An EFT-Inspired Introduction to NP in Isotope Shifts

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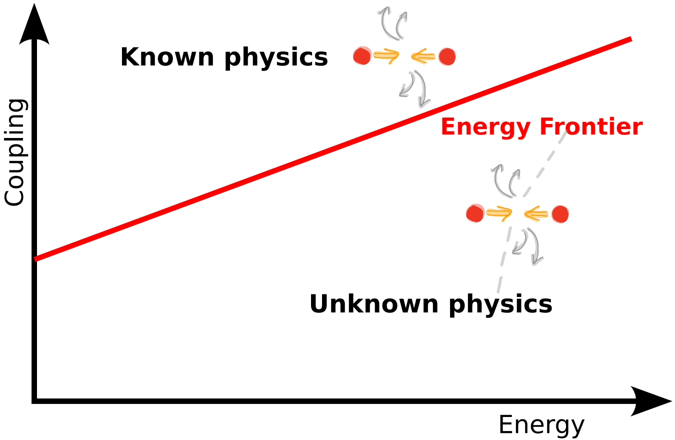
QuantumFrontiers
Cluster of Excellence

Leibniz Universität Hannover

YOUNGST@RS - EFTs and Beyond, 5^{th} December 2024

Where is the New Physics?



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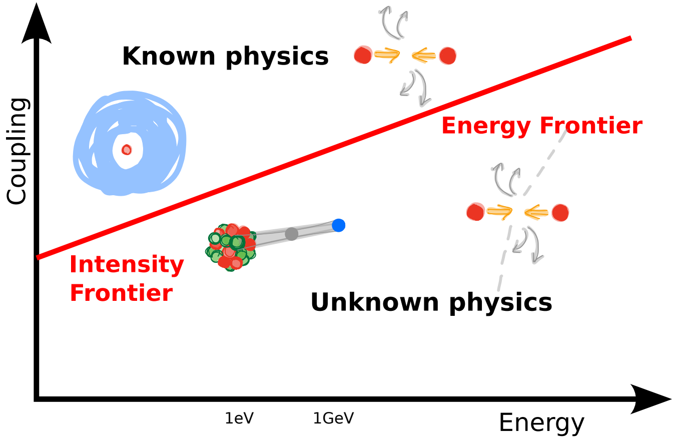


Outline

Outline

Why Isotope Shifts?

The most accurately measured numbers in physics are ratios of atomic clock transition frequencies:

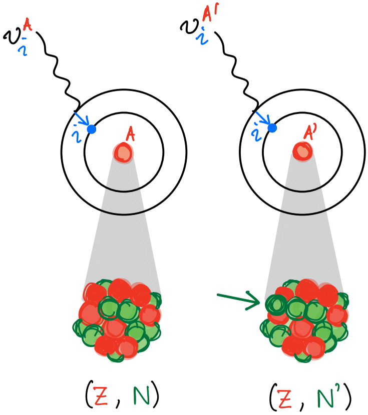
- $\nu_{\mathrm{Al}^+}/\nu_{\mathrm{Hg}^+} = 1.052871833148990438(55)$ (NIST; $\sigma_\nu/\nu \sim 5.2 \times 10^{-17}$)
  [Rosenband et al. Science 319, 1808 (2008)]
- $\nu_{\mathrm{Yb}}/\nu_{\mathrm{Sr}} = 1.207507039343337749(55)$ (RIKEN; $\sigma_\nu/\nu \sim 4.6 \times 10^{-17}$)
  [Nemitz et al. Nat. Photonics 10, 258 (2016)]
- $\nu_{\mathrm{E3}}/\nu_{\mathrm{E2}} = 0.932829404530965376(32)$ (PTB; $\sigma_\nu/\nu \sim 3.4 \times 10^{-17}$)
  [Lange et al. PRL 126 011102 (2021)]
- $\nu_{\mathrm{In}^+}/\nu_{\mathrm{Yb}^+} = 1.973773591557215789(9)$ (PTB; $\sigma_\nu/\nu \sim 4.4 \times 10^{-18}$)
  [Hausser et al. arXiv: 2402.16807 (2024)]

$\Rightarrow$ These are sensitive to "everything", but we cannot calculate the spectrum below around 1% accuracy.

So what can we do with these?

[slide by Julian Berengut]

Isotope Shifts



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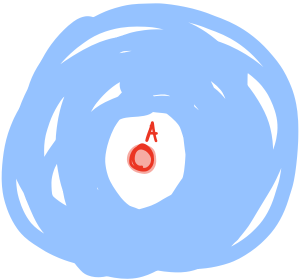

$$\frac{m_e}{m_A} \ll 1, \qquad \frac{r_{\text{nucleus}}}{r_{\text{atom}}} \ll 1$$

$\Rightarrow$ Can assume factorisation of electronic and nuclear contributions.

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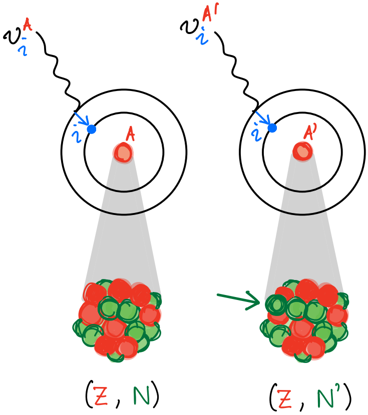

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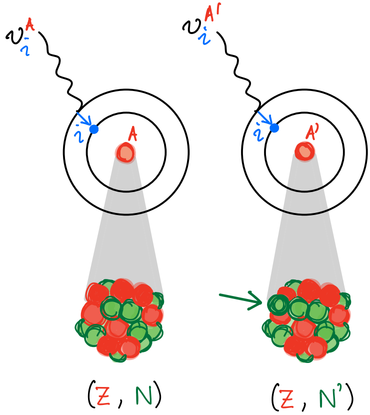

Isotope shifts:

$$\begin{aligned}\nu_i^{AA'} &\equiv \nu_i^A - \nu_i^{A'} \\ &= K_i \mu^{AA'} + F_i \delta\langle r^2\rangle^{AA'} + \ldots\end{aligned}$$

i: transition index

AA': isotope pair index

$K_i, F_i, \ldots$: electronic coeffs.

