kifit

Towards a Global Overview of Isotope Shift Data

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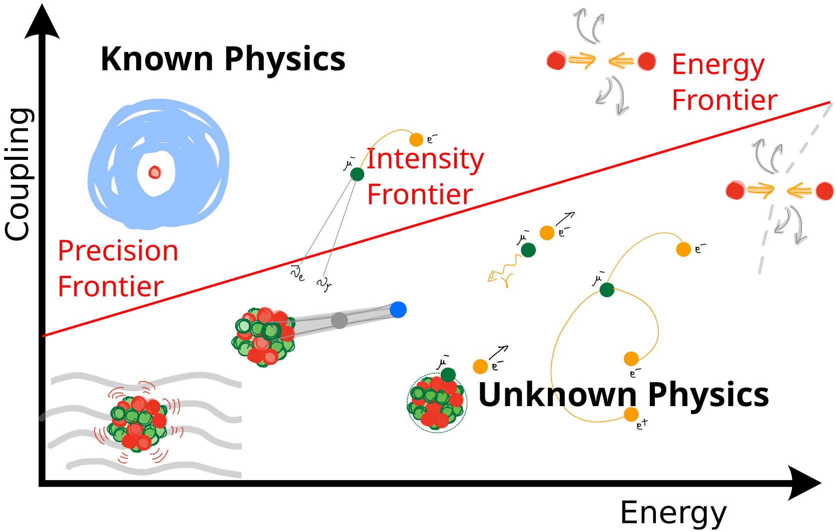
Based on work with

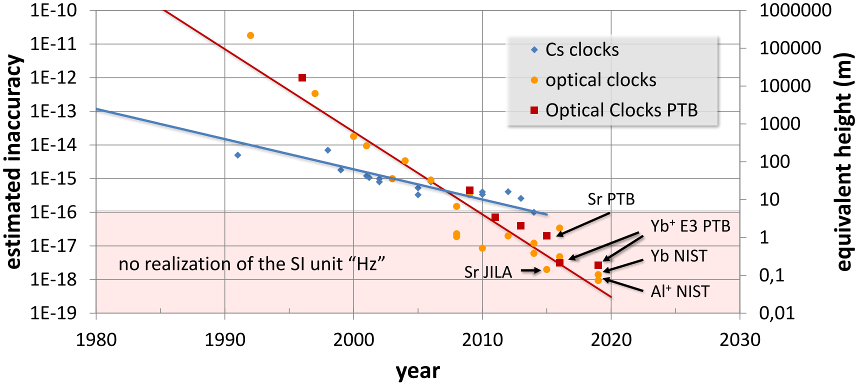
E. Fuchs, A. Mariotti, J. Richter, M. Robbiati

PhysTeV 2025 BSM Session, Les Houches

Where is the New Physics?



Evolution of Clock Precision



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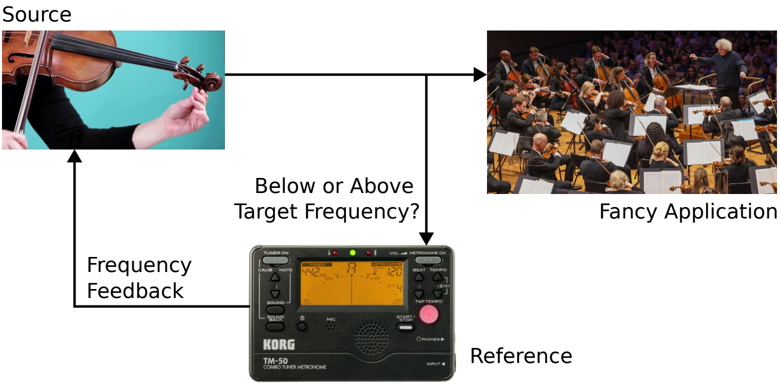

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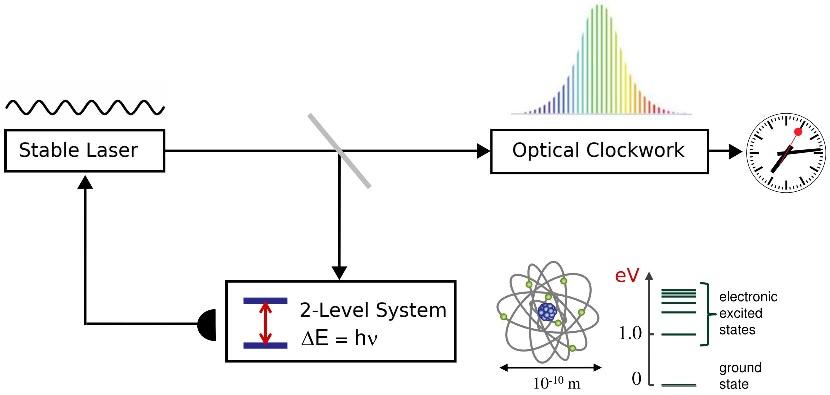

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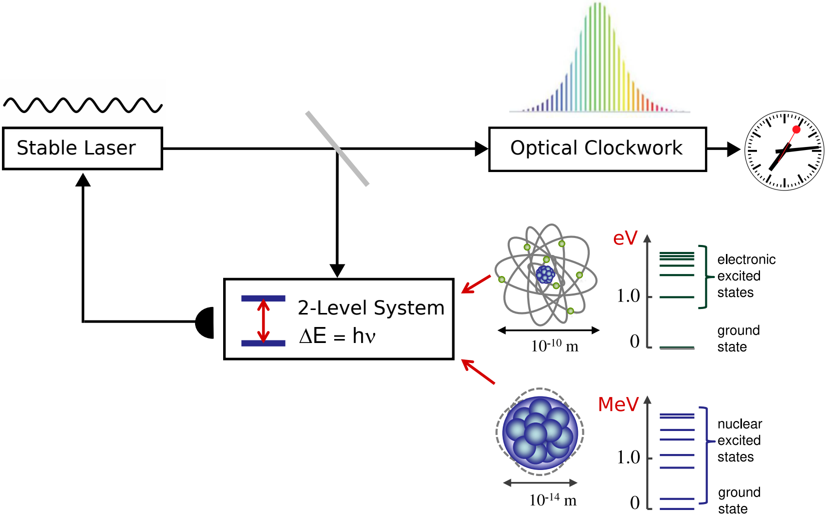

