Isotope shift of atomic levels and search for the “New Physics”

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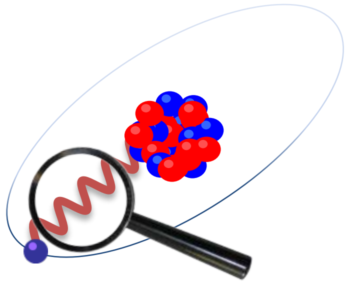
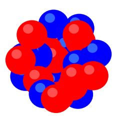
Isotope shift: Basic ideas



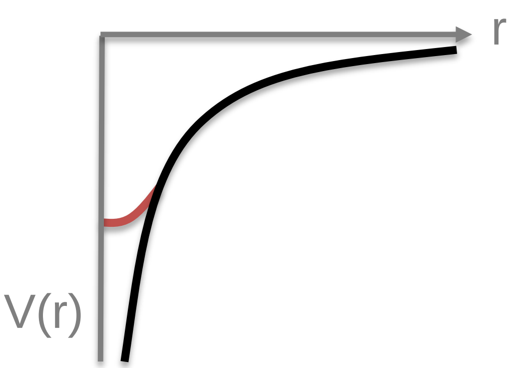
Is the electron-nucleus interaction just an interaction of two point-like charges, one of which (nucleus) is infinitely heavy?

$$V(r) = -\frac{Ze^2}{r}$$

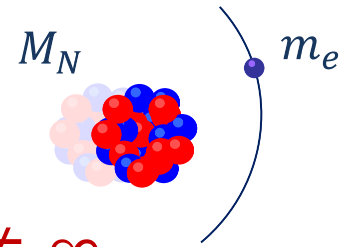
Field shift
due to non-zero charge radii



$$\langle r^2 \rangle \neq 0$$



Mass shift
due to finite nuclear mass



$$M_N \neq \infty$$

Both corrections lead to shift of energy levels. How to estimate this shift?

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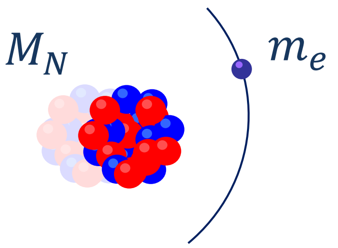
Nuclear recoil correction

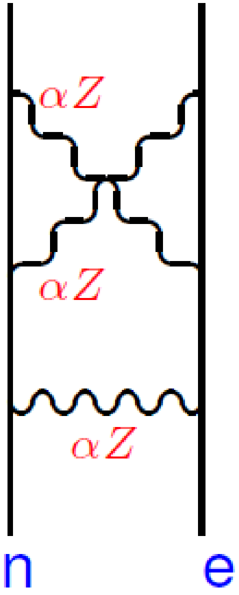
Mass shift
due to finite nuclear mass



Mass shift has been discussed already in non-relativistic quantum mechanics.

In the non-relativistic approach, for single-electron ions, we have just to introduce the reduced mass:

$$m_e \rightarrow \frac{m_e M_N}{m_e + M_N}$$



Accurate relativistic treatment for the hydrogen-like ions gives us:

$$\Delta E_1 \cong \frac{m_e}{M_N} m_e c^2 \left\{ \frac{(\alpha Z)^2}{2n^2} + \frac{(\alpha Z)^4}{2n^3} \left(\frac{1}{j + 1/2} - \frac{1}{n} \right) + \cdots \right\}$$

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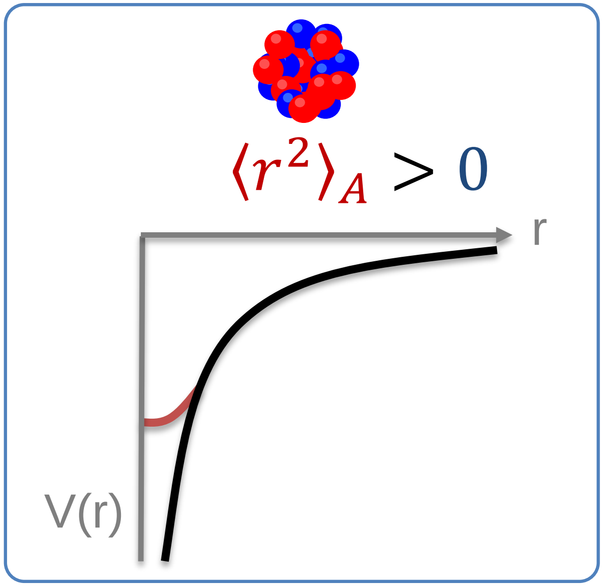
Finite nuclear size: Non-relativistic treatment

We assume that nuclear charge is uniformly distributed within a sphere of radius:

$$R = r_0\, A^{1/3}$$



Electrostatic potential due to the nucleus deviates from pure Coulomb one and is given by:

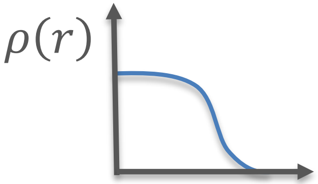
$$V(r) = \begin{cases} \dfrac{Ze^2}{2R}\left(\dfrac{r^2}{R^2} - 3\right), & r \le R \\ -\dfrac{Ze^2}{r}, & r > R \end{cases}$$

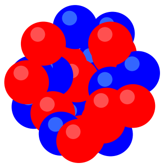
We just need to plug it in Schrödinger equation

First-order energy shift in the non-relativistic approach:

$$\Delta E \approx \langle \psi_{nlm_l} | V' | \psi_{nlm_l} \rangle \propto \frac{Z^4 R^2}{n^3}$$

Finite nuclear size effect





The potential induced by the nuclear charge distribution $\rho(r)$ is defined as:

$$V_N(\boldsymbol{r}) = 4\pi\alpha Z \int_0^\infty dr' r'^2 \rho(r') \frac{1}{r_>} \qquad r_> = \mathrm{Max}\{r, r'\}$$