$\mu^{AA'}, \delta\langle r^2\rangle^{AA'}, \ldots$: nuclear coeffs.

Z: number of protons

N, N': number of neutrons in A, A'

Isotope Shifts: Mass Shift & Field Shift

$$\nu_i^{AA'} = K_i \mu^{AA'} + F_i \delta \langle r^2 \rangle^{AA'} + \ldots$$

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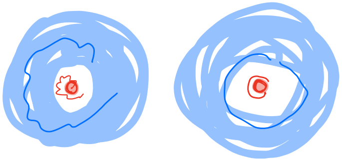
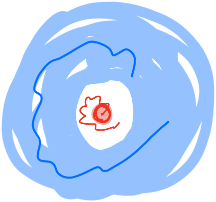
Mass Shift

$$\propto \mu^{AA'} = \frac{1}{M^A} - \frac{1}{M^{A'}}$$



Mass Shift: Nuclear Mass Effect

$M_N \neq M_{N'} \Rightarrow T_N \neq T_{N'} \Rightarrow$ Correction to electronic kinetic energy.



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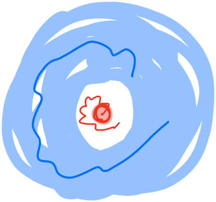

- Perturbation due to nuclear recoil

$$\delta H = \frac{\mathbf{p}_N^2}{2M_N} = \frac{\left(\sum_i \mathbf{p}_i\right)^2}{2M_N} = \frac{\sum_i \mathbf{p}_i^2 + \sum_{i\neq j} \mathbf{p}_i \cdot \mathbf{p}_j}{2M_N} \propto \frac{1}{M_A}$$

in center of mass $\mathbf{p}_N + \sum_i \mathbf{p}_i = 0$

M_N: Nuclear mass
M_A: Atomic mass, $M_A \sim M_N$

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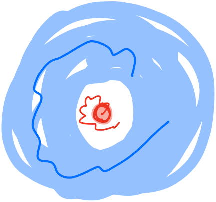

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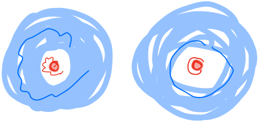
$\Rightarrow$ Contribution to isotope shift:



$$\delta E_i = K_i \left(\frac{1}{M_{A'}} - \frac{1}{M_A}\right) \equiv K_i \mu^{AA'}$$

K_i: Mass shift constant

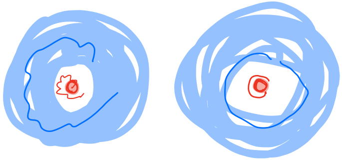
Isotope Shifts: Mass Shift & Field Shift

$$\nu_i^{AA'} = K_i \mu^{AA'} + F_i \delta\langle r^2\rangle^{AA'} + \dots$$

Mass Shift

Different motion of nuclei in A, A'
$\Rightarrow$ Correction to e^- kin. energy

$$\propto \mu^{AA'} = \frac{1}{M^A} - \frac{1}{M^{A'}}$$



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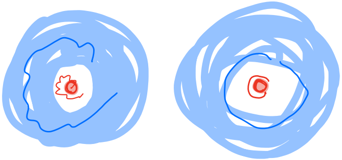
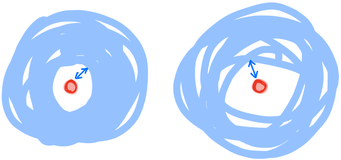
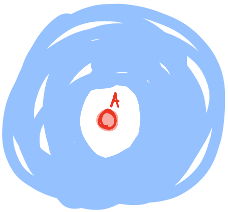


Field Shift

$$\propto \delta \langle r^2 \rangle^{AA'} = \langle r^2 \rangle^A - \langle r^2 \rangle^{A'}$$



Field Shift: Nuclear Size Effect



- **Well outside the atom,** spherically symm. charge distribution ⇒ Coulomb potential

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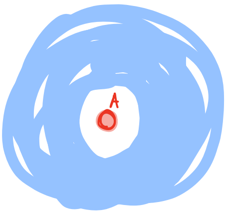

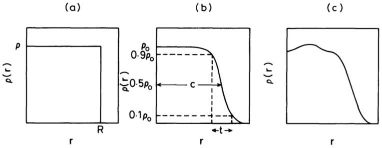

- **Well outside the atom,** spherically symm. charge distribution $\Rightarrow$ Coulomb potential
- **Inside the atom,** electron wavefct. affected by non-Coulombic nuclear potential, dep. on
  - Radial coordinate r
  - Nuclear **charge radius** $\langle r^2 \rangle = \frac{\int \rho_N(\mathbf{r}) r^2 \mathrm{d}\mathbf{r}^3}{\int \rho_N(\mathbf{r}) \mathrm{d}\mathbf{r}^3}$

$$\rho_N(\mathbf{r}) = \begin{cases} \rho_0 & r < R \\ 0 & r \geq R \end{cases}, \quad \rho_N(\mathbf{r}) = \frac{\rho_0}{1 + e^{\frac{r-c}{a}}}, \quad \dots$$

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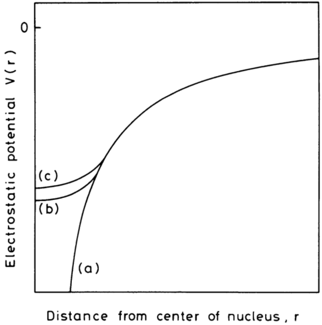

(a) Coulomb $V = -\frac{Ze}{4\pi r}$
(b) Finite size nucleus
(c) Larger nucleus

The larger the nucleus, the shallower the potential.