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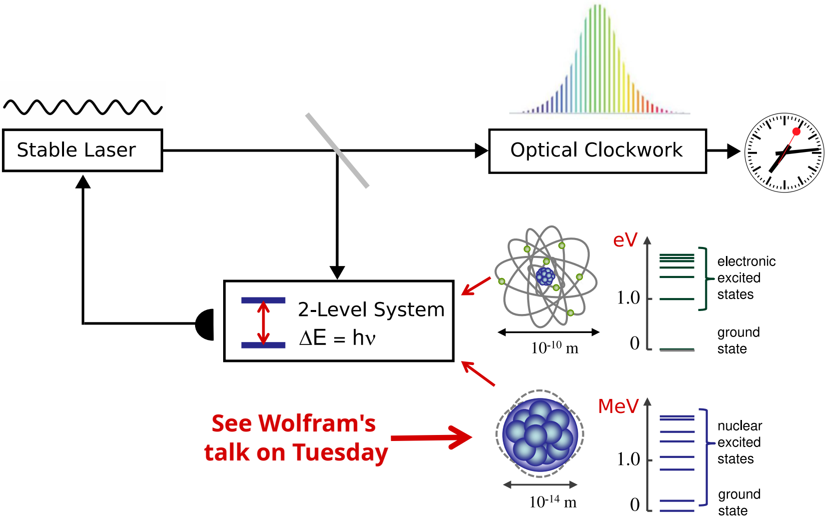

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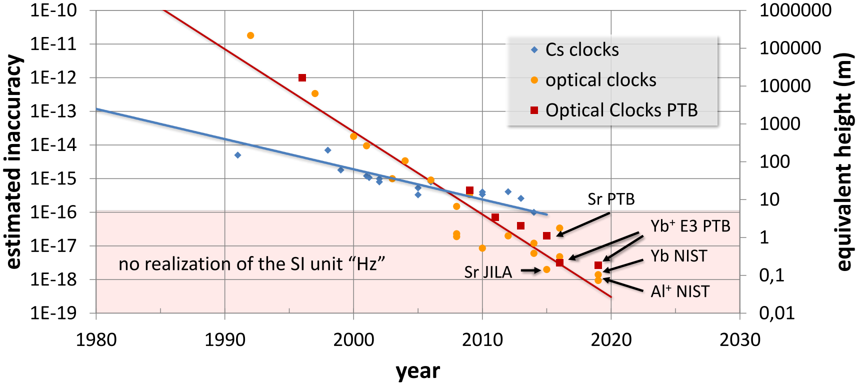


Why Isotope Shifts?

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.

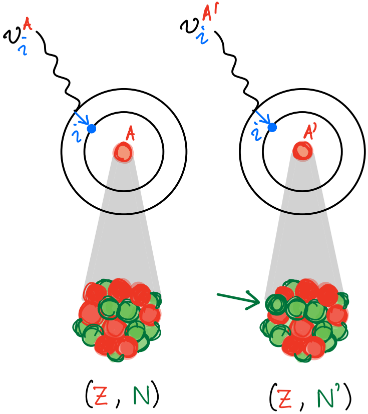
So what can we do with these?

[slide by Julian Berengut]

Outline

Outline

Isotope Shifts



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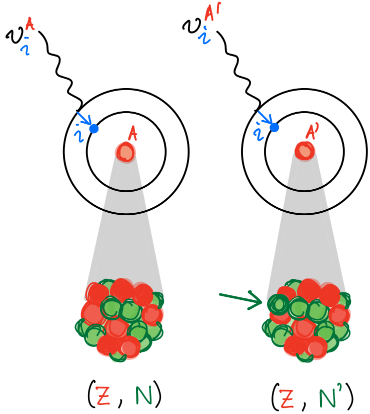


Isotope shifts:

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

- 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

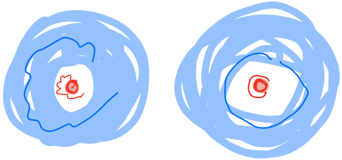
$$\nu_i^{AA'} = K_i \mu^{AA'} + F_i \delta\langle r^2\rangle^{AA'} + \dots$$

Mass Shift

Nuclear motion in A vs. A'

$\Rightarrow$ Correction to e^- kin. energy

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



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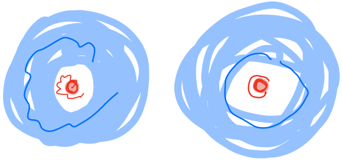
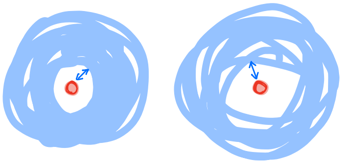
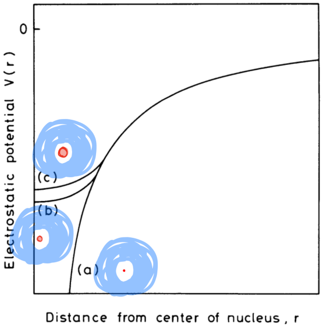


Field Shift

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



Field Shift: Nuclear Size Effect



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

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

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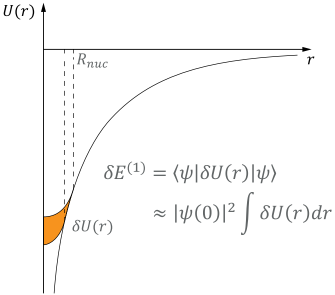

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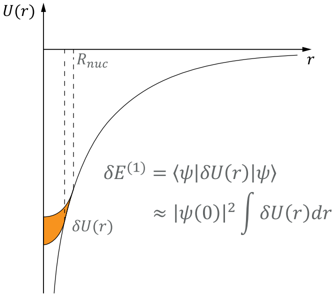