And can be plugged in the Dirac equation

$$\left(-i\hbar c\boldsymbol{\alpha}\cdot\widehat{\boldsymbol{\nabla}} + V(\boldsymbol{r}) + m_e c^2 \beta\right)\psi(\boldsymbol{r}) = E\,\psi(\boldsymbol{r})$$

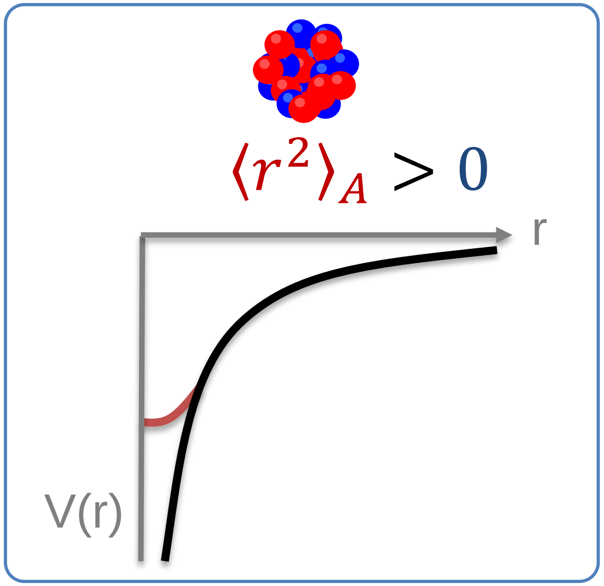
Solution of the Dirac equation is most conveniently written in the bi-spinor form:

$$\psi_{nj\mu_j}(r) = \frac{1}{r}\begin{pmatrix} g_{nj}(r)\,\Omega_{lj\mu_j}(\hat{\boldsymbol{r}}) \\ i\,f_{nj}(r)\,\Omega_{l'j\mu_j}(\hat{\boldsymbol{r}}) \end{pmatrix}$$

We can re-write Dirac equation for the radial components!

Finite nuclear size: Relativistic treatment

Rather similar approach to the non-relativistic case. Again, we need to choose proper charge distribution and plug it in Dirac equation:



$$\left(\frac{df_{nj}(r)}{dr} - \frac{\kappa}{r} f_{nj}(r)\right) = -(E - V(r) - m_e c^2) g_{nj}(r)$$

$$\left(\frac{dg_{nj}(r)}{dr} + \frac{\kappa}{r} g_{nj}(r)\right) = (E - V(r) + m_e c^2) f_{nj}(r)$$

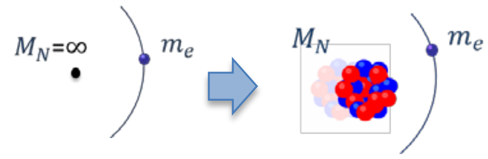
One can find the relativistic correction (Shabaev 1993)

$$\Delta E \approx \frac{(\alpha Z)^2}{10\, n} \left[1 + (\alpha Z)^2\, \phi_{nj}(\alpha Z)\right] \left(2\, \frac{\alpha Z}{n} \frac{R}{\hbar/mc}\right)^{2\gamma} m_e c^2$$

where $\gamma = \sqrt{1 - (\alpha Z)^2}$

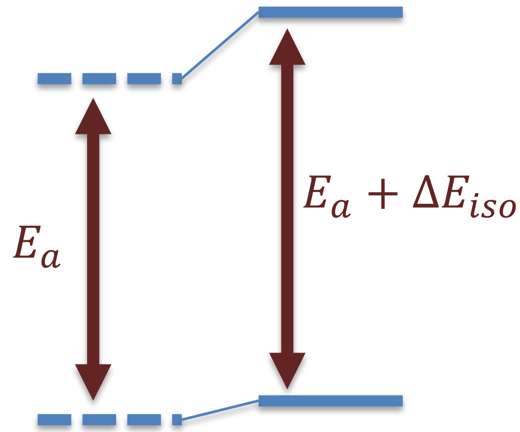
Isotope shift: Basic ideas

The isotope-dependent part of the transition energy can be conveniently represented as a sum of two terms:



$$\Delta E_{iso} = \frac{m_e}{M_N} K + \frac{R^2}{\lambda_C^2} F$$

Nuclear part   Atomic part



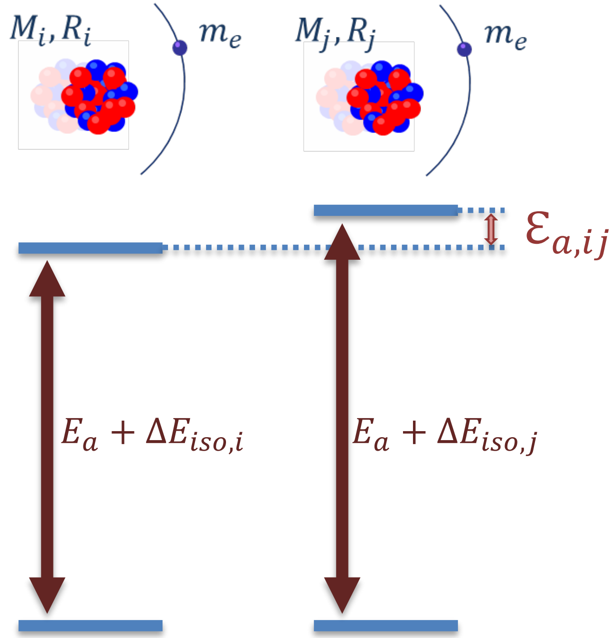
In our theory this expression is exact! That means that mass-shift K and field-shift F constants have (weak) dependence on nuclear parameters.

In real life, in contrast to theory, we can not make nucleus infinitely heavy and point like. Therefore, in order to “see” ΔE_{iso} we need to measure particular transition **for two isotopes**.