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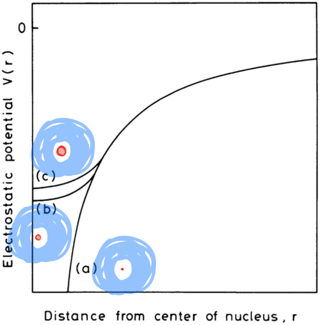

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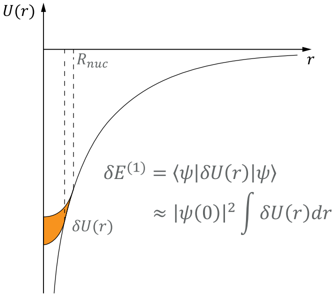

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$\Rightarrow$ Shift in $\langle r^2 \rangle \Rightarrow$ Energy shift

$$\delta E_i \equiv F_i \delta \langle r^2 \rangle^{AA'}$$

F_i : Field shift constant
$\delta\langle r^2\rangle^{AA'} = \langle r^2\rangle^A - \langle r^2\rangle^{A'}$: Charge radius variance

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Mass Shift

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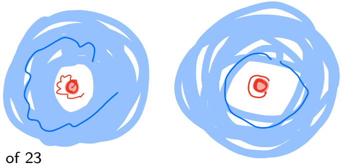
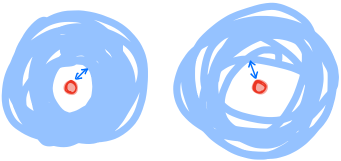


Field Shift

Different nuclear charge distributions in A, A'
$\Rightarrow$ Different contact interactions betw. e^- & nuclei

$$\propto \delta \langle r^2 \rangle^{AA'} = \langle r^2 \rangle^{A} - \langle r^2 \rangle^{A'}$$



The King-Plot: Trade Data for Nuclear Physics

[W. King, J. Opt. Soc. Am. 53, 638 (1963)]

Issue: Large uncertainty on charge radius variance $\delta\langle r^2\rangle^{AA'}$

$$\nu_1^{AA'} = K_1 \mu^{AA'} + F_1 \delta\langle r^2\rangle^{AA'}$$

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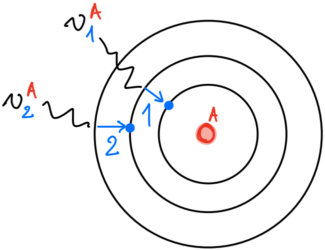

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$\Rightarrow$ Measure isotope shifts for 2 transitions

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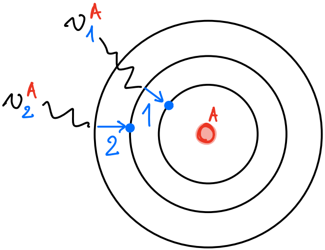

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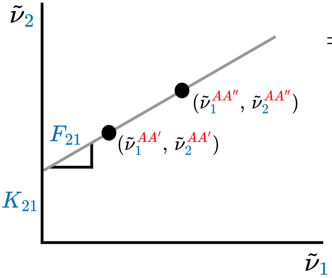


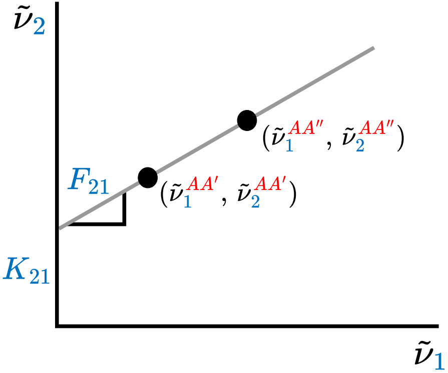
$\Rightarrow$ Eliminate charge radius variance $\delta\langle r^2\rangle^{AA'}$

$$\tilde{\nu}_2^{AA'} = K_{21} + F_{21}\tilde{\nu}_1^{AA'}$$

$\tilde{\nu}_i^{AA'} \equiv \nu_i^{AA'}/\mu^{AA'}$ $\Rightarrow$ data

$F_{21} \equiv F_2/F_1$ $K_{21} \equiv K_2 - F_{21}K_1$ $\Rightarrow$ fit

The King-Plot: Fit to Isotope Shift Data



$$\tilde{\nu}_2^{AA'} = K_{21} + F_{21}\tilde{\nu}_1^{AA'}$$
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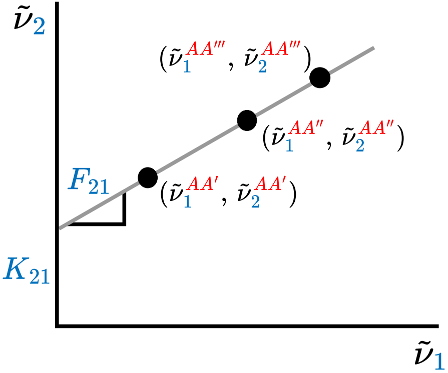

