An Overview of Atomic Methods to Estimate Nuclear Charge Radii from Isotope Shifts + Addressing large differences among the APV results in ^{133}Cs

B. K. Sahoo

Atomic, Molecular and Optical Physics Division
Physical Research Laboratory, Ahmedabad , India

Outline

- Theory of Atomic Energy Levels
- Isotope Shifts (IS)
- All-order methods to determine wave functions
- Different approaches for property evaluation
- Challenges in Isotope Shift calculations
- Atomic Parity Violating Amplitudes in ^{133}Cs
- Future directions and Summary

Hydrogen-like Systems

H-like systems: $h(m_e, N) = \frac{P_N^2}{2M_A} + \frac{p_e^2}{2m_e} + V_N(r_e, R_N)$

$$\rho_e = r_e - R_N \quad \text{and} \quad R_0 = \frac{M_N R_N + m_e \sum_i r_i}{M_N + Z m_e}$$

Effective momenta and mass:

$$\mu_A = \frac{M_N m_e}{M_N + m_e} \sim m_e \quad \text{and} \quad \pi_e = -i\hbar \frac{\partial}{\partial \rho_e}$$

Schroedinger Eq: $h|\psi\rangle = \varepsilon\,|\psi\rangle$ with $h \simeq \frac{\pi_e^2}{2m_e} + V_N(\rho_e)$

Relativistic Hamiltonian: $h \simeq c\,\vec{\alpha}\cdot\vec{\pi} + \beta m_e c^2 + V_N(\rho_e)$

Multi-electron Systems

Hamiltonian:

$$H_{at} = \frac{P_N^2}{2M_N} + \sum_i \left[\frac{p_i^2}{2m_e} + V_N(R_N, r_i)\right] + \frac{1}{2}\sum_{i,j} \frac{1}{|\vec{r}_i - \vec{r}_j|}$$

We can express: $H_{at}(M_N, R_N, r_e) = H_N + H_0 + H_{MS} + H_{FS}$

where $H_{MS} = -\frac{1}{2}\frac{M_N}{(M_N + m_e)^2}\sum_{i,j}[\vec{p_i} \cdot \vec{p}_j]$

$$= -\frac{1}{2}\frac{M_N}{(M_N+m_e)^2}\sum_i p_i^2 \; - \; \frac{1}{2}\frac{M_N}{(M_N+m_e)^2}\sum_{i,j\neq i}[\vec{p_i} \cdot \vec{p}_j]$$

and $H_{FS}(r_e) = -\frac{\partial V_N(R_N, r_e)}{\partial \langle R_N^2 \rangle}\, \delta\langle R_N^2 \rangle$

Energy Level Shifts (isotope shift (IS))

Modified energy: $E = E_0 + \Delta E^{MS} + \Delta E^{FS}$

$$\Delta E^{MS} = \Delta E^{(1)}_{NMS} + \Delta E^{(1)}_{SMS} + \mathcal{O}\left(\mu_A^2\right)$$

with $E^{(1)}_{NMS} = \mu_A K^{NMS}$ and $E^{(1)}_{SMS} = \mu_A K^{SMS}$

Similarly, $E^{FS} \approx \Delta E^{(1)}_{FS} + \mathcal{O}\left(\boldsymbol{\delta}\langle \boldsymbol{r^2_{rms}}\rangle\right)^2$ with $E^{(1)}_{FS} = -F\,\boldsymbol{\delta}\langle \boldsymbol{r^2_{rms}}\rangle$

Measuring ISs in two transitions *a* & *b* of isotopes (King's plot):

$$\frac{\nu_b^{AA'}}{\mu_{AA'}} \simeq \frac{F_b}{F_a}\frac{\nu_a^{AA'}}{\mu_{AA'}} + \left(K_b^{MS} - \frac{F_b}{F_a} K_a^{MS}\right)$$

where $K^{MS} = K^{NMS} + K^{SMS}$ and $\mu_{AA'} = \mu_A - \mu_{A'}$

Relativistic Expressions and Challenges

In the first-order approximation, IS constants are needed to be determined:

$$F_i = \left\langle \frac{\delta V_{nuc}(r)}{\delta \langle r_N^2 \rangle} \right\rangle$$

Computational Challenging

$$K^{NMS} = \frac{1}{2}\left\langle p^2 - \frac{\alpha_e Z}{r}\left(\alpha \cdot p + \left(\alpha \cdot C^1\right)^2\right)\right\rangle$$

$$K^{SMS} = \frac{1}{2}\left\langle \sum_{kl} p_k \cdot p_l - \frac{\alpha_e Z}{r_k}\left(\alpha_k \cdot p_l + (\alpha_k \cdot C_k^1)(\alpha_l \cdot C_l^1)\right)\right\rangle$$

Typical approach to estimate first-order energy

In the presence of an interaction Hamiltonian H_{int}, we can express the total Hamiltonian $H = H_0 + \lambda\, H_{int}$ and energy $E_n = E_n^{(0)} + \Delta E_n(\lambda)$.