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$\Rightarrow$ Shift in $\langle r^2 \rangle \Rightarrow$ Energy shift

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

F_i : (Electronic) field shift constant

$\delta \langle r^2 \rangle^{AA'}$: Charge radius variance

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

Isotope Shifts: Mass Shift & Field Shift

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

Mass Shift

Nuclear motion in A vs. A'

⇒ Correction to e^- kin. energy

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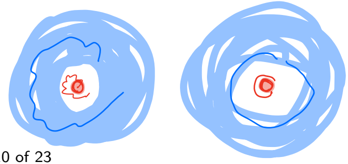
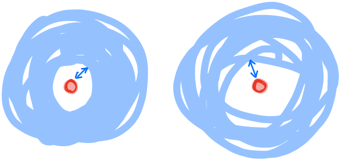


Field Shift

Nuclear charge distr. in A vs. A'

⇒ Difference in contact interactions between e^- & nuclei in A vs. A'

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



Outline

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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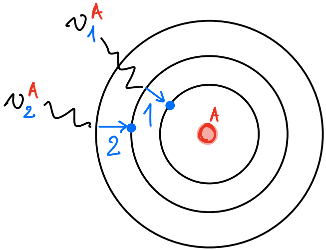

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$\Rightarrow$ Measure isotope shifts for 2 transitions

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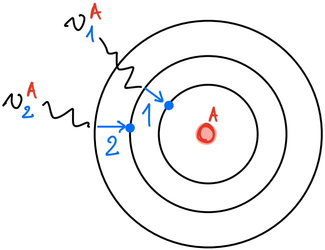

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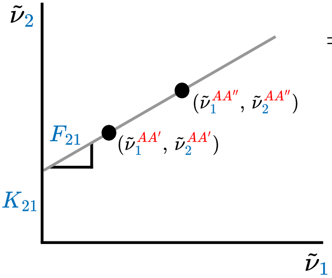
$\Rightarrow$ Eliminate charge radius variance $\delta\langle r^2\rangle^{AA'}$

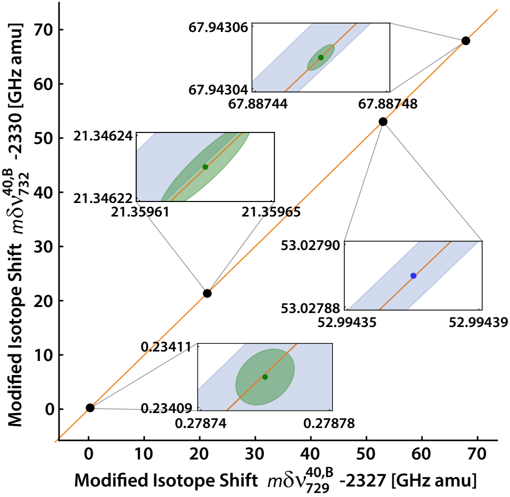
$$\tilde{\nu}_2^{AA'} = K_{21} + F_{21}\tilde{\nu}_1^{AA'}$$

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

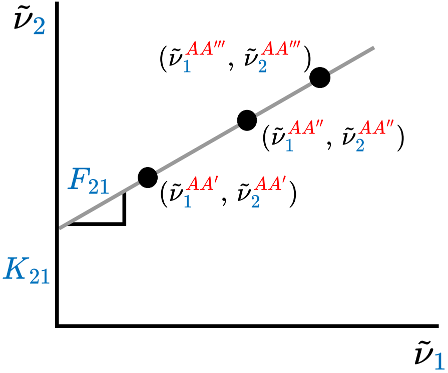
$F_{21} \equiv F_2/F_1$ $K_{21} \equiv K_2 - F_{21}K_1$ $\Rightarrow$ fit



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



The King-Plot: Fit to Isotope Shift Data



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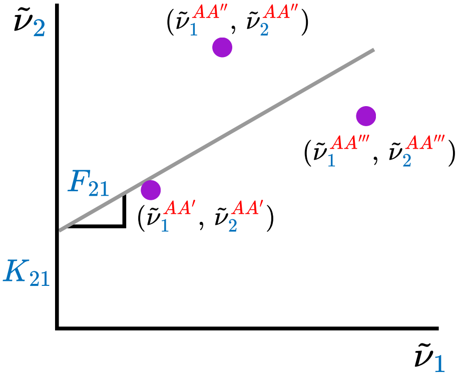

$$\tilde{\nu}_2^{AA'} = K_{21} + F_{21}\tilde{\nu}_1^{AA'} + ?$$
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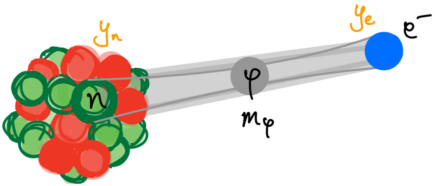
Outline

Dark Portals

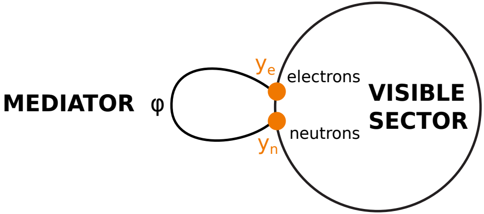


Question that can be addressed by King plot analyses:

Given a mediator mass m_φ in the **eV-GeV** range, ...

...how large can the coupling $y_e y_n$ be?