Isotope shift: Standard formulation

Within the standard formulation, K and F constants are assumed to depend only on the electronic transition but not on the isotope. In this case, the isotope shift of the transition energy a between the isotopes i and j is:

$$\mathcal{E}_{a,ij} = \underbrace{\left(\frac{m_e}{M_i} - \frac{m_e}{M_j}\right)}_{\mu_{ij}} K_a + \underbrace{\left(\frac{R_i^2}{\lambda_C^2} - \frac{R_j^2}{\lambda_C^2}\right)}_{\mathcal{R}_{ij}} F_a$$

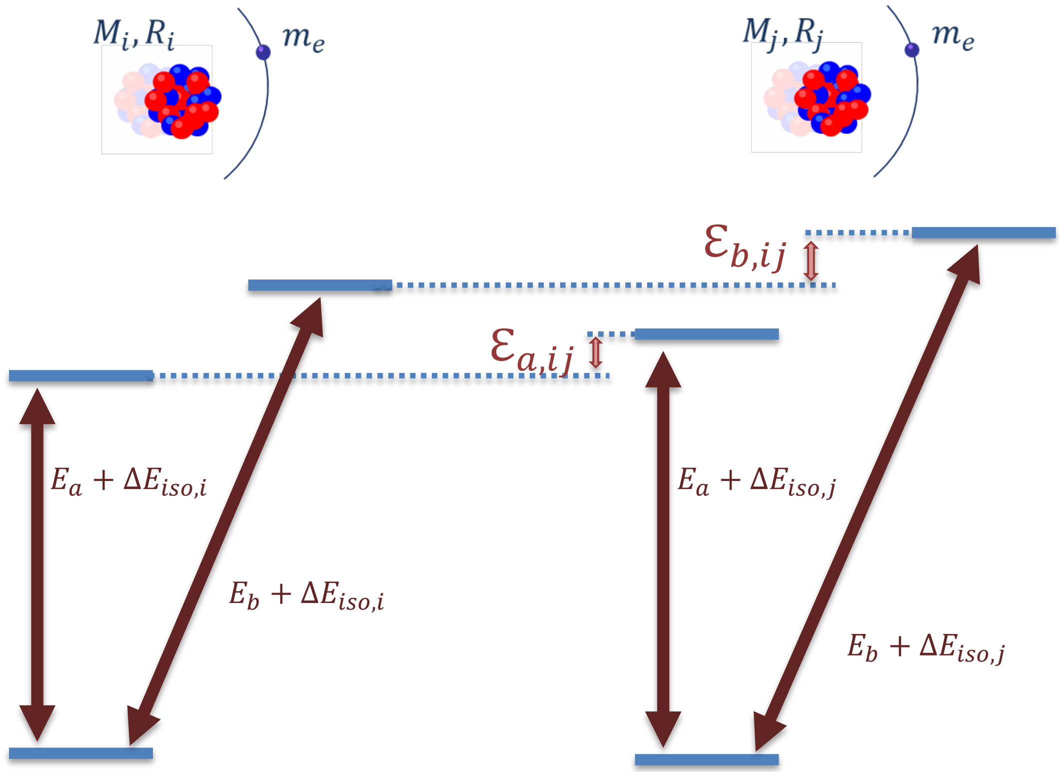


By introducing the modified energy $\epsilon_{a,ij} = \mathcal{E}_{a,ij}/\mu_{ij}$ we can finally obtain:

$$\epsilon_{a,ij} = K_a + \frac{\mathcal{R}_{ij}}{\mu_{ij}} F_a$$

We want to eliminate isotope-dependent constant

King's plot: Standard formulation



By considering two transitions (a and b) and two isotopes we can eliminate isotope-dependent constant:

$$
\begin{cases}
\epsilon_{a,ij} = K_a + \dfrac{\mathcal{R}_{ij}}{\mu_{ij}} F_a \\
\epsilon_{b,ij} = K_b + \dfrac{\mathcal{R}_{ij}}{\mu_{ij}} F_b
\end{cases}
$$

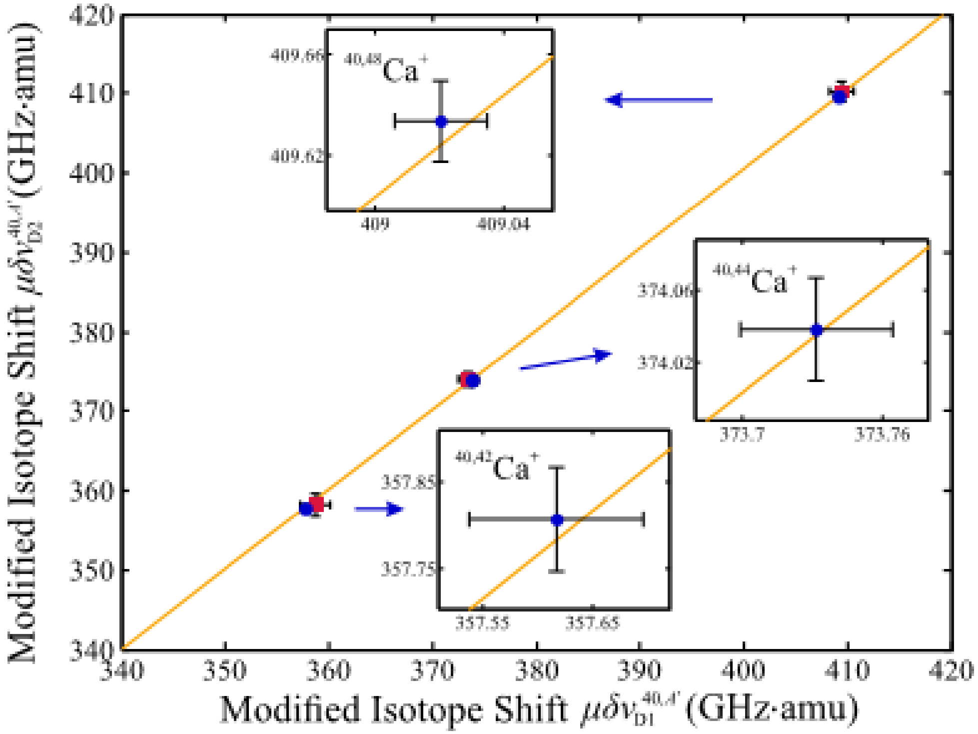
$$
\epsilon_{b,ij} = \left(K_b - \frac{F_b}{F_a} K_a \right) + \frac{F_b}{F_a} \epsilon_{a,ij}
$$