For the (N/S)MS: $H_{int} = K^{N/SMS}$ and $\lambda = \mu_A$

For the FS: $H_{int} = F$ and $\lambda = \delta\langle r_{rms}^2 \rangle$

In the perturbative analysis:

$$|\Psi_n\rangle = |\Psi_n^{(0)}\rangle + \lambda|\Psi_n^{(1)}\rangle + \lambda^2|\Psi_n^{(2)}\rangle + \cdots$$

and $$E_n(\lambda) = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots$$

Taylor series: $$E_n(\lambda) = E_n(0) + \lambda \frac{dE_n}{d\lambda}\Big|_{\lambda\to 0} + \frac{\lambda^2}{2}\frac{d^2E_n}{d\lambda^2}\Big|_{\lambda\to 0} + \cdots$$

Finite-field (FF) approach: $$E_n^{(1)} = \lambda \frac{dE_n}{d\lambda}\Big|_{\lambda\to 0} \approx \frac{E_n(+\lambda) - E_n(-\lambda)}{2\,\lambda}$$

Points to be noted about the FF approach

- Calculations to be carried out for $+\lambda$ and $-\lambda$. Again, to minimize numerical errors, calculations should be carried out for a number of λ values.
- Neglects $\mathfrak{O}(\boldsymbol{\lambda^2})$ contributions, which may not be small.
- Choice of $\boldsymbol{\lambda}$ depends on properties of interest ($\boldsymbol{F}$, $\boldsymbol{K^{NMS}}$, and $\boldsymbol{K^{SMS}}$ may not be calculated accurately by considering same $\boldsymbol{\lambda}$).
- Also, choice of λ can be atomic state dependent.
- It will be difficult to account contributions interactions among the FS and MS interactions, as well as the second-order effects. i.e.

$$H_\lambda = H_{at} + \lambda_F F + \lambda_{MS} K^{MS}$$

$$\boldsymbol{E_\lambda = E_0^{(0,0)} + \lambda_F E_0^{(1,0)} + \lambda_F^2 E_0^{(2,0)} + \cdots}$$
$$+\lambda_{MS} E_0^{(0,1)} + \lambda_{MS}^2 E_0^{(0,2)} + \cdots$$
$$+\lambda_F \lambda_{MS} E_0^{(1,1)} + \cdots$$

Approaches to evaluate the first-order energy

In the perturbative theory: $|\Psi_n\rangle = |\Psi_n^{(0)}\rangle + \lambda|\Psi_n^{(1)}\rangle + \lambda^2|\Psi_n^{(2)}\rangle + \cdots$

$$E_n(\lambda) = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots$$

The expectation value evaluation (EVE) approach:

$$E_n^{(1)} = \langle H_{int}\rangle = \frac{\langle \Psi_n^{(0)}|H_{int}|\Psi_n^{(0)}\rangle}{\langle \Psi_n^{(0)}|\Psi_n^{(0)}\rangle}$$

Analytical Response (AR) approach:

$$\left(H_0 - E_n^{(0)}\right)|\Psi_n^{(1)}\rangle = \left(E_n^{(1)} - H_{int}\right)|\Psi_n^{(0)}\rangle$$

In many-body methods, the AR approach is more difficult to implement than the EVE approach. However, the AR approach has several advantages over the EVE approach in the coupled-cluster theory.