Dark Portals and Isotope Shift Measurements



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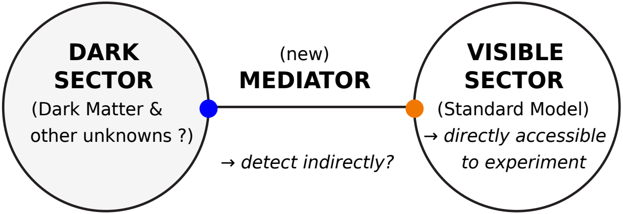

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King-Plot Bounds on New Bosons [arXiv:1704.05068,2005.06144]

Use King-Plots to search for new physics PRD 96, 093001 (2017)

DESY 17-055, FERMILAB-PUB-17-077-T, LAPTh-009/17, MIT-CTP-4898

Probing new light force-mediators by isotope shift spectroscopy

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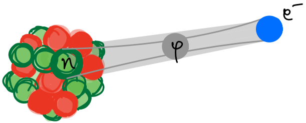

New effective Yukawa-potential

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

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

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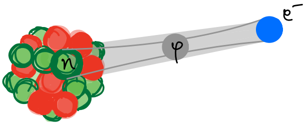

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Induces new term in the King-relation:

$$\tilde{\nu}_2^{AA'} = K_{21}\tilde{\mu}^{AA'} + F_{21}\tilde{\nu}_1^{AA'} + \alpha_{\text{NP}} X_{21}\tilde{\gamma}^{AA'}$$

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

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

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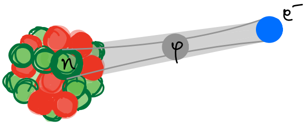

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$X_{21} = X_2 - F_{21}X_1$: NP electronic coefficient

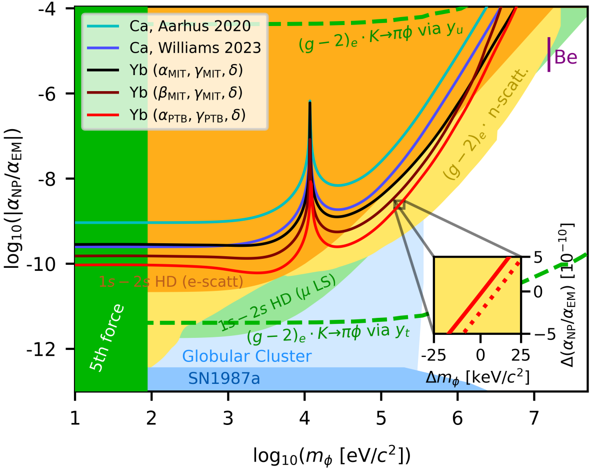
$\tilde{\gamma}^{AA'} \equiv (A - A')/\mu^{AA'}$: NP nucl. coeff.

⇒ Extract α_{NP} from fraction of volumes spanned by frequency vectors:

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

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

New Spectroscopy Bounds on New Physics [2403.07792]



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

Outline

Isotope Shifts

King Plots

Sensitivity To New Physics

`kifit`

Outlook & Conclusions

`kifit`: (Global) King Plot Fit

Idea:

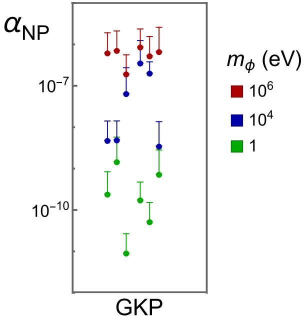
- Define consistent way of combining isotope shift measurements:

  Which is the "right" upper bound?

- Starting from fit of [arXiv:1602.04822], develop a King plot fit that can handle new isotope shift data

⇒ **Combine elements, perform a global fit to isotope shift data**

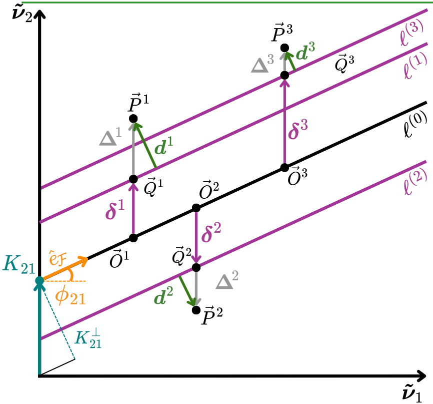
See also [arXiv:1602.04822]



2σ *Ca bounds on* α_{NP}

[arXiv:1906.04105, PRL 115, 053003 (2015), AME 2020 (CPC 45 030003 (2021))]

kifit: Construction of the Loglikelihood Function



$\vec{P}^a \equiv (\tilde{\nu}_1^a, \tilde{\nu}_2^a)\,,\ a = 1, \ldots, n$: Data pts

$\ell^{(0)}$: King line without NP (linear fit)

$K_{21}^{\perp}$, ϕ_{21}: Fit parameters

$\boldsymbol{\delta}^a$: Predicted NP shift in $\tilde{\nu}_2^a$

$\ell^{(a)}$: Pred. King line for isotope pair a

$\|\boldsymbol{d}^a\|$: Distance of $\vec{P}^a$ from $\ell^{(a)}$

$\Sigma^{ab} = \mathrm{cov}(\|\boldsymbol{d}^a\|, \|\boldsymbol{d}^b\|)$

$$\Rightarrow -\log\mathcal{L} \propto \frac{1}{2}\sum_{a=1}^{n}\sum_{b=1}^{n}\left[\log\Sigma^{ab} + \|\boldsymbol{d}^a\|\left(\Sigma_{\boldsymbol{d}}^{ab}\right)^{-1}\|\boldsymbol{d}^b\|\right]$$

$\Rightarrow$ Minimise $-\log\mathcal{L}$ to find preferred window for NP coupling α_{NP}

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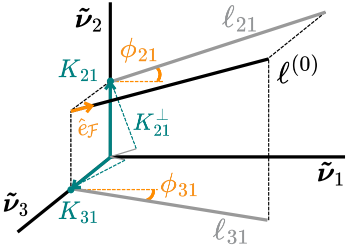

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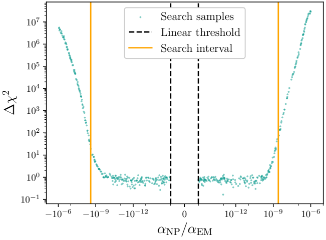
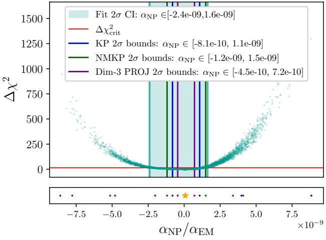
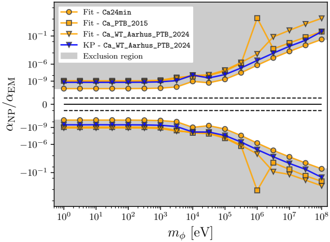
`kifit`: From the Search Grid to the Exclusion Plot