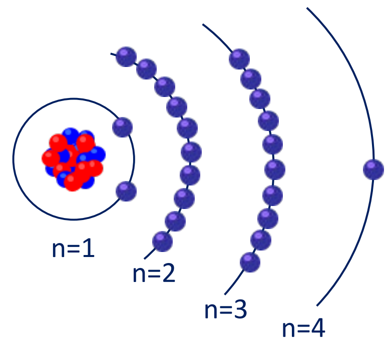
Fixing one of the isotopes (say, j) and plotting $\epsilon_{b,ij}$ $(= y_i)$ against $\epsilon_{a,ij}$ $(= x_i)$ for different isotopes i, one gets the linear dependence of the form $y_i = A + B x_i$

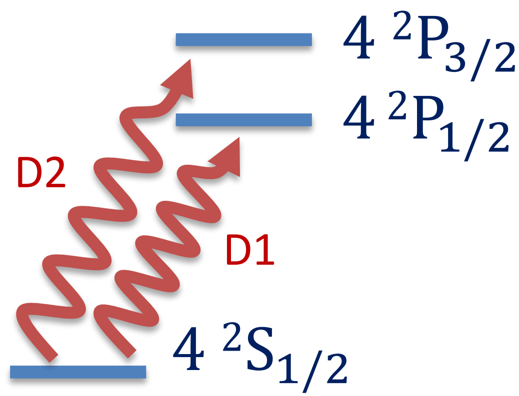
King's plot: Standard formulation

Recently, high-precision measurements have been performed in collaboration with TU Darmstadt to compare isotope shifts for the $S_{1/2} \rightarrow P_{1/2}$ and $S_{1/2} \rightarrow P_{3/2}$ transitions in Ca^+ ion.

Ca⁺ ion: symmetric Argon core + 1 electron







C. Shi *et al.*, Appl. Phys. B (2017) 123:2

Isotope shift: Ca^+ puzzle

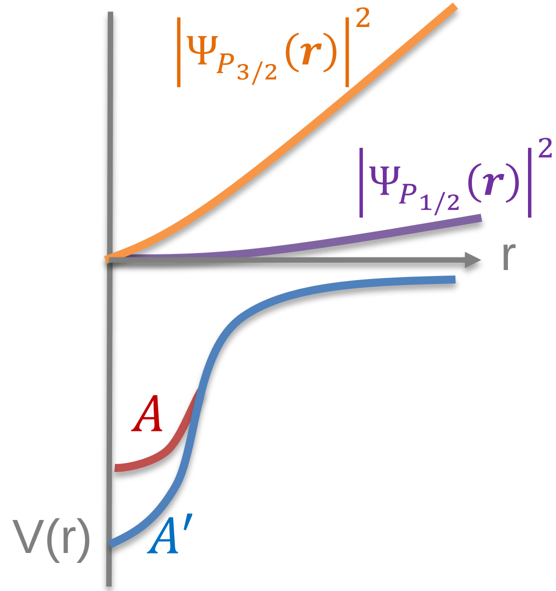
Recently, high-precision measurements have been performed at the QUEST institute to compare isotope shifts for the $S_{1/2} \rightarrow P_{1/2}$ and $S_{1/2} \rightarrow P_{3/2}$ transitions in Ca^+ ion.

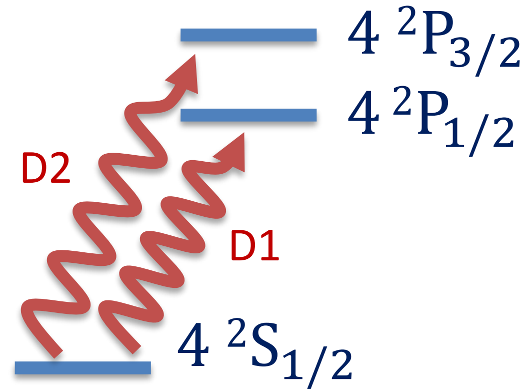
These transitions exhibit different behavior with respect to the field shift.

$$f = \frac{F_{D2}}{F_{D1}}$$

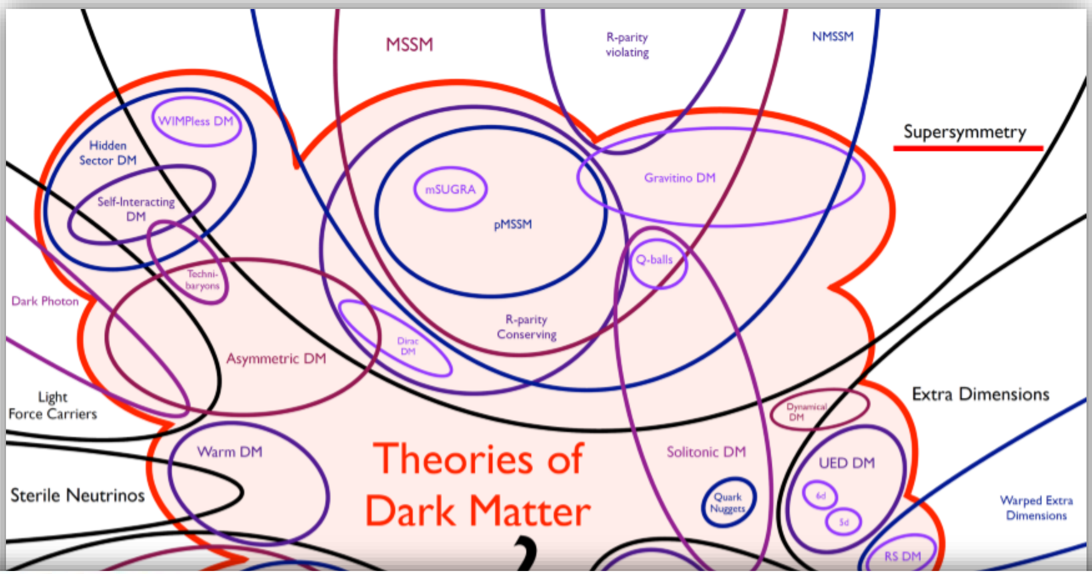
Theoretical model	f
Hydrogenic	1.0051
Dirac-Fock	1.0010
Dirac-Fock + Core Pol.	1.0009
CCSD	1.0029
CCSD(T)	1.0048
MBPT	1.0011
CI+MBPT	1.0014 (4)
Experimental value	1.0085 (12)