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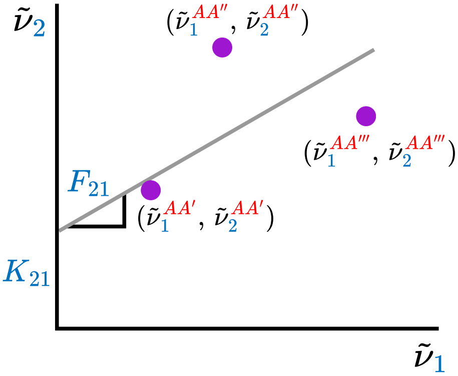
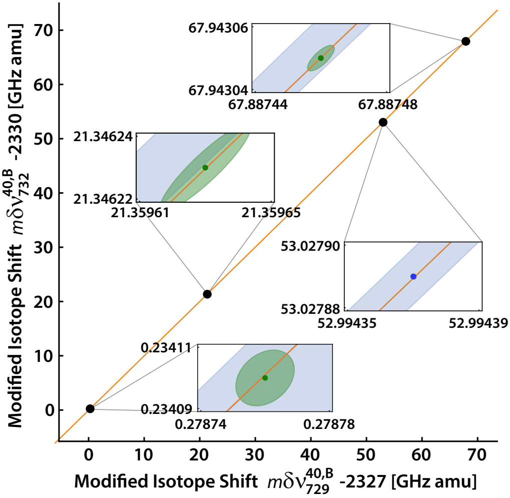
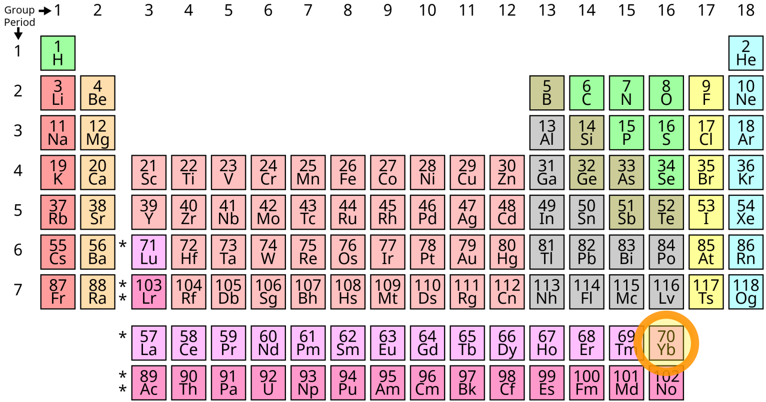


$$\begin{aligned}
\tilde{\nu}_2^{AA'} &= K_{21} + F_{21}\tilde{\nu}_1^{AA'} + ? \\
\tilde{\nu}_2^{AA''} &= K_{21} + F_{21}\tilde{\nu}_1^{AA''} + ? \\
\tilde{\nu}_2^{AA'''} &= K_{21} + F_{21}\tilde{\nu}_1^{AA'''} + ?
\end{aligned}$$

Example of a Linear King Plot: Ca^+ [arXiv:2311.17337]



Ytterbium and its Stable Isotopes



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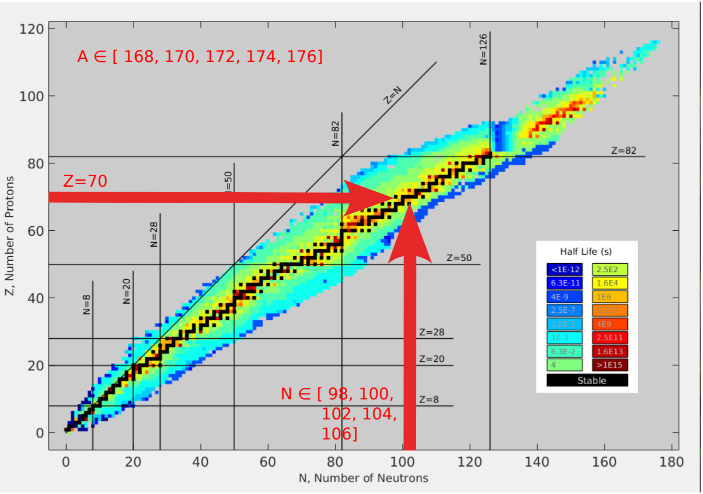
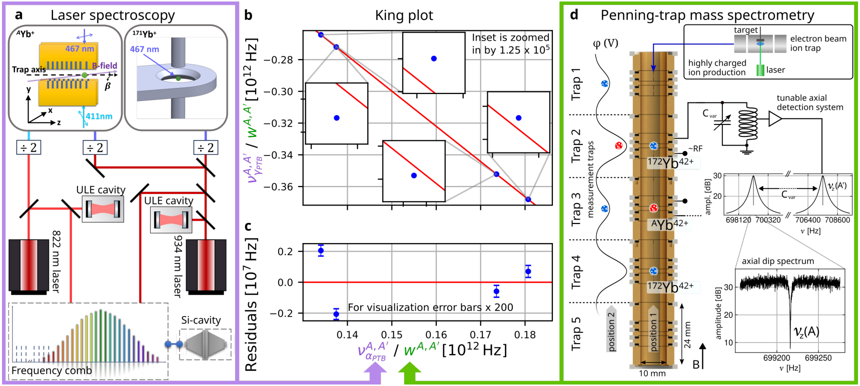
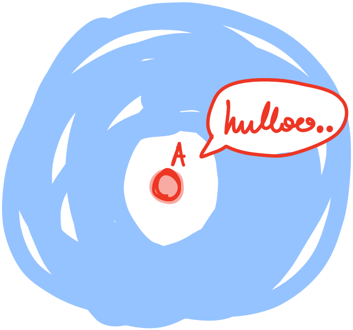


PTB + MPIK = New Yb King Plot [arXiv:2403.07792]



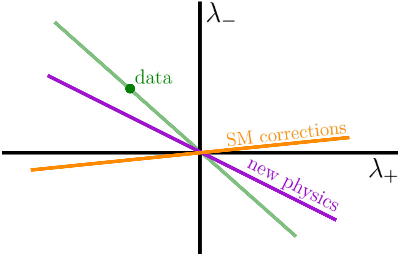
Observed King plot nonlinearity: $\sim 20.17(2)$ kHz

Nuclear Finite-Size Effects



Outline

The Nonlinearity Decomposition Plot



- Plane of King linearity ($\mathbf{1} = (1, 1, 1, 1)$)

$$\tilde{\boldsymbol{\nu}}_j \approx F_{j1} \tilde{\boldsymbol{\nu}}_1 + K_{j1} \mathbf{1} \,, \qquad j > 1.$$