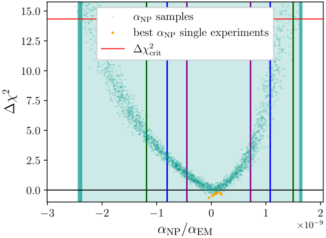
1. Search Phase



2. Experiment Phase

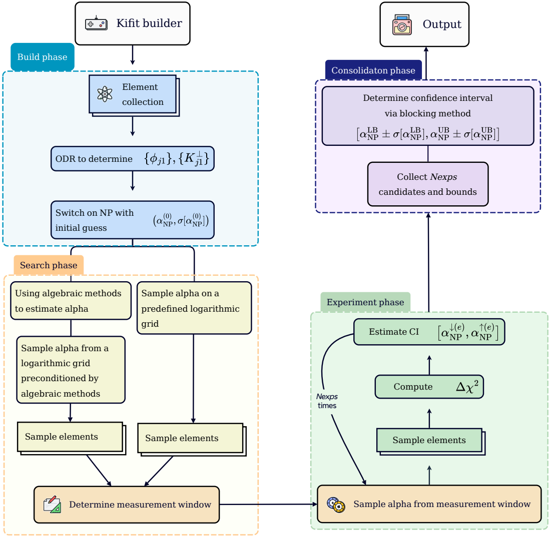


4. Scan over m_ϕ Values

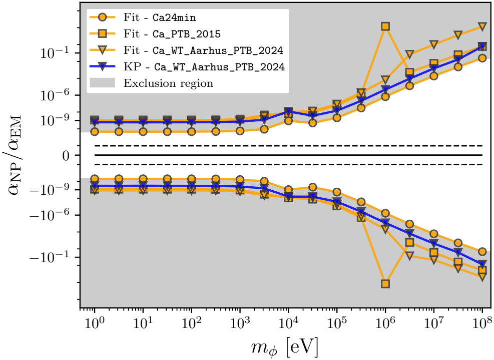


3. Experiment Phase (Zoom)

kifit Algorithm



`kifit` vs. Algebraic Methods



`Ca24min`, `Ca_PTB_2015`:
Minimal data sets
(2 transitions, 3 isotope pairs)

`Ca_WT_Aarhus_PTB_2024`=
=`Ca24min`+`Ca_PTB_2015`:
(4 transitions, 3 isotope pairs)

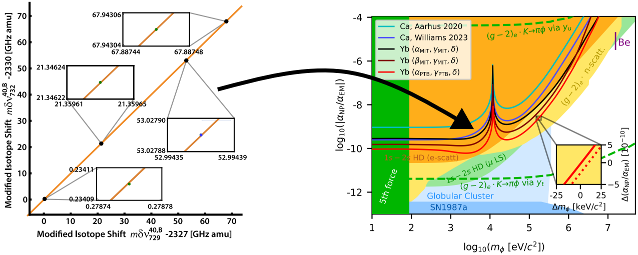
Algebraic bound shown here:
KP(`Ca_WT_Aarhus_PTB_2024`)=
=KP(`Ca24min`)

Sizeable difference between fit & algebraic results for minimal data sets, better agreement for larger data sets.

Outline

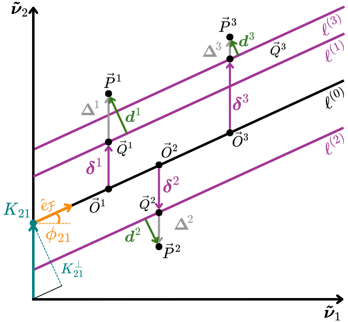
Conclusions

- Initial idea: King plots have a "tradition" of being linear
  $\Rightarrow$ Use them to set bounds on NP



Conclusions

- Initial idea: King plots have a “tradition” of being linear
  ⇒ Use them to set bounds on NP
- `kifit`: 1st step towards a global overview of isotope shift data
  - ⇒ Combine isotope shift data from different elements
  - ⇒ Tool to search for new bosons mediating between neutrons & electrons



Conclusions

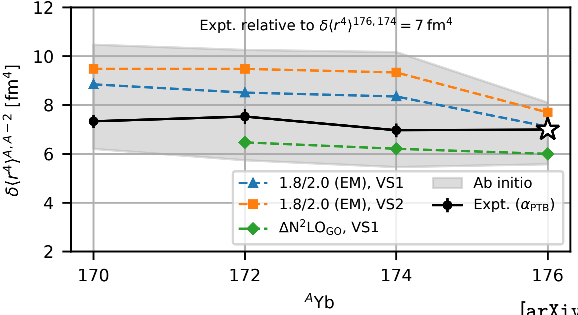
- Initial idea: King plots have a "tradition" of being linear
  ⇒ Use them to set bounds on NP
- `kifit`: 1st step towards a global overview of isotope shift data
  - ⇒ Combine isotope shift data from different elements
  - ⇒ Tool to search for new bosons mediating between neutrons & electrons
- Generalise framework to account for NLO nuclear effects?
  - ⇒ Decomposition of nonlinearities?
  - ⇒ Tool to test nuclear physics models?

Outlook

Dialog between theory and experiment is needed:

- Worth measuring transitions in metastable isotopes?
- Complementary experimental input?
- Predictions/ power counting for nuclear effects?

Use isotope shift data to gain information about the nucleus:



[arXiv:2403.07792]

Towards a Global Search for New Physics with Isotope Shifts
arXiv:2506.07303

kifit: https://github.com/QTI-TH/kifit

Ytterbium King Plot

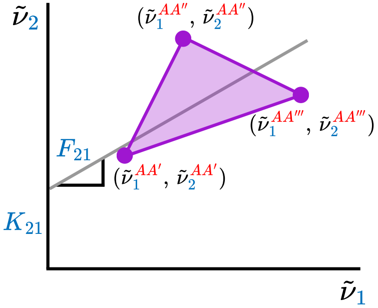
Phys.Rev.Lett. 134 (2025) 6, 063002 arXiv:2403.07792

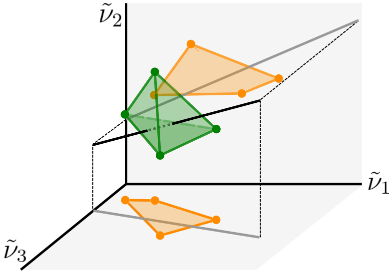
Thank you for your attention.