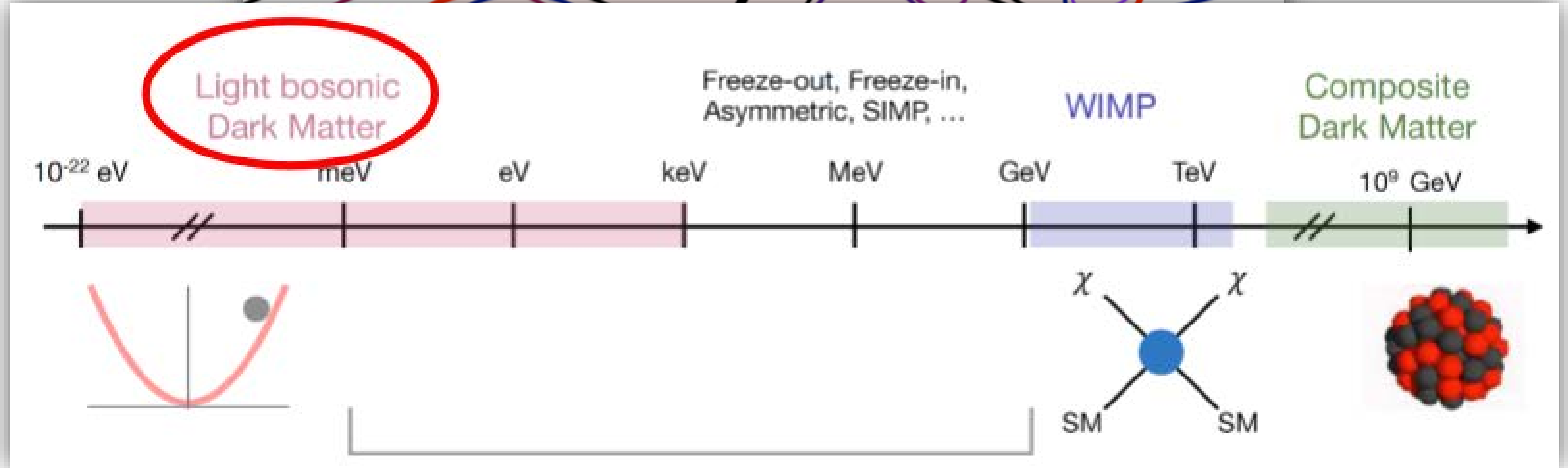
What is the reason for this big disagreement between experiment and theory? Many-electron or nuclear effects? QED?





Search for the "New Physics"





Isotope shift: New physics

We assume that interaction between nucleus and electrons is also mediated by hypothetical boson particle with mass m_ϕ:

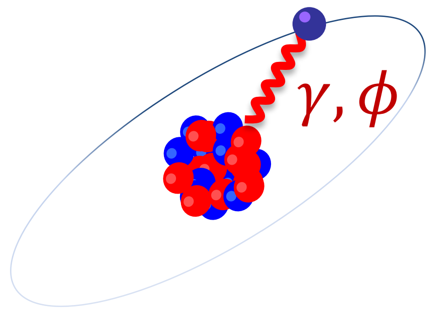
$$\hat{H} = \hat{H}_0 + \sum_i \alpha_{NP}\, A\, \frac{e^{-m_\phi r_i}}{r_i}$$

With a new particle, the isotope-dependent part of the transition energy becomes:

$$\Delta E_{iso} = \frac{m_e}{M_N} K + \frac{R^2}{\lambda_C^2} F + \frac{\alpha_{NP}}{\alpha} A\, X_\phi$$

where the "new-physics" isotope shift constant defined as:

$$X_\phi = \left\langle \Psi_{\rm atom} \middle| \sum_i \frac{\alpha\, e^{-m_\phi r_i}}{r_i} \middle| \Psi_{\rm atom} \right\rangle$$



Two parameters of hypothetical boson particle:

