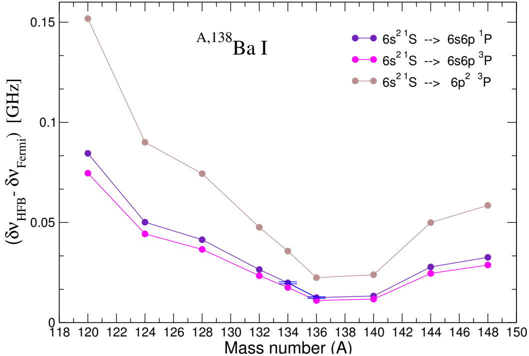
Higher order corrections from realistic charge distributions



Decomposition of expansion and corrections terms for the $^2P_{1/2} - ^2S_{1/2}$ transition in Li-like ^{150,142}Nd. Experimental (statistical) uncertainty from Brandau et al., PRL **100** (2008) 973201

Higher order corrections from realistic charge distributions

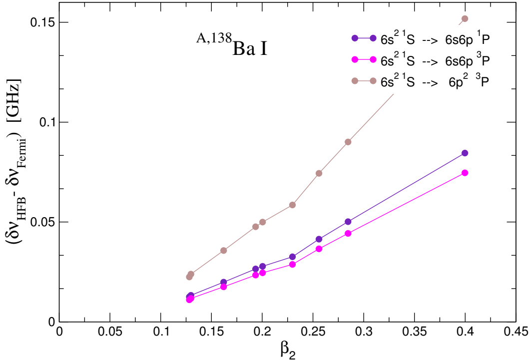


Higher order corrections, $\delta\nu_{k,\mathrm{corr}}^{(1)A,138}$, from realistic charge distributions for selected transitions in neutral barium (Ba I).

Wave functions from

C. Nazé, J.G. Li, and M. Godefroid, Phys. Rev. A **91**, 032511 (2015)

Higher order corrections from realistic charge distributions



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C. Naze, J.G. Li, and M. Godefroid, Phys. Rev. A **91**, 032511 (2015)

Applications: Simultaneous extraction of $\delta\langle r^2\rangle$ and $\delta\langle r^4\rangle$ values

A. Papoulia, Master thesis, Lund University, 2015
B.G Carlsson, J. Ekman and A. Papoulia, in preparation

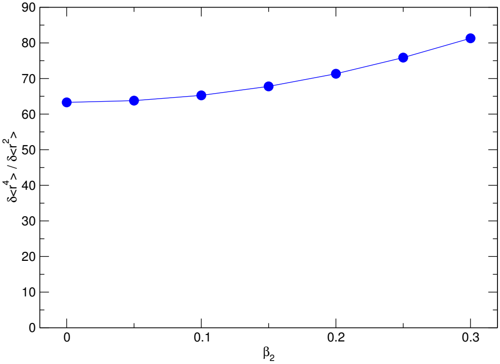
Simultaneous extraction of $\delta\langle r^2\rangle$ and $\delta\langle r^4\rangle$ values

Using the reformulated fiels shift and experimental isotope shifts for at least four analogue transitions in an isotope pair it is principle possible to extract $\delta\langle r^2\rangle$, $\delta\langle r^4\rangle$, $\delta\langle r^6\rangle$ and $\delta\langle r^8\rangle$

However, this is an extremely challenging task and would rely on experimental data and calculations without uncertainties.

Extracting $\delta\langle r^2\rangle$ and $\delta\langle r^4\rangle$ is more realistic, although extremely challenging, and would provide additional information of nuclear charge distributions.

Simultaneous extraction of $\delta\langle r^2\rangle$ and $\delta\langle r^4\rangle$ values



The ratio $\delta\langle r^4\rangle^{A.A'}/\delta\langle r^2\rangle^{A,A'}$ as a function of the deformation parameter β_2 of the larger isotope.

$\delta\langle r^2\rangle^{1/2} = 5.0$ and 5.1 fm, respectively. $t = 2.3$ fm for both isotopes.