Backup slides

King-Plot Method in Presence of Nuclear Effects: The Generalised King Plot

[arXiv:2005.06144]





⇒ Test King linearity

⇒ Account for one King nonlinearity

⇒ Put bound on 2^{nd} nonlinearity

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

α_{NP} from Determinants

(No-Mass King-Plot:)

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

Choose your King-Plot

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

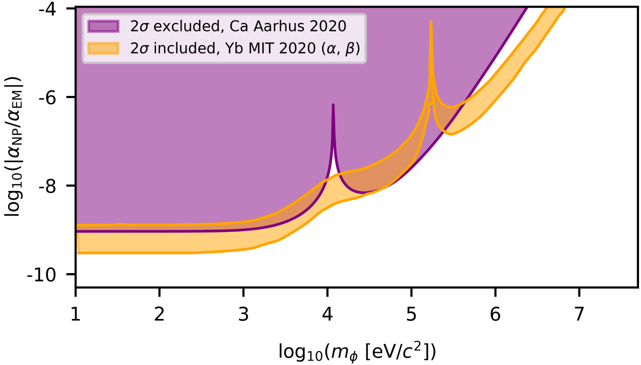
Type of King-Plot	Isotope-Pairs	Transitions	
Generalised King-Plot:	n	$n-1$	[PRR 2, 043444 (2020)]
No-Mass King-Plot:	n	n	[PRR 2, 043444 (2020)]

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

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

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

Upper Bounds on $|\alpha_{\rm NP}|$ 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 NP Yukawa potential and electronic wavefunction

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

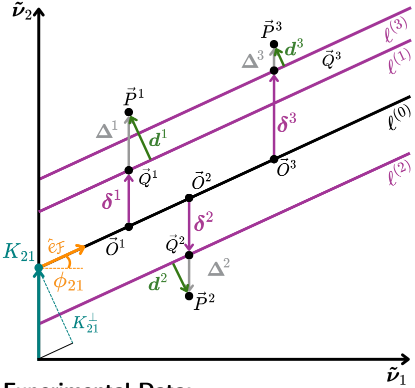
$|\psi(r)|^2$: electron density in absence of new physics,

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 Yukawa potential.
- For tight bounds on α_{NP}, one X_i needs to be large.

kifit Construction



Experimental Data:

$\vec{P}^a \equiv (\tilde{\nu}_1^a, \tilde{\nu}_2^a)$, $a = 1, \ldots, n$: Data pts.

Linear Fit to Data:

$\ell^{(0)}$: King line w/o NP $\Leftrightarrow$ $(K_{21}^{\perp}, \phi_{21})$

$$\hat{\boldsymbol{e}}_{\boldsymbol{F}} \equiv \frac{\boldsymbol{\mathcal{F}}}{\|\boldsymbol{\mathcal{F}}\|}, \quad \boldsymbol{\mathcal{F}} \equiv (1, \tan\phi_{21}, \ldots, \tan\phi_{m1})^{\top}$$

$$\boldsymbol{\mathcal{K}} \equiv (0, K_{21}, \ldots, K_{m1})^{\top}$$

Prediction:

$$\vec{Q}^a = \boldsymbol{\mathcal{K}}' + \tilde{\nu}_1^a \boldsymbol{\mathcal{F}} + \boldsymbol{\sigma}[\boldsymbol{\delta^a}], \quad a = 1, \ldots, n.$$

$$\boldsymbol{\mathcal{K}}' = \boldsymbol{\mathcal{K}} + \langle\tilde{\gamma}\rangle$$

$$\sigma[\delta_j^a] = \frac{\alpha_{\rm NP}}{\alpha_{\rm EM}} \left(\tilde{\gamma}^a - \langle\tilde{\gamma}\rangle^j\right) X_{j1}$$

$$\langle\tilde{\gamma}\rangle^j = \frac{\sum_{a=1}^n \tilde{\gamma}^a \sigma[\tilde{\nu}_j^a]}{\sum_{b=1}^n \sigma[\tilde{\nu}_j^b]}, \quad j = 2, \ldots, m$$

$\boldsymbol{\delta^a}$: Predicted NP shift in $\tilde{\nu}_2^a$

$\ell^{(a)}$: Predicted King line for isotope pair a

Log-likelihood Construction:

$$\boldsymbol{\Delta}^a \equiv \vec{P}^a - \vec{Q}^a = \tilde{\boldsymbol{\nu}}^a - \left(\boldsymbol{\mathcal{K}}' + \tilde{\nu}_1^a \boldsymbol{\mathcal{F}} + \boldsymbol{\sigma}[\boldsymbol{\delta^a}]\right)$$

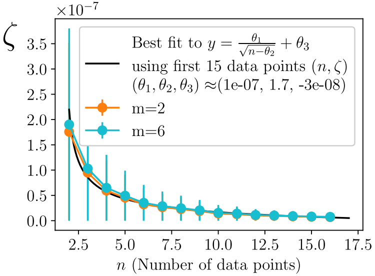
$$\boldsymbol{d}^a = \boldsymbol{\Delta}^a - (\boldsymbol{\Delta}^a \cdot \hat{\boldsymbol{e}}_{\boldsymbol{F}})\, \hat{\boldsymbol{e}}_{\boldsymbol{F}}, \quad a = 1, \ldots, n.$$