- Project isotope-shift data onto $\tilde{\boldsymbol{\nu}}_1$, $\mathbf{1}$, Λ_+, Λ_- with $\Lambda_\pm \perp (\tilde{\boldsymbol{\nu}}_1, \mathbf{1})$:

$$\tilde{\boldsymbol{\nu}}_j = (\tilde{\boldsymbol{\nu}}_1, \mathbf{1}, \boldsymbol{\Lambda}_+, \boldsymbol{\Lambda}_-)\,(F_{j1}, K_{j1}, \lambda_+, \lambda_-)^T$$

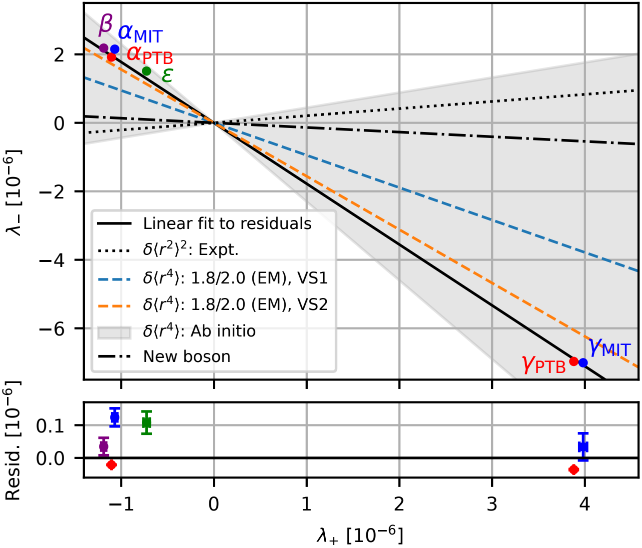
In presence of just one nonlinearity,

$$\tilde{\boldsymbol{\nu}}_j \approx F_{j1} \tilde{\boldsymbol{\nu}}_1 + K_{j1} \mathbf{1} + G_{j1}^{(4)} \boldsymbol{\delta} \widetilde{\langle \mathbf{r}^4 \rangle} \,, \qquad j > 1.$$

slope: $\frac{\lambda_-}{\lambda_+} \equiv \frac{G_{j1}^{(4)} \boldsymbol{\delta} \widetilde{\langle \mathbf{r}^4 \rangle}_-}{G_{j1}^{(4)} \boldsymbol{\delta} \widetilde{\langle \mathbf{r}^4 \rangle}_+} = \frac{\boldsymbol{\delta} \widetilde{\langle \mathbf{r}^4 \rangle}_-}{\boldsymbol{\delta} \widetilde{\langle \mathbf{r}^4 \rangle}_+} \Rightarrow$ transition-universal

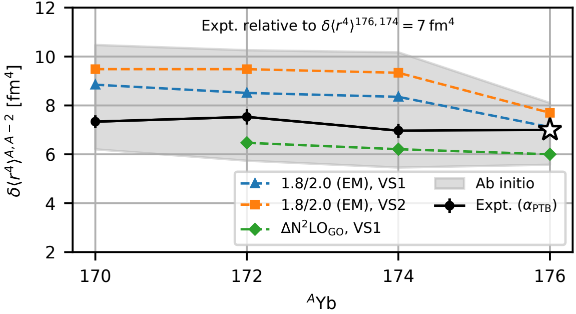
[arXiv:2004.11383, arXiv:2201.03578]

The Nonlinearity Decomposition Plot [arXiv:2403.07792]



Extracting Nuclear Physics from Isotope-Shift Measurements

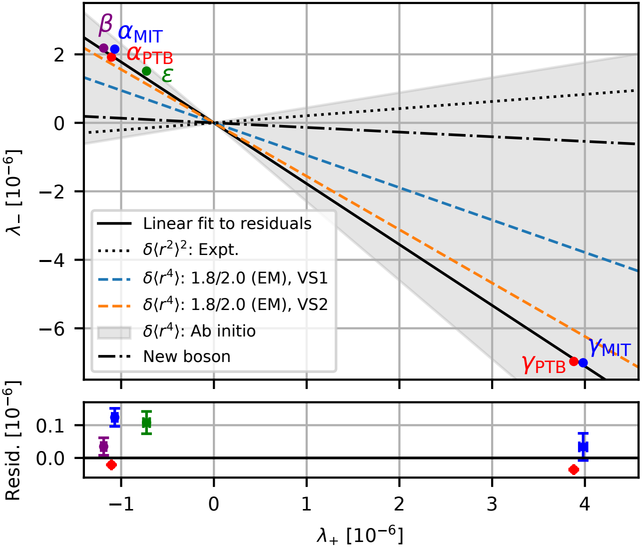
- **Assuming $\delta\langle r^4\rangle$ dominates,** what does the isotope-shift data tell us about the evolution of $\delta\langle r^4\rangle$ along the isotope chain?



blue, **orange**, **green**: Calculations by group of Prof. Achim Schwenk

black: new spectroscopic method, fixed at $\star$

The Nonlinearity Decomposition Plot [arXiv:2403.07792]



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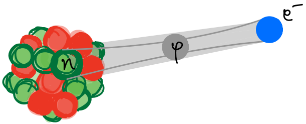
Introduction to King Plots

New Nuclear Physics

New Physics

King-Plot Bounds on New Bosons [arXiv:1704.05068]



New effective Yukawa-potential

$$V_\phi(r) = -\alpha_{\mathrm{NP}}(A - Z)\frac{e^{-m_\phi r}}{r}$$

with $\alpha_{\mathrm{NP}} = (-1)^s \frac{y_e y_n}{4\pi}$, $s = 0, 1, 2$ (spin)

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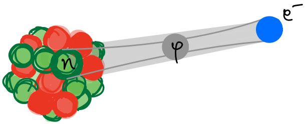

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Induces new term in the King-relation:

$$\tilde{\nu}_2^{AA'} = K_{21}\tilde{\mu}^{AA'} + F_{21}\tilde{\nu}_1^{AA'} + G_{21}^{(4)}\delta\langle\widetilde{r^4}\rangle^{AA'} + \alpha_{\mathrm{NP}}X_{21}\tilde{\gamma}^{AA'}$$

$X_{21} = X_2 - F_{21}X_1$: NP electronic coefficient

$\tilde{\gamma}^{AA'} \equiv (A-A')/\mu^{AA'}$: NP nucl. coeff.