Coupled-cluster vs. Perturbation Methods

Many-body perturbation theory (MBPT):

$$|\Psi_0\rangle = |\Phi_0\rangle + \lambda\left|\Phi_0^{(1)}\right\rangle + \lambda^2\left|\Phi_0^{(2)}\right\rangle + \lambda^3\left|\Phi_0^{(3)}\right\rangle + \cdots$$

where $|\Phi_0\rangle$ is the (Dirac)-Hartree-Fock mean-field wave function and each order is given by: $\left|\Phi_0^{(n)}\right\rangle = \sum_{k\neq 0}^{N}\left|\Phi_k^{(0)}\right\rangle\ C_{0k}^{(n)}$

Coupled-cluster (CC) theory (gold standard):

$$|\Psi_0\rangle = |\Phi_0\rangle + T_I|\Phi_0\rangle + \left(T_{II} + \frac{1}{2}T_I^2\right)|\Phi_0\rangle + \cdots + T_N|\Phi_0\rangle$$

$$= e^T|\Phi_0\rangle \qquad \text{where} \quad \mathrm{T} = \mathrm{T_I} + \mathrm{T_{II}} + \cdots + T_N$$

With the same computational effort, the CC method includes electron correlation effects to all-orders and more physical effects.

Energy equation in (R)CC theory (FF approach)

Energy expression: $E_0 = \langle H_0 \rangle = \dfrac{\langle \Psi_0 | H_0 | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$

$$E_0 = \frac{\langle \Phi_0 | e^{T^+} H_0 e^T | \Phi_0 \rangle}{\langle \Phi_0 | e^{T^+} e^T | \Phi_0 \rangle} = \frac{\sum_K \langle \Phi_0 | e^{T^+} e^T | \Phi_K \rangle \langle \Phi_K | e^{-T} H_0 e^T | \Phi_0 \rangle}{\langle \Phi_0 | e^{T^+} e^T | \Phi_0 \rangle}$$

$$= \langle \Phi_0 | e^{-T} H_0 e^T | \Phi_0 \rangle = \left\langle \Phi_0 \middle| \left(H_0 e^T \right)_c \middle| \Phi_0 \right\rangle$$

Excitation amplitudes: $\boxed{\left\langle \Phi_K \middle| \left(H_0 e^T \right)_c \middle| \Phi_0 \right\rangle = 0}$

In the FF approach of RCC theory, the same equations are used for IS.

Expectation value evaluation (EVE) approach

IS evaluating expression:

$$\langle H_{int} \rangle = \frac{\langle \Psi_0 | H_{int} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} = \frac{\langle \Phi_0 | e^{T^+} H_{int} e^{T} | \Phi_0 \rangle}{\langle \Phi_0 | e^{T^+} e^{T} | \Phi_0 \rangle}$$

- Possesses two non-terminating series.
- Unmanageable with two-body operators like SMS operator.
- It does not satisfy the Hellmann-Feynman theorem.
  (energy and property evaluating equations are different)

$$\Rightarrow e^{T^+} H_{int} e^{T} = H_{int} + H_{int}T + T^+ H_{int} + T^+ H_{int} T + \frac{1}{2} H_{int} T^2 + \cdots$$

And $\quad e^{T^+} e^{T} = 1 + T^+ T + \frac{1}{2} T^+ T^2 + \cdots$

Analytic Response approach in (R)CC method

In the AR RCC method, we express

$$H_\lambda = H_0 + \lambda H_{int} \quad \text{and} \quad |\Psi_0\rangle \simeq |\Psi_0^{(0)}\rangle + \lambda\,|\Psi_0^{(1)}\rangle$$

First-order Eqn: $(H_0 - E_0^{(0)})|\Psi_n^{(1)}\rangle = (E_0^{(1)} - H_{int})\,|\Psi_0^{(0)}\rangle$

$$|\Psi_0\rangle = e^T|\Phi_0\rangle = e^{T^{(0)}+\lambda T^{(1)}}|\Phi_0\rangle$$

$$\Rightarrow \left|\Psi_0^{(0)}\right\rangle = \; e^{T^{(0)}}\,|\Phi_0\rangle$$

and $$\left|\Psi_0^{(1)}\right\rangle = \; e^{T^{(0)}}\left(1 + T^{(1)}\right)|\Phi_0\rangle$$

It yields that:

$$\langle H_{int}\rangle \equiv E_0^{(1)} = \langle\Phi_0\left|(H_0 e^{T^{(0)}}T^{(1)})_c + \left(H_{int}e^{T^{(0)}}\right)_c\right|\Phi_0\rangle$$