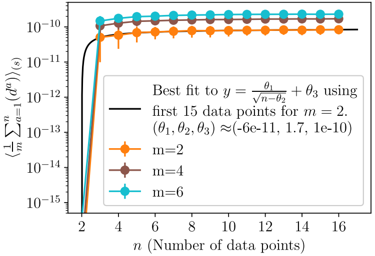
$\|\boldsymbol{d}^a\|$: Distance of $\vec{P}^a$ from $\ell^{(a)}$

$$-\log\mathcal{L} \propto \frac{1}{2} \sum_{a,b=1}^{n} \left[\log\Sigma^{ab} + \|\boldsymbol{d}^a\| \left(\Sigma_{\boldsymbol{d}}^{ab}\right)^{-1} \|\boldsymbol{d}^b\|\right]$$

$$\Sigma^{ab} = \mathrm{cov}(\|\boldsymbol{d}^a\|, \|\boldsymbol{d}^b\|)$$

The Issue with Small Sample Sizes





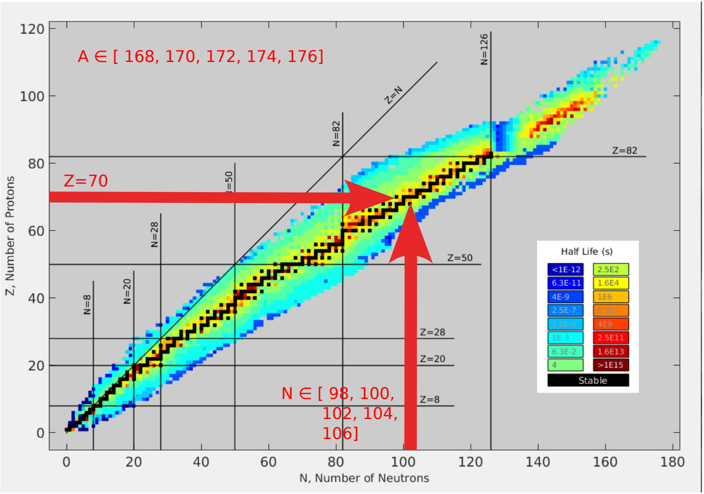
Goodness of a fit to $f(x) = ax + b$ as a function of the number n of data points (x, y):
$\forall n$, 500 mock data sets with Gaussian uncertainties $\sigma_{\text{meas}} = \sigma_{\text{pos}} = 10^{-10}$
$\Rightarrow \sigma_x/x,\ \sigma_y/y \sim \mathcal{O}(10^{-10})$

Top: Average rel. uncertainty on the $2(n-1)$ fit parameters $\{a^i, b^i\}_{i=2}^{n}$ used to fix the line in n-dim. space.

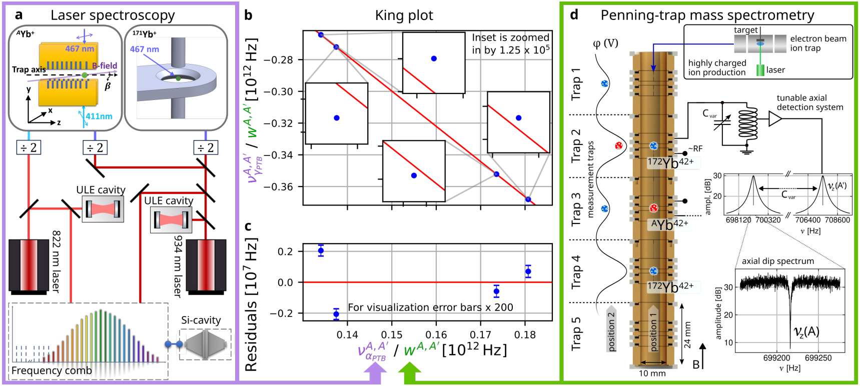
$$\zeta = \left\langle \sqrt{\sum_{j=2}^{m} \left(\frac{(m_j^{(s)} - m_j)^2}{m_j^2} + \frac{(c_j^{(s)} - c_j)^2}{c_j^2} \right)} \right\rangle_{(s)}$$

Bottom: Avg. distance of the data points from best fit line: $\left\langle \frac{1}{m} \sum_{a=1}^{n} (d^a) \right\rangle_{(s)}$

Ytterbium and its Stable Isotopes



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

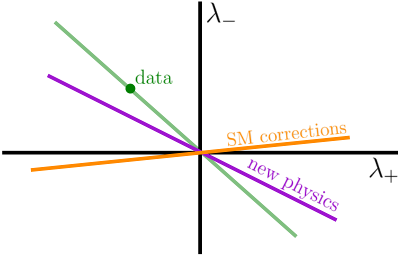


Frequencies: $\frac{\delta\nu}{\nu} \sim \mathcal{O}(10^{-9})$ Mass ratios $\eta_A = \frac{m_A}{m_{172}}$: $\frac{\delta\eta}{\eta} \sim \mathcal{O}(10^{-12})$

$\Rightarrow$ Hz-precision for isotope shifts

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

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 $\Lambda_\pm \perp (\tilde{\boldsymbol{\nu}}_1, \mathbf{1})$:

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

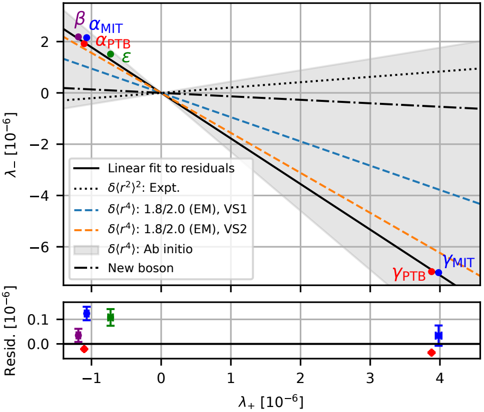
In presence of just one nonlinearity,

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

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

[arXiv:2004.11383, arXiv:2201.03578]

The Nonlinearity Decomposition Plot



Notation	Transition	Refs.
$\alpha_{\rm MIT,PTB}$	${}^2S_{1/2} \to {}^2D_{5/2}$ E2 in Yb^+	MIT, t.w.
β	${}^2S_{1/2} \to {}^2D_{3/2}$ E2 in Yb^+	MIT
$\gamma_{\rm MIT,PTB}$	${}^2S_{1/2} \to {}^2F_{7/2}$ 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: $\frac{\lambda_-^{(\tau)}}{\lambda_+^{(\tau)}} = \frac{G_\tau^{(4)}\boldsymbol{\delta\langle r^4\rangle_-}}{G_\tau^{(4)}\boldsymbol{\delta\langle r^4\rangle_+}} = \frac{\boldsymbol{\delta\langle r^4\rangle_-}}{\boldsymbol{\delta\langle r^4\rangle_+}} \equiv \frac{\lambda_-}{\lambda_+} \Rightarrow$ transition-universal

Extracting Nuclear Physics from Isotope-Shifts

- **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?