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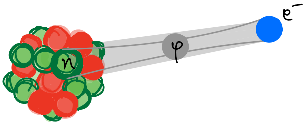

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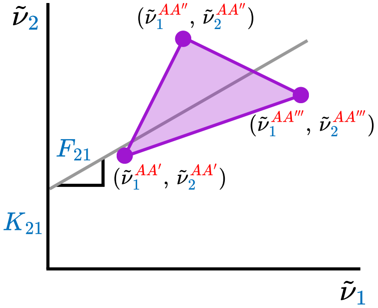
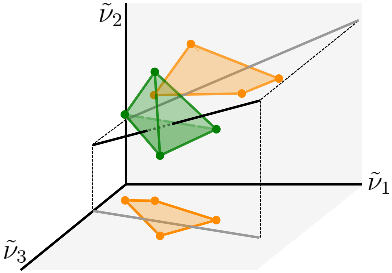
$\Rightarrow$ Extract $\alpha_{\rm NP}$ from fraction of volumes spanned by frequency vectors:

$$\alpha_{\rm NP} = \frac{Vol.}{Vol.|_{th,\alpha_{\rm NP}=1}} = \frac{2\det\left(\vec{\tilde{\nu}}_1, \vec{\tilde{\nu}}_2, \vec{\tilde{\nu}}_3, \vec{\tilde{\mu}}\right)}{\varepsilon_{ijk}\det\left(X_i\vec{\tilde{\gamma}}, \vec{\nu}_j, \vec{\nu}_k, \vec{\tilde{\mu}}\right)}$$

$\{\vec{\nu}_i\}$: data vect. in isotope-pair space, $\vec{\tilde{\mu}} \equiv (1,1,1,1)$, X_i, $\vec{\tilde{\gamma}}$: theory input

King-Plot Method in Presence of Nuclear Effects: The Generalised King Plot [PRR 2, 043444 (2020)]





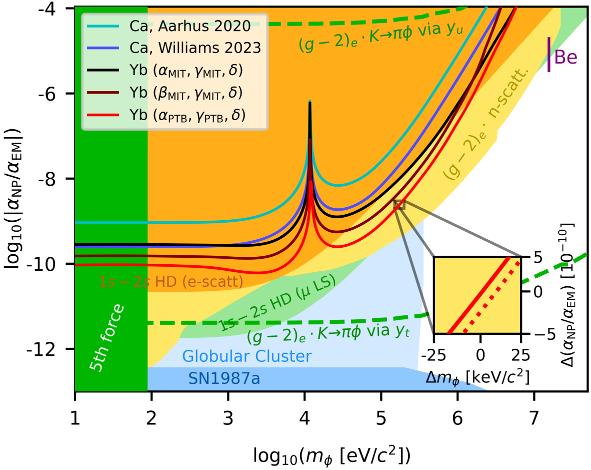
⇒ test King linearity

⇒ account for one King nonlinearity

⇒ put bound on 2nd

⇒ **King-plot method also works in presence of nuclear effects.**

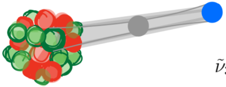
New Spectroscopy Bounds on New Physics

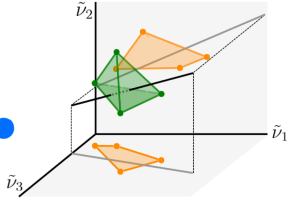


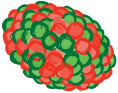
- $m_\phi \to 0$: $>$ size atom
- $m_\phi \to \infty$: not sensitive to contact interactions
- "Peaks" due to cancellations among electronic coefficients

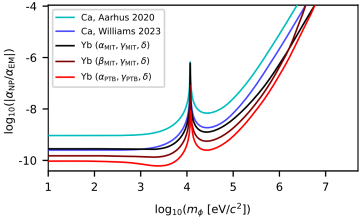
Conclusions

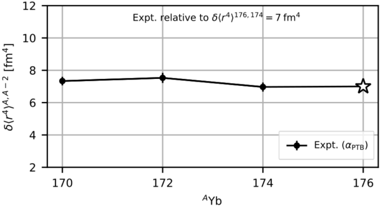
Atomic clocks are sensitive probes for











New mediators between n & e$^-$ **Nuclear structure**

Check out our paper on the arXiv:

Yb King plot: `arXiv:2403.07792`

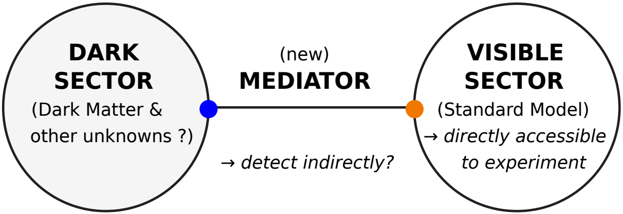
Stay tuned for:

- `Kifit`: Global King-plot analysis
- King-plot analysis of highly-charged Ca ions

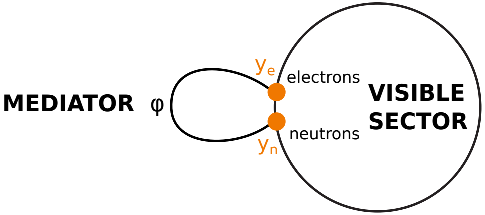
Thank you for your attention.