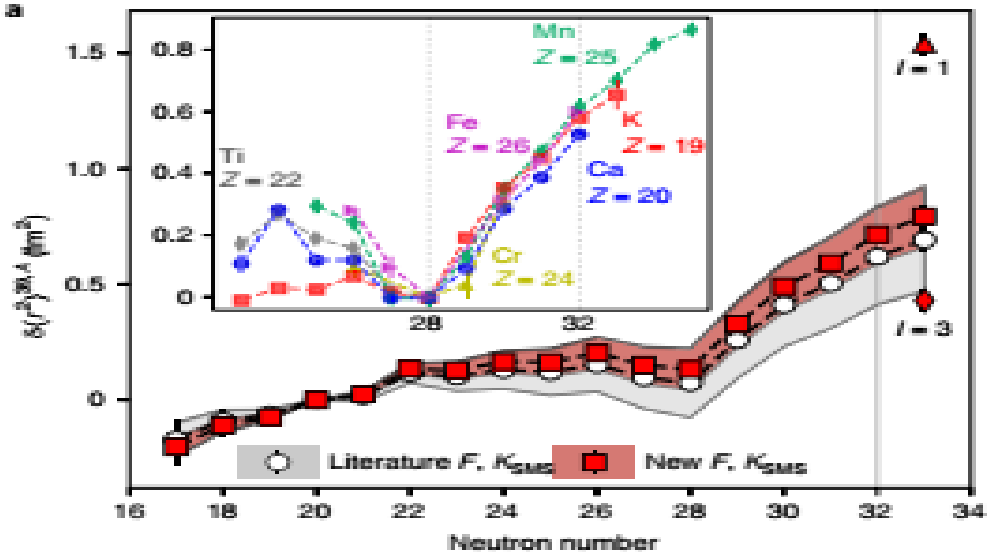
Advantages of AR approach in the RCC method

- All the terms are terminated.
- It satisfies the Hellmann-Feynman theorem (as it is derived from energy expression).
- Free from choice of any perturbative parameter.
- Computational efforts are less than other approaches of the RCC method.
- Second-order IS effects can be easily evaluated by:

$$E_0^{(2)} = \langle \Psi_0^{(0)} \Big| H_{int} | \Psi_0^{(1)} \rangle$$

$$= \frac{\langle \Phi_0 | e^{T^{(0)^+}} H_{int} e^{T^{(0)}} T^{(1)} | \Phi_0 \rangle}{\langle \Phi_0 | e^{T^{(0)^+}} e^{T^{(0)}} | \Phi_0 \rangle}$$

A few notable results from the AR-RCC method



nature physics
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https://doi.org/10.1038/s41567-020-01136-5
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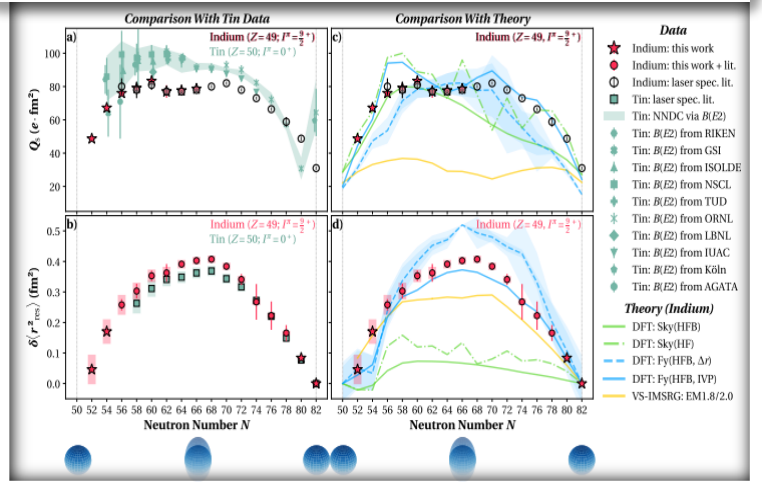
Charge radii of exotic potassium isotopes challenge nuclear theory and the magic character of $N = 32$