Extracting Nuclear Physics from Isotope-Shifts

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$\Rightarrow$ **"Put the King plot on it's head.":** Experimental data (under control)

- **King Plot** (in transition space): Eliminate charge radius variance $\delta\langle r^2\rangle^{AA'}$

$$
\begin{aligned}
\nu_i^{AA'} &= F_i \delta\langle r^2\rangle^{AA'} && + K_i \mu^{AA'} && + \boldsymbol{G_i^{(4)}} \delta\langle r^4\rangle^{AA'} \\
\nu_1^{AA'} &= F_1 \delta\langle r^2\rangle^{AA'} && + K_1 \mu^{AA'} && + \boldsymbol{G_1^{(4)}} \delta\langle r^4\rangle^{AA'} \\
\hline
\Rightarrow \nu_i^{AA'}/\mu^{AA'} &= F_{i1} \nu_1^{AA'}/\mu^{AA'} && + K_{i1} && + \boldsymbol{G_{i1}^{(4)}} \delta\langle r^4\rangle^{AA'}/\mu^{AA'}
\end{aligned}
$$

$\Rightarrow$ Fit F_{i1}, K_{i1}, $\boldsymbol{G_{i1}^{(4)} = G_i^{(4)} - F_{i1} G_1^{(4)}}$ (double-index electronic coeff.): AMBiT
Accuracy severely limited due to strong many-body correlations, both $G^{(4)}, F$ dep. on nucl. size & shape $\Rightarrow$ Large cancellations in $G_{i1}^{(4)}$ $\Rightarrow$ Large errors on $G_{i1}^{(4)}$

Extracting Nuclear Physics from Isotope-Shifts

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\hline
\Rightarrow \nu_i^{AA'}/\mu^{AA'} &= F_{i1}\nu_1^{AA'}/\mu^{AA'} && + K_{i1} && + \boldsymbol{G_{i1}^{(4)}}\delta\langle \boldsymbol{r}^4\rangle^{AA'}/\mu^{AA'}
\end{aligned}
$$

$\Rightarrow$ Fit F_{i1}, K_{i1}, $\boldsymbol{G_{i1}^{(4)} = G_i^{(4)} - F_{i1}G_1^{(4)}}$ (double-index electronic coeff.): AMBiT

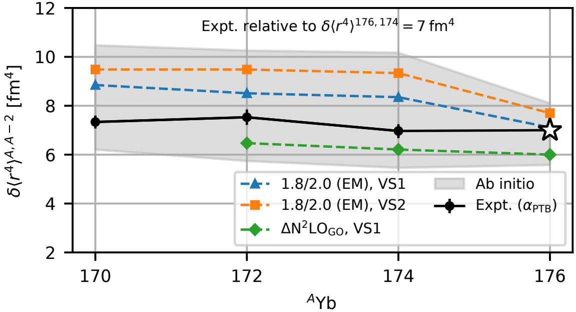
- **$\boldsymbol{\delta\langle r^4\rangle}$-Extraction** (in isotope pair space): Eliminate mass shift coeff. K_i

$$
\begin{aligned}
\nu_i^{AA'} &= F_i\delta\langle r^2\rangle^{AA'} + K_i\mu^{AA'} + \boldsymbol{G_i^{(4)}}\delta\langle \boldsymbol{r}^4\rangle^{AA'} \\
\nu_i^{RR'} &= F_i\delta\langle r^2\rangle^{RR'} + K_i\mu^{RR'} + \boldsymbol{G_i^{(4)}}\delta\langle \boldsymbol{r}^4\rangle^{RR'} \\
\hline
\nu_i^{AA'} - \frac{\mu^{AA'}}{\mu^{RR'}}\nu_1^{AA'} &= F_i\left(\delta\langle r^2\rangle^{AA'} - \frac{\mu^{AA'}}{\mu^{RR'}}\delta\langle r^2\rangle^{AA'}\right) + \boldsymbol{G_i^{(4)}}\underbrace{\left(\delta\langle \boldsymbol{r}^4\rangle^{AA'} - \frac{\mu^{AA'}}{\mu^{RR'}}\delta\langle \boldsymbol{r}^4\rangle^{RR'}\right)}_{\boldsymbol{Q^{AA'RR'}}}
\end{aligned}
$$

$\Rightarrow$ Fit F_i, $\delta\langle r^2\rangle^{AA'}$: [Angeli, Marinova], $\boldsymbol{G_i^{(4)}}$: AMBiT

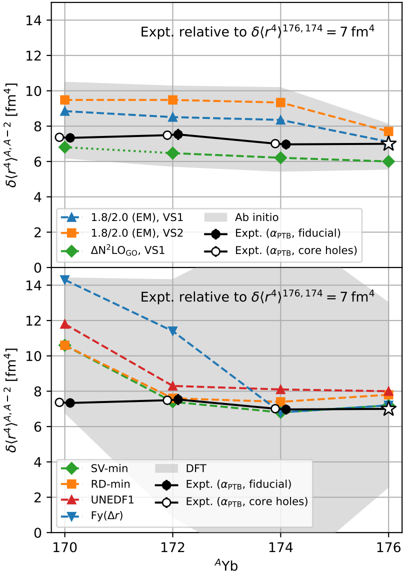
Extracting Nuclear Physics from Isotope-Shifts

- **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 $\star$

$\delta\langle r^4\rangle$ 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