Mass m_ϕ

Coupling $\alpha_{NP} = g_n g_e$

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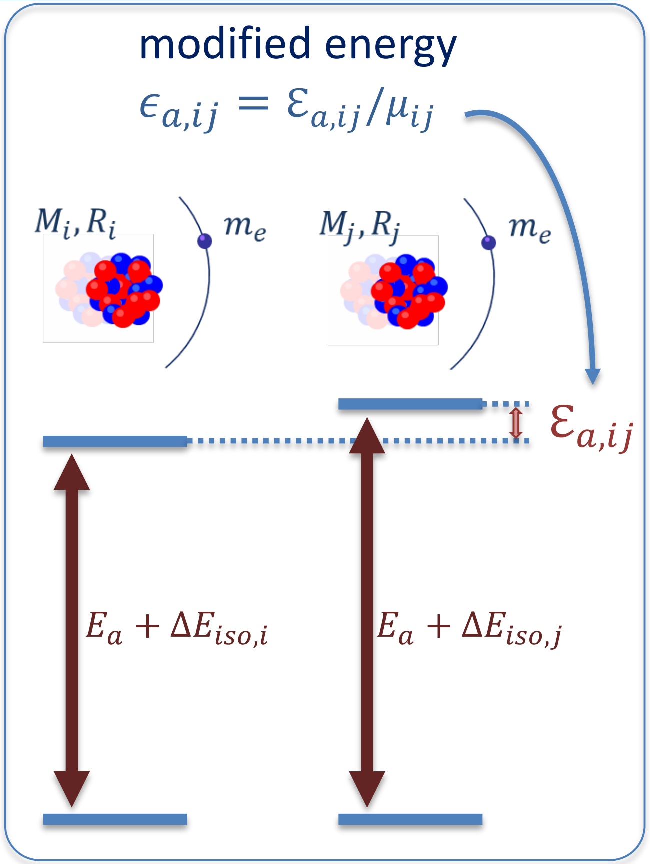
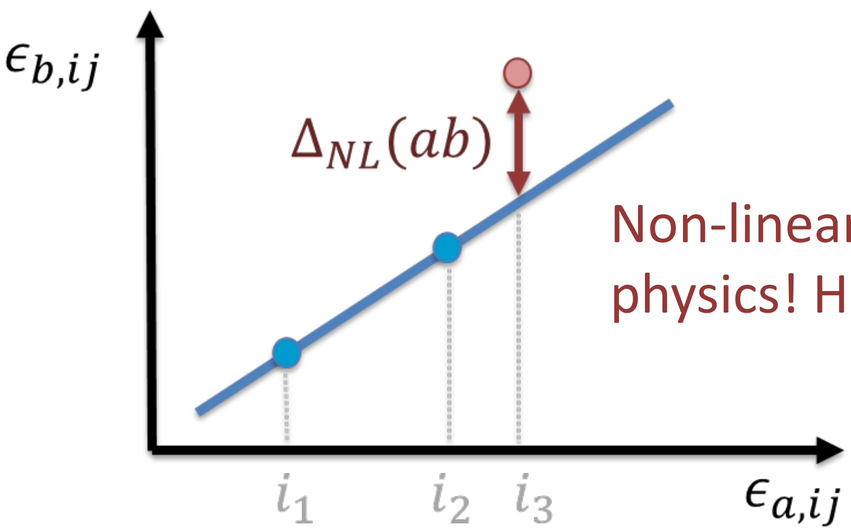
Isotope shift: New physics

An additional (hypothetical) interaction leads to the additional term in the modified energy:

$$\epsilon_{a,ij} = K_a + \frac{\mathcal{R}_{ij}}{\mu_{ij}} F_a + \frac{\alpha_{NP}}{\alpha} \frac{A_i - A_j}{\mu_{ij}} X_{\phi,a}$$

This „new physics“ term depends on the isotopes! This leads to the **violation of the linearity** of King‘s plot!





Non-linearity of King‘s plot can be the sign of new physics! How large are this non-linearity?

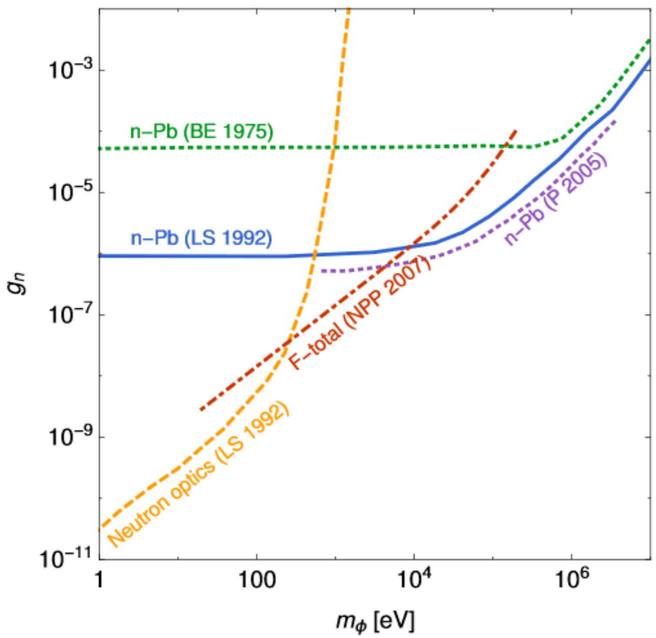
Isotope shift: New physics

The present isotope shift experiments allow measurements at the kHz level. Which parameters should have a “new physics” boson in order to be seen at this level of experimental accuracy?

TABLE III. Ratios of the “new-physics” coupling constant α_{NP} to the fine-structure constant α which would result in a non-linearity of King’s plot of 1 kHz, for different values of masses of the hypothetical boson m_ϕ.

	Transitions	$m_\phi = 10$ eV	$m_\phi = 10^2$ eV	$m_\phi = 10^3$ eV	$m_\phi = 10^4$ eV	$m_\phi = 10^5$ eV	$m_\phi = 10^6$ eV	$m_\phi = 10^7$ eV
α_{NP}/α	(a,b)	6×10^{-12}	6×10^{-12}	6×10^{-12}	7×10^{-12}	5×10^{-11}	1.2×10^{-8}	1.2×10^{-5}
	(b,c)	4×10^{-11}	4×10^{-11}	4×10^{-11}	4×10^{-11}	2.5×10^{-10}	2×10^{-8}	2×10^{-6}