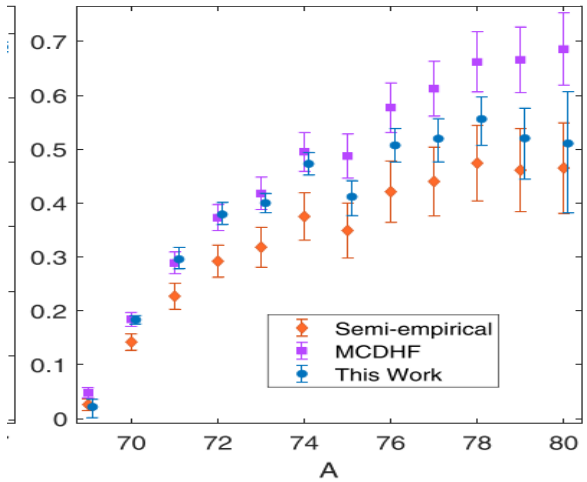
Á. Koszorús[1,17] ✉, X. F. Yang[1,2] ✉, W. G. Jiang[3,4,5], S. J. Novario[3,4], S. W. Bai[2], J. Billowes[6], C. L. Binnersley[6], M. L. Bissell[6], T. E. Cocolios[1], B. S. Cooper[6], R. P. de Groote[7,8], A. Ekström[5], K. T. Flanagan[6,9], C. Forssén[5], S. Franchoo[10], R. F. Garcia Ruiz[11,12], F. P. Gustafsson[1], G. Hagen[4], G. R. Jansen[4], A. Kanellakopoulos[1], M. Kortelainen[7,8], W. Nazarewicz[13], G. Neyens[1,12], T. Papenbrock[3,4], P.-G. Reinhard[14], C. M. Ricketts[6], B. K. Sahoo[15], A. R. Vernon[1,6] and S. G. Wilkins[16]

Electromagnetic Properties of Indium Isotopes Elucidate the Doubly Magic Character of ^{100}Sn



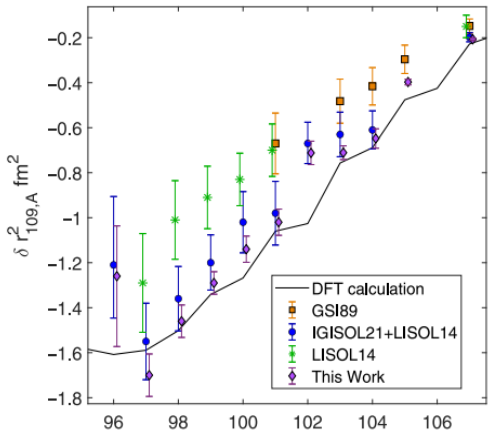
Nature Physics (accepted)

All-optical differential radii in zinc



PHYSICAL REVIEW RESEARCH **5**, 043142 (2023)

Reconciling mean-squared radius differences in the silver chain through improved measurement and *ab initio* calculations



PHYSICAL REVIEW RESEARCH **6**, 033040 (2024)

IS studies in Al and implication to particle physics

The largest CKM matrix element V_{ud} can be extracted from the superallowed $0^+ \rightarrow 0^+$ beta transition between states with isospin $T = 1$. It is usually parameterized as:

$$V_{ud}^{-2} \propto ft(1+\delta_R')(1+\delta_{NS}-\delta_C)(1+\Delta_R^V)$$

where $f(Q)$ is the statistical rate function, t is the half-life of beta, Δ is the nucleus independent correction and δ is the nucleus dependent correction.

This study requires accurate estimate of

$$\langle r_{rms}^2 \rangle^{26m,27}$$

Nuclear Charge Radius of ^{26m}Al and Its Implication for V_{ud} in the Quark Mixing Matrix

$$\langle r_{rms}^2 \rangle^{26m,27} = 0.429(45)(76)$$

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Energies of Al from RCC theory

Method	$3p\ ^2P_{1/2}$	$3p\ ^2P_{3/2}$	$4s^2S_{1/2}$
EAs			
DHF	42823.87	42714.35	21311.66
RMBPT(2)	48637.77	48514.21	22760.10
RCCSD	47841.74	47725.64	22849.31
RCCSDT	48223.08	48114.72	22914.98
Extra	37.88	37.73	3.18
+Breit	−7.65	−1.16	−1.04
+VP	−0.26	−0.25	0.05
+SE	4.46	4.18	−0.74
Final	48258(25)	48155(25)	22917(15)
Experiment	48278.48(3)	48166.42(3)	22930.72(3)
EEs	$^2P_{1/2}$–$^2S_{1/2}$	$^2P_{3/2}$–$^2S_{1/2}$	$^2P_{1/2}$–$^2P_{3/2}$
This work	25341(30)	25238(30)	103
Experiment	25347.756	25235.695	112.061

RCC results for IS constants in Al using FF and AR

FF vs. AR

TABLE III. Calculated IS factors F, K^{SMS} for selected levels in Al using FF approach of the RCC method.