Backup slides

Dark Portals



Dark Portals and Isotope Shift Measurements



α_{NP} from Determinants

(No-Mass King-Plot:)

$$
\begin{aligned}
\vec{\nu}_1 =& K_1\vec{\mu} + F_1\overrightarrow{\delta\langle r^2\rangle} + \alpha_{\mathsf{NP}} X_1\vec{\gamma} \\
\vec{\nu}_2 =& K_2\vec{\mu} + F_2\overrightarrow{\delta\langle r^2\rangle} + \alpha_{\mathsf{NP}} X_2\vec{\gamma} \\
\vec{\nu}_3 =& K_3\vec{\mu} + F_3\overrightarrow{\delta\langle r^2\rangle} + \alpha_{\mathsf{NP}} X_3\vec{\gamma} \\
\Rightarrow \det\left(\vec{\nu}_1, \vec{\nu}_2, \vec{\nu}_3\right) =& \alpha_{\mathsf{NP}} \det\left(\vec{K}, \vec{F}, \vec{X}\right) \det\left(\vec{\mu}, \overrightarrow{\delta\langle r^2\rangle}, \vec{\gamma}\right) \\
\Rightarrow \alpha_{\mathsf{NP}} =& \frac{Vol}{Vol|_{th,\alpha_{\mathsf{NP}}=1}} = \frac{\det\left(\vec{\nu}_1, \vec{\nu}_2, \vec{\nu}_3\right)}{\det\left(\vec{K}, \vec{F}, \vec{X}\right) \det\left(\vec{\mu}, \overrightarrow{\delta\langle r^2\rangle}, \vec{\gamma}\right)} \\
=& \frac{\det\left(\vec{\nu}_1, \vec{\nu}_2, \vec{\nu}_3\right)}{\frac{1}{2}\varepsilon_{ijk} \det\left(X_i\vec{\gamma}, \vec{\nu}_j, \vec{\nu}_k\right)}
\end{aligned}
$$

Choose your King-Plot

Extraction of α_{NP} using the "determinant method" requires

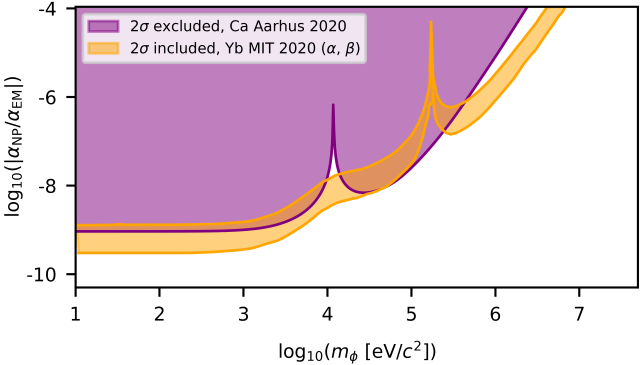
Type of King-Plot	Isotope-Pairs	Transitions	
Generalised King-Plot:	n	$n-1$	[PRR 2, 043444 (2020)]
No-Mass King-Plot:	n	n	[PRR 2, 043444 (2020)]

$n \geq 3$ (else cannot search for nonlinearities)

$$\alpha_{\mathrm{NP}} = \frac{V}{V|_{\mathrm{th},\alpha_{\mathrm{NP}}=1}} = \frac{(n-2)!\,\det\left(\vec{\tilde{\nu}}_1,\ldots,\vec{\tilde{\nu}}_{n-1},\vec{\tilde{\mu}}\right)}{\varepsilon_{i_1,\ldots,i_{n-1}}\det\left(X_{i_1}\vec{\tilde{\gamma}},\vec{\tilde{\nu}}_{i_2},\ldots,\vec{\tilde{\nu}}_{i_{n-1}},\vec{\tilde{\mu}}_{i_n}\right)}$$

$$\alpha_{\mathrm{NP}} = \frac{v}{v|_{\mathrm{th},\alpha_{\mathrm{NP}}=1}} = \frac{(n-1)!\,\det\left(\vec{\nu}_1,\vec{\nu}_2,\ldots,\vec{\nu}_n\right)}{\varepsilon_{i_1,i_2,\ldots,i_n}\det\left(X_{i_1}\vec{\gamma},\vec{\nu}_{i_2},\ldots,\vec{\nu}_{i_n}\right)}$$

Upper Bounds on $|\alpha_{\mathrm{NP}}|$ vs. New Mediator Mass m_ϕ



Nonlinear King plot relation:

$$\tilde{\nu}_2^{AA'} = K_{21}\tilde{\mu}^{AA'} + F_{21}\tilde{\nu}_1^{AA'} + G_{21}^{(2)}\delta\langle r^2\rangle^2 + G_{21}^{(4)}\delta\langle r^4\rangle + \ldots?$$

X Coefficients

Overlap of new physics potential and electronic wavefunction

$$X_i = \int \mathrm{d}^3 r \frac{e^{-m_\phi r}}{r} \left[|\psi_b(r)|^2 - |\psi_a(r)|^2 \right]$$

$|\psi(r)|^2$: electron density in absence of new physics,

a, b initial, final states

Requirement for searches for new light bosons:

- At least one of ψ_a or ψ_b should have good overlap with new potential.
- For tight bounds on α_{NP}, one X_i needs to be large.