V. A. Yerokhin, R. A. Müller, A. Surzhykov, P. Micke, and P. O. Schmidt, Phys. Rev. A 101, 012502 (2020)

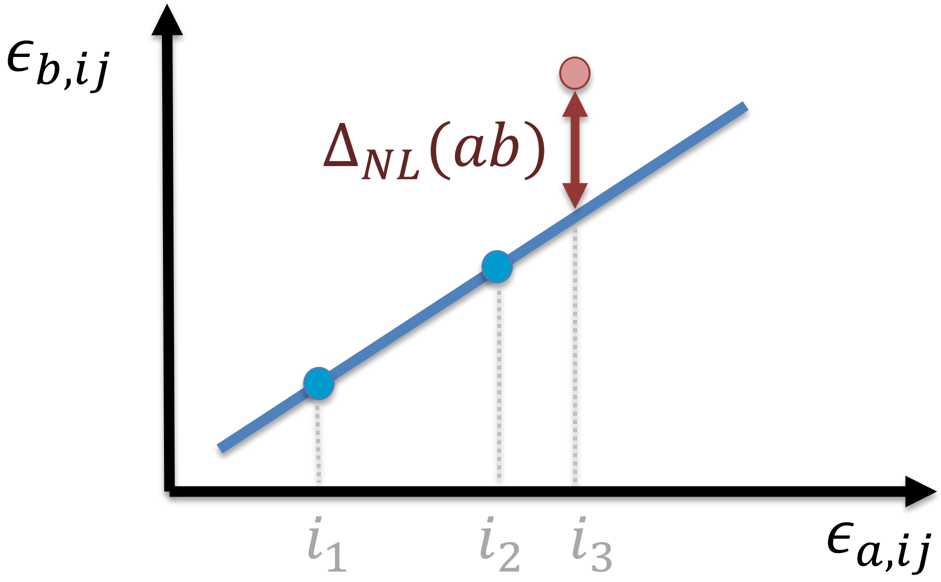


Various theories propose various parameters of a potential boson particle.

Various experimental studies place various bounds on these theories.

But wait… could be yet another reasons for the non-linearity of King‘s plot?

Non-linearity of King's plot: How to quantify?



The nonlinearity of a 3-point curve is defined as a shift of the ordinate of the third point from the straight line defined by the first two points:

$$\Delta_{NL}(ab) = \mu_{3j}\left[\epsilon_{b,3j} - \epsilon_{b,1j} - \frac{\epsilon_{b,2j} - \epsilon_{b,1j}}{\epsilon_{a,2j} - \epsilon_{a,1j}}\left(\epsilon_{a,3j} - \epsilon_{a,1j}\right)\right]$$

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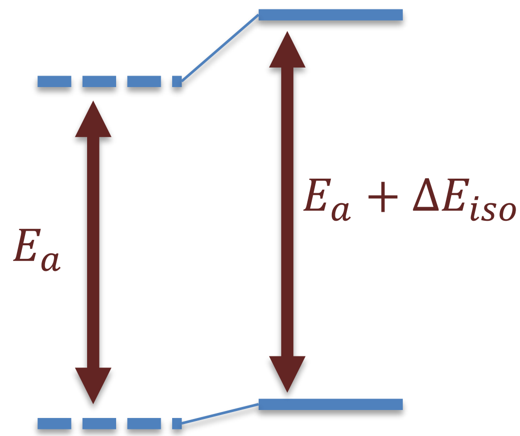
Isotope shift: Basic ideas

The isotope-dependent part of the transition energy can be conveniently represented as a sum of two terms:

$$\Delta E_{iso} = \frac{m_e}{M_N} K + \frac{R^2}{\lambda_C^2} F$$

Nuclear part   Atomic part



In our theory this expression is exact! That means that mass-shift K and field-shift F constants have (weak) dependence on nuclear parameters.

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King's plot: Extended formulation

Now comes important issues: what if mass- and field constants not only on the transition but also on the isotope:

$$K_{a,i} = K_a + \delta K_{a,i}$$

$$F_{a,i} = F_a + \delta F_{a,i}$$

What are the consequences for our theory?

The expressions for the modified energy reads: $\epsilon_{a,ij} = K_{a,ij} + \frac{\mathcal{R}_{ij}}{\mu_{ij}} F_{a,ij}$

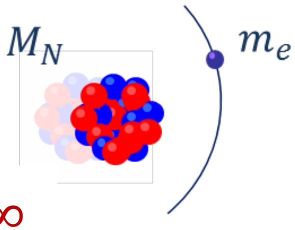
with $K_{a,ij} = K_a + \delta K_{a,ij}$ and $F_{a,ij} = F_a + \delta F_{a,ij}$

The relation between isotope shifts of two transitions is given now:

$$\epsilon_{b,ij} = \underbrace{\left(K_{b,ij} - \frac{F_{b,ij}}{F_{a,ij}} K_{a,ij} \right)}_{A = A_{ij}} + \underbrace{\frac{F_{b,ij}}{F_{a,ij}}}_{B = B_{ij}} \epsilon_{a,ij}$$

Since coefficients A and B depend now on isotope the King's plot is not anymore linear!

Theory of the isotope shift: Mass shift



The mass shift of energy levels is induced by the nuclear recoil effect. Within the Breit approximation the recoil effect is induced by the operator:

$$H_{rec} = \frac{m_e}{M_N}\left(\widetilde{H}_{rnms} + \widetilde{H}_{rsms}\right)$$

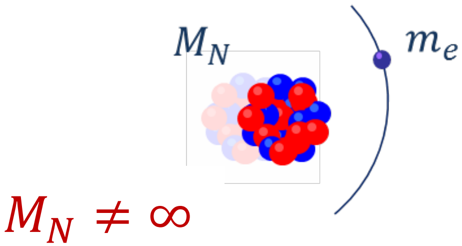
Here relativistic normal and specific mass shifts are given by:

$$\widetilde{H}_{\rm rnms} = \frac{1}{2}\sum_k \left[\boldsymbol{p}_k^2 - \frac{Z\alpha}{r_k}\left(\boldsymbol{\alpha}_k + \frac{(\boldsymbol{\alpha}_k \cdot \boldsymbol{r}_k)\,\boldsymbol{r}_k}{r_k^2}\right)\cdot \boldsymbol{p}_k\right]$$

$$\widetilde{H}_{\rm rsms} = \frac{1}{2}\sum_{k\neq l} \left[\boldsymbol{p}_k \cdot \boldsymbol{p}_l - \frac{Z\alpha}{r_k}\left(\boldsymbol{\alpha}_k + \frac{(\boldsymbol{\alpha}_k \cdot \boldsymbol{r}_k)\,\boldsymbol{r}_k}{r_k^2}\right)\cdot \boldsymbol{p}_l\right]$$

How to calculate energy shift due to these opearors? To apply perturbation theory!