Method	$3p\ ^2P_{1/2}$	$3p\ ^2P_{3/2}$	$4S$
F MHz/fm^2			
DHF	59.22	59.31	−12.44
RMBPT(2)	70.20	70.29	−10.71
RCCSD	63.72	63.86	−10.90
RCCSDT	67.53	67.84	−10.19
+Basis	0.04	0.03	−0.01
+Breit	−0.08	0.14	−0.10
+VP	−0.07	−0.25	−0.15
+SE	−0.59	−0.37	−0.17
Final	66.8(5)	67.4(5)	−10.6(3)
K^{NMS} GHz u			
DHF	703.20	702.28	350.17
RMBPT(2)	798.79	797.72	373.96
RCCSD	785.58	784.58	375.44
RCCSDT	791.91	791.04	376.50
+Basis	0.59	0.58	0.05
+Breit	0.14	0.23	−0.04
+VP	1.02	0.80	0.23
+SE	0.48	0.17	−0.04
Final	794.14	792.65	376.7
Scaling	794	792	377
K^{SMS} GHz u			
DHF	−736.93	−742.37	−13.68
RMBPT(2)	−491.51	−499.01	36.02
RCCSD	−589.84	−597.02	50.96
RCCSDT	−597.14	−599.83	52.75
+Basis	−1.09	−1.10	−0.03
+Breit	0.43	0.06	−0.02
+VP	−0.08	−0.32	0.02
+SE	−0.64	−1.37	0.64
Final	−598.52	−602.56	53.36

TABLE IV. Calculated IS factors F, K^{SMS} for selected levels in Al using AR-RCC method.

Method	$3p\ ^2P_{1/2}$	$3p\ ^2P_{3/2}$	$4S$
F MHz/fm^2			
DHF	−0.09	~0.0	−13.44
RCCSD	63.29	63.22	−10.45
RCCSDT	69.58	69.30	−8.74
+Basis	0.02	0.02	~0.0
+Breit	−0.06	−0.05	0.01
+QED	−0.44	−0.43	0.08
Final	69.1	68.84	-8.65
K^{NMS} GHz u			
DHF	1920.03	1914.46	431.69
RCCSD	790.83	790.05	364.69
RCCSDT	755.59	760.54	362.74
Basis	0.87	0.90	−0.03
+Breit	−0.16	−0.08	−0.05
+QED	0.22	0.14	−0.04
Final	756.52	761.5	362.62
Scaling	794	792	377
K^{SMS} GHz u			
DHF	−977.25	−980.86	−50.31
RCCSD	−607.06	−614.91	48.23
RCCSDT	−598.14	−600.66	56.58
+Basis	−1.17	−1.21	−0.36
+Breit	−0.34	−0.15	0.41
+QED	−0.14	−0.11	0.00
Final	−599.76	−602.13	56.63

RCC results for Potassium (FF approach)

State	DHF	RMBPT(2)	RCCSD	RCCSDT	+Basis	+Breit	+QED	Total	Experiment
				Energies					
EAs									
$4s\ ^2S_{1/2}$	32370.48	35077.13	35077.13	34972.90	16.47	−1.45	−6.80	34988(20)	35009.813971(2)
$4p\ ^2P_{1/2}$	21006.44	22010.82	22027.81	22018.00	8.30	−2.32	**0.47**	22024(10)	22024.628(1)
$4p\ ^2P_{3/2}$	20959.39	21951.66	21967.69	21957.90	8.26	−0.35	**0.18**	21966(10)	21966.918(1)
$5s\ ^2S_{1/2}$	13406.99	14028.06	13988.83	13979.84	3.63	−0.46	−0.16	13983(5)	13983.263(5)
$5p\ ^2P_{1/2}$	10011.64	10313.36	10308.65	10307.84	2.57	−0.79	**0.16**	10310(3)	10308.414(2)
$5p\ ^2P_{3/2}$	9995.43	10293.90	10289.13	10288.24	2.55	−0.15	**0.07**	10291(3)	10289.68
$6s\ ^2S_{1/2}$	7335.04	7574.11	7558.63	7555.61	1.42	−0.19	−0.63	7557(3)	7559.1036
EEs									
$4s\ ^2S_{1/2} - 4p\ ^2P_{1/2}$	11364.04	13066.31	13049.32	13015.90	8.17	0.87	−7.27	12964(25)	12985.185724
$4s\ ^2S_{1/2} - 4p\ ^2P_{3/2}$	11411.09	13125.47	13109.44	13015.00	8.21	−1.10	−6.98	13022(25)	13042.896027
$4s\ ^2S_{1/2} - 5s\ ^2S_{1/2}$	18963.49	21049.07	21088.30	20993.06	12.84	−0.99	−6.64	21005(21)	21026.551
$4s\ ^2S_{1/2} - 5p\ ^2P_{1/2}$	22358.84	24763.77	24768.48	24665.06	13.90	−0.66	−6.96	24678(21)	24701.382
$4s\ ^2S_{1/2} - 5p\ ^2P_{3/2}$	22375.05	24783.23	24788.00	24684.66	13.92	−1.30	−6.87	24697(21)	24720.139
$4s\ ^2S_{1/2} - 6s\ ^2S_{1/2}$	25035.44	27503.02	27518.50	27417.29	15.05	−1.26	−6.17	27431(21)	27450.7104