Recipe for the Nonlinearity Decomposition Plot

[PRL 125, 123002 (2020), PRL 128, 163201 (2022)]

1. Arrange the isotope-shift data for all transitions $\tau \in \{\alpha, \beta, \gamma, \delta, \epsilon\}$ in n-vectors $\tilde{\boldsymbol{\nu}}_\tau$, where n is the number of isotope pairs (here 4):

$$\tilde{\boldsymbol{\nu}}_\tau = \left(\tilde{\nu}_\tau^{168,170}, \tilde{\nu}_\tau^{170,172}, \tilde{\nu}_\tau^{172,174}, \tilde{\nu}_\tau^{174,176}\right)$$

2. Choose a reference transition, say δ.
3. Plane of King linearity is defined by the relations ($\mathbf{1} = (1,1,1,1)$)

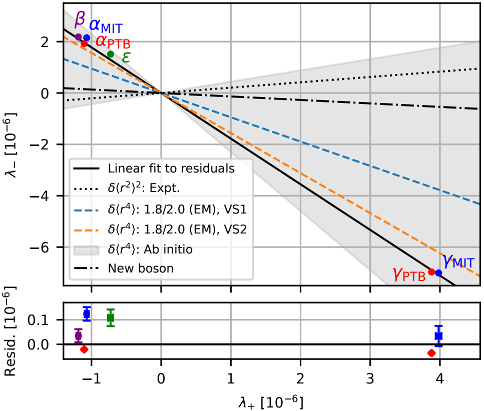
$$\tilde{\boldsymbol{\nu}}_\tau \;\approx\; F_{\tau\delta}\tilde{\boldsymbol{\nu}}_\delta + K_{\tau\delta}\mathbf{1}\,.$$

4. Define two $(n = 4)$−vectors $\Lambda_\pm$ that are orthogonal to $\tilde{\boldsymbol{\nu}}_\delta$, $\mathbf{1}$.
5. Project all isotope-shift data onto the four vectors $\tilde{\boldsymbol{\nu}}_\delta$, $\mathbf{1}$, Λ_+, Λ_-:

$$\tilde{\boldsymbol{\nu}}_\tau = \begin{pmatrix}\tilde{\boldsymbol{\nu}}_\delta & \mathbf{1} & \boldsymbol{\Lambda}_+ & \boldsymbol{\Lambda}_-\end{pmatrix}\begin{pmatrix}F_{\tau\delta} & K_{\tau\delta} & \lambda_+^{(\tau)} & \lambda_-^{(\tau)}\end{pmatrix}^T$$

6. Plot all points $(\lambda_+^{(\tau)}, \lambda_-^{(\tau)})$ in the same plane.

The Nonlinearity Decomposition Plot



Notation	Transition	Refs.
$\alpha_{\mathrm{MIT,PTB}}$	${}^2S_{1/2} \to {}^2D_{5/2}$ E2 in Yb^+	MIT, t.w.
β	${}^2S_{1/2} \to {}^2D_{3/2}$ E2 in Yb^+	MIT
$\gamma_{\mathrm{MIT,PTB}}$	${}^2S_{1/2} \to {}^2F_{7/2}$ E3 in Yb^+	MIT, t.w.
δ	${}^1S_0 \to {}^3P_0$ in Yb	Kyoto
ϵ	${}^1S_0 \to {}^1D_2$ in Yb	Mainz

- $\delta\langle r^2\rangle^2$ estimated using Angeli & Marinova Tables of experimental nuclear ground state charge radii
- $\delta\langle r^4\rangle$: Calculations by group of Prof. Achim Schwenk, TU Darmstadt

In presence of just one nonlinearity, e.g. $G^{(4)}\delta\langle r^4\rangle$,

slope: $\frac{\lambda_-^{(\tau)}}{\lambda_+^{(\tau)}} = \frac{G_\tau^{(4)}\boldsymbol{\delta}\langle\mathbf{r^4}\rangle_-}{G_\tau^{(4)}\boldsymbol{\delta}\langle\mathbf{r^4}\rangle_+} = \frac{\boldsymbol{\delta}\langle\mathbf{r^4}\rangle_-}{\boldsymbol{\delta}\langle\mathbf{r^4}\rangle_+} \equiv \frac{\lambda_-}{\lambda_+} \Rightarrow$ transition-universal

Extracting Nuclear Physics from Isotope-Shift Measurements

- **Assuming $\delta\langle r^4\rangle$ dominates,** what does the isotope-shift data tell us about the evolution of $\delta\langle r^4\rangle$ along the isotope chain?

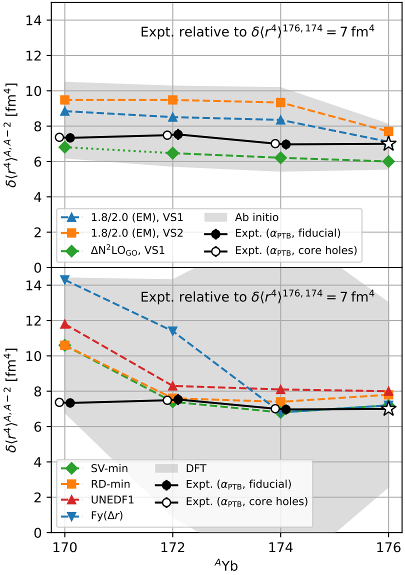
$\Rightarrow$ **"Put the King plot on it's head.":**

1. Instead of eliminating $\delta\langle r^2\rangle$ from the system of equations, we use experimental data (Angeli & Marinova) to determine it.
2. Perform a fit to determine the field shift coefficient F_τ from the data.
3. Use theoretical input for the electronic coefficient $G_\tau^{(4)}$ (J. Berengut)
4. Solve for object

$$Q^{AA',RR'} \equiv \delta\langle r^4\rangle^{AA'} - \frac{\mu^{AA'}}{\mu^{RR'}}\delta\langle r^4\rangle^{RR'} \,,$$

where RR': reference isotope pair, AA': any of remaining isotope pairs.

$\delta\langle r^4\rangle$ Calculations: Ab initio vs. DFT



- Experimental $\delta\langle r^4\rangle^{AA'}$ values relative to $\delta\langle r^4\rangle^{176,174} = 7$ fm^4 extracted from isotope shifts from the α transition using atomic theory (fiducial, core holes)
- Above: ab initio calculations (t.w.)
- Below: density functional theory calculations (PRL.128.163201)
- Gray bands: estimated theory uncertainties