Simultaneous extraction of $\delta\langle r^2\rangle$ and $\delta\langle r^4\rangle$ values

Approach 1:

Neglect $\delta\langle r^6\rangle$ and $\delta\langle r^8\rangle$ terms in the expression for the reformulated field shift:

$$\delta\nu_{k,\mathrm{FS}}^{(1)A,A'} \approx F_{k,0}\delta\langle r^2\rangle^{A,A'} + F_{k,2}\delta\langle r^4\rangle^{A,A'}$$

Using experimental isotope shifts for two transitions, 1 and 2, in an isotope pair, $\delta\langle r^4\rangle^{A,A'}$ is then given by

$$\delta\langle r^4\rangle^{A,A'} = \frac{\lambda_1^{A,A'} - \lambda_2^{A,A'}}{\frac{F_{1,2}}{F_{1,0}} - \frac{F_{2,2}}{F_{2,0}}}$$

Simultaneous extraction of $\delta\langle r^2\rangle$ and $\delta\langle r^4\rangle$ values

Approach 2:

Constructing radial moments $\delta\langle y_2\rangle^{A,A'}$ and $\delta\langle y_4\rangle^{A,A'}$ that are orthogonal inside the nuclear volume:

$$\delta\nu_{k,\mathrm{FS}}^{(1)A,A'} = c_{k,0}\delta\langle y_2\rangle^{A,A'} + c_{k,2}\delta\langle y_4\rangle^{A,A'}$$

- $c_{k,0}$ and $c_{k,2}$ are linear combinations of $F_{k,N}$
- $\delta\langle y_2\rangle^{A,A'}$ and $\delta\langle y_4\rangle^{A,A'}$ are linear combinations of $\delta\langle r^2\rangle^{A,A'}$ and $\delta\langle r^4\rangle^{A,A'}$.

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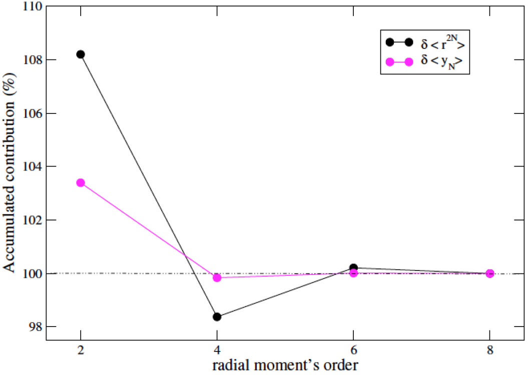
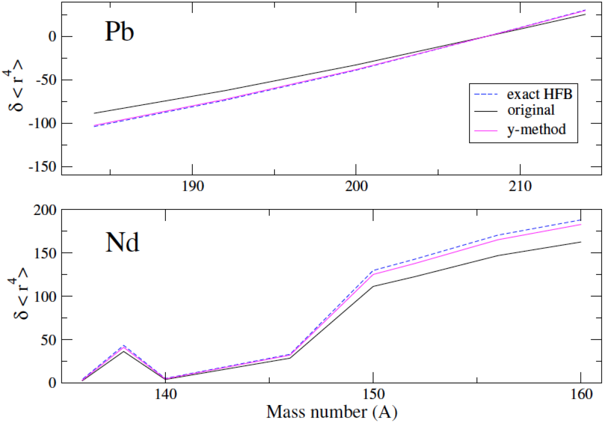
Simultaneous extraction of $\delta\langle r^2\rangle$ and $\delta\langle r^4\rangle$ values



Convergence in frequency field shift as a function of radial moment order using original, but truncated, reformulated field shift (black) and orthogonal radial moments within nuclear volume (purple) in the case of Li-like ^{200,208}Pb.

Simultaneous extraction of $\delta\langle r^2\rangle$ and $\delta\langle r^4\rangle$ values



Extraction of $\delta\langle r^4\rangle$ values from "pseudo-experimental" field shifts in Li-like Pb and Nd isotopes.

Simultaneous extraction of $\delta\langle r^2\rangle$ and $\delta\langle r^4\rangle$ values

- For the $^2P_{1/2} -^2 S_{1/2}$ and $^2P_{3/2} -^2 S_{1/2}$ transitions in Li-like Nd $\delta\nu_{k,\mathrm{FS}}^{A,A'}$ needs to be determined with a relative uncertainty of approximately 10^{-5} in order to extract $\delta\langle r^4\rangle$ with 20% accuracy
- However, using pair of transitions where the electronic factors are less linear dependent a relative uncertainty of 10^{-4} may be sufficient.

Conclusions and outlook

- Knowledge of nuclear shapes and deformation is important for the extraction of accurate $\delta\langle r^2\rangle$ values
- The extraction of $\delta\langle r^2\rangle$ values benefits from nuclear Hartree-Fock calculations
- The extraction of $\delta\langle r^2\rangle$ and $\delta\langle r^4\rangle$ values are in principle possible, but requires more effort on both the experimental and theory side.
- In the future it will be investigated whether the method of reformulated field shift is applicable also to $K\alpha$ isotope shifts and muonic atoms

Thank you!

Nuclear charge and radial electron densities
in ground states of selected noble gases