TABLE IV. FS constants (in MHz/fm^{-1}) at different levels of approximation in the FF approach.

	DHF	RMBPT(2)	RCCSD	RCCSDT	+Basis	+Breit	+QED	Total
				F constants				
State								
$4s\ ^2S_{1/2}$	−80.25	−106.91	−106.16	−105.50	−0.14	0.13	1.24	−105.5(15)
$4p\ ^2P_{1/2}$	5.05	4.38	4.65	4.55	~ 0.0	~ 0.0	−0.04	4.55(5)
$4p\ ^2P_{3/2}$	5.17	4.58	4.85	4.75	~ 0.0	−0.01	−0.04	4.75(5)
$5s\ ^2S_{1/2}$	−21.20	−25.83	−25.32	−25.25	−0.02	0.03	0.29	−25.24(30)
$5p\ ^2P_{1/2}$	1.92	1.82	1.91	1.88	~ 0.0	−0.01	−0.02	1.87(2)
$5p\ ^2P_{3/2}$	1.88	1.78	1.86	1.84	~ 0.0	~ 0.0	−0.01	1.83(2)
$6s\ ^2S_{1/2}$	−8.54	−10.65	−10.40	−10.35	−0.03	0.01	0.11	−10.37(12)
Transition								
$4s\ ^2S_{1/2}$−$4p\ ^2P_{1/2}$	−85.30	−111.29	−110.81	−110.05	−0.14	0.13	1.28	−110.1(13)
$4s\ ^2S_{1/2}$−$4p\ ^2P_{3/2}$	−85.42	−111.49	−111.01	−110.25	−0.14	0.14	1.28	−110.3(13)
$4s\ ^2S_{1/2}$−$5s\ ^2S_{1/2}$	−59.05	−81.08	−80.84	−80.25	−0.12	0.11	0.95	−80.3(15)
$4s\ ^2S_{1/2}$−$5p\ ^2P_{1/2}$	−82.17	−108.73	−108.07	−107.38	−0.14	0.14	1.26	−107.4(15)
$4s\ ^2S_{1/2}$−$5p\ ^2P_{3/2}$	−82.13	−108.69	−108.02	−107.34	−0.14	0.13	1.27	−107.3(15)
$4s\ ^2S_{1/2}$−$6s\ ^2S_{1/2}$	−71.71	−96.26	−95.76	−95.15	−0.11	0.12	1.13	−95.1(15)

NMS and SMS constants of K from FF approach

TABLE V. NMS constants (in GHz amu) at different levels of approximation in the FF approach.

State	DHF	RMBPT(2)	RCCSD	RCCSDT	+Basis	+Breit	+QED	Total	Scaling [39]
$4s\ ^2S_{1/2}$	531.52	575.83	575.32	574.33	0.24	−0.08	-0.29	575(3)	575.77
$4p\ ^2P_{1/2}$	345.22	361.64	361.97	361.88	0.12	−0.53	-0.09	362(2)	362.22
$4p\ ^2P_{3/2}$	344.85	361.05	361.36	361.26	0.12	−0.51	-0.52	361(2)	361.27
$5s\ ^2S_{1/2}$	220.21	230.37	229.78	229.67	0.05	−0.03	-0.09	230(1)	229.97
$5p\ ^2P_{1/2}$	164.58	169.52	169.47	169.47	0.03	−0.09	-0.06	169.5(5)	169.53
$5p\ ^2P_{3/2}$	164.38	169.25	169.19	169.20	0.04	−0.05	-0.13	169.1(5)	169.22
$6s\ ^2S_{1/2}$	120.62	124.82	124.53	124.49	0.06	−0.12	-0.15	124.3(2)	124.32
$4s\ ^2S_{1/2}-4p\ ^2P_{1/2}$	186.30	214.19	213.35	212.45	0.12	0.45	-0.20	213(4)	213.55
$4s\ ^2S_{1/2}-4p\ ^2P_{3/2}$	186.67	214.78	213.96	213.07	0.12	0.43	0.23	214(4)	214.50
$4s\ ^2S_{1/2}-5s\ ^2S_{1/2}$	311.31	345.46	345.54	344.66	0.19	-0.05	-0.20	345(3)	345.80
$4s\ ^2S_{1/2}-5p\ ^2P_{1/2}$	366.94	406.31	405.85	404.86	0.21	0.01	-0.23	405.5(4)	406.24
$4s\ ^2S_{1/2}-5p\ ^2P_{3/2}$	367.14	406.58	406.13	405.13	0.20	-0.03	-0.16	406(6)	406.55
$4s\ ^2S_{1/2}-6s\ ^2S_{1/2}$	410.90	451.01	450.79	449.84	0.18	0.04	-0.14	451(4)	451.45