Theory of the isotope shift: Mass shift



The mass shift of energy levels is induced by the nuclear recoil effect. Within the Breit approximation the recoil effect is induced by the operator:

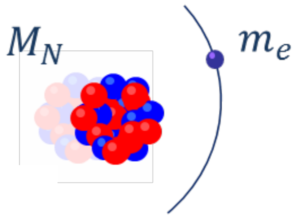
$$H_{rec} = \frac{m_e}{M_N}\left(\widetilde{H}_{rnms} + \widetilde{H}_{rsms}\right)$$

The leading, first-order, energy shift is given by the expectation value of the nuclear recoil operator on the atomic wave function of the reference state:

$$\Delta E_{rec} = \frac{m_e}{M_N} \underbrace{\left\langle \Psi_{\text{atom}} \middle| \widetilde{H}_{rnms} + \widetilde{H}_{rsms} \middle| \Psi_{\text{atom}} \right\rangle}_{K}$$

We did not obtain anything new. But! This is only first order perturbation!

Quadratic nuclear recoil effect



$M_N \neq \infty$

Within the Breit approximation, the quadratic mass shift is induced by the second-order perturbation of the operator H_{rec}. But… second-order calculations are rather complicated. We want to avoid them and make a trick.

First, we construct the nuclear-recoil-corrected wave function, by including the recoil operator into the Dirac Coulomb-Breit Hamiltonian and solving it.

$$(H_{DCB} + H_{rec})\Psi_N(\boldsymbol{r}) = E\,\Psi_N(\boldsymbol{r})$$

Second, we determine the leading isotope-dependent correction as:

$$\delta K_{rec} \equiv \frac{m_e}{M_N} K^{(2)} = \frac{1}{2}\left[\langle \widetilde{H}_{rnms} + \widetilde{H}_{rsms} \rangle_N - \langle \widetilde{H}_{rnms} + \widetilde{H}_{rsms} \rangle\right]$$

Where $\langle \ldots \rangle_N$ is calculated with the nuclear-recoil-corrected wave function.

Relativistic isotope shift constants for Ar ions

The quadratic nuclear recoil effect is the main source of non-linearity of King's plot for light atoms.

$$K_{a,i} = K_a + \frac{m_e}{M_N} K_a^{(2)}$$

TABLE I. Relativistic isotope-shift constants for Be-like, B-like, and C-like argon, in a.u.

Label	Transition	Ion	$K^{(1)}$	$K^{(2)}$	F
a	$(1s)^2 2s2p\ ^3P_2 - ^3P_1$	Ar^{14+}	−0.1072 (3) −0.107 [b] −0.1072 [c]	0.289 (3)	−0.000 326 (1) −0.000 3 [b] −0.000 33 [c]
b	$(1s)^2(2s)^2 2p\ ^2P_{3/2} - ^2P_{1/2}$	Ar^{13+}	−0.1900 (3) −0.1913 [a] −0.1908 [c]	−0.202 (35)	−0.001 43 (1) −0.001 4 (1) [a] −0.001 45 [c]
c	$(1s)^2(2s)^2(2p)^2\ ^3P_1 - ^3P_0$	Ar^{12+}	−0.0740 (16) −0.0735 [c]	0.310 (68)	−0.000 118 (5) −0.000 13 [c]

R. S. Orts, Z. Harman, J. R. C. López-Urrutia, A. N. Artemyev, H. Bruhns, A. J. G. Martínez, U. D. Jentschura, C. H. Keitel, A. Lapierre, V. Mironov, V. M. Shabaev, H. Tawara, I. I. Tupitsyn, J. Ullrich, and A. V. Volotka, Phys. Rev. Lett. **97**, 103002 (2006).

N. A. Zubova, A. V. Malyshev, I. I. Tupitsyn, V. M. Shabaev, Y. S. Kozhedub, G. Plunien, C. Brandau, and T. Stöhlker, Phys. Rev. A **93**, 052502 (2016).

C. Nazé, S. Verdebout, P. Rynkun, G. Gaigalas, M. Godefroid, and P. Jönsson, At. Dat. Nucl. Dat. Tabl. **100**, 1197 (2014).

$$\Delta_{NL}(ab) = 5 - 30\ kHz$$

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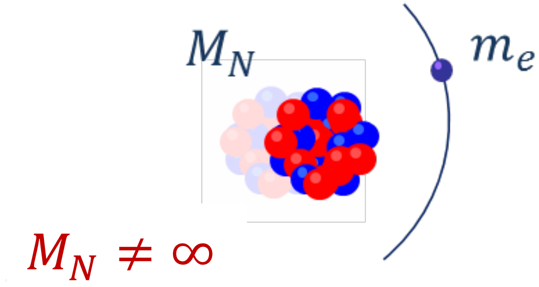
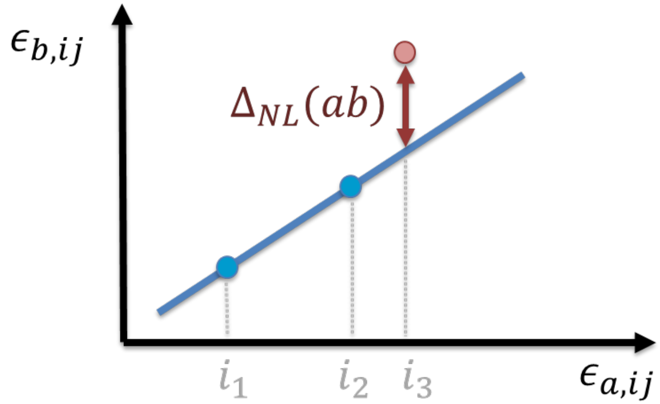
Summary and outlook

In this work we performed relativistic calculations of the isotope-shift constants for the 2P fine-structure transitions in Be-like, B-like, and C-like argon.



For the first time, the quadratic recoil constant $K^{(2)}$ in these systems was calculated.



For the fine-structure transitions in highly-charged argon ions, nonlinearities from 5 to 30 kHz were found.

The nonlinear effects in the King plot arising within the Standard Model and the accuracy of their theoretical description put limitations on possible constraints on hypothetical new long-range forces between the electron and the nucleus.