TABLE VI. SMS constants (in GHz amu) at different levels of approximation in the FF approach.

State	DHF	RMBPT(2)	RCCSD	RCCSDT	+Basis	+Breit	+QED	Total
$4s\ ^2S_{1/2}$	−200.14	−61.60	−18.96	−35.64	−0.45	0.56	0.27	−35.53
$4p\ ^2P_{1/2}$	−57.05	−21.14	−9.09	−16.84	−0.08	0.07	0.25	−16.85
$4p\ ^2P_{3/2}$	−58.77	−23.67	−11.94	−19.52	−0.08	0.48	0.25	−19.12
$5s\ ^2S_{1/2}$	−46.39	−1.72	5.05	4.80	−0.13	0.04	−0.06	4.71
$5p\ ^2P_{1/2}$	−19.89	−6.47	−3.75	−4.94	−0.03	−0.01	−0.09	−4.98
$5p\ ^2P_{3/2}$	−20.52	−7.34	−4.69	−5.85	−0.03	0.14	0.02	−5.8(3)
$6s\ ^2S_{1/2}$	−18.07	0.88	3.03	3.37	−0.07	0.03	0.03	3.33
$4s\ ^2S_{1/2}-4p\ ^2P_{1/2}$	-143.09	−40.46	−9.87	−18.8	−0.37	0.49	0.02	−18.68
$4s\ ^2S_{1/2}-4p\ ^2P_{3/2}$	−140.54	−37.93	−7.02	−16.12	−0.37	0.08	0.02	−16.41
$4s\ ^2S_{1/2}-5s\ ^2S_{1/2}$	−153.75	−59.88	-24.01	−40.44	−0.32	0.52	0.33	−40.24
$4s\ ^2S_{1/2}-5p\ ^2P_{1/2}$	−180.25	−55.13	−15.21	−30.7	−0.42	0.57	0.36	−30.55
$4s\ ^2S_{1/2}-5p\ ^2P_{3/2}$	−179.62	−54.26	−14.27	−29.79	−0.42	0.42	0.25	−29.73
$4s\ ^2S_{1/2}-6s\ ^2S_{1/2}$	−182.07	−60.72	−21.99	−39.01	−0.38	0.53	0.24	−38.86

IS constants of K from AR approach

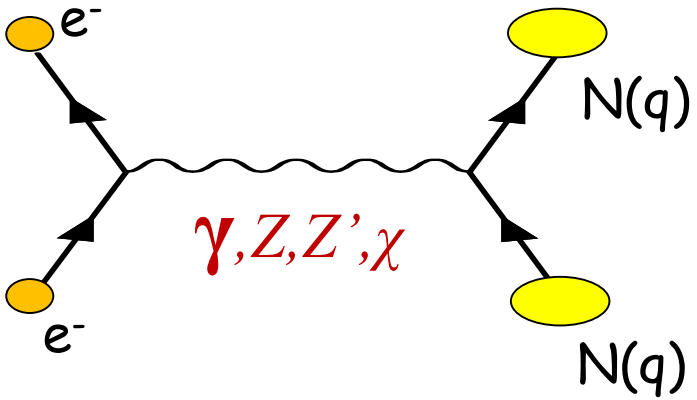
State	DHF	RCCSD	RCCSDT	+Basis	+Breit	+QED	Total
			F values (in MHz/fm^{-1})				
$4s\ ^2S_{1/2}$	−73.08	−105.20	−103.62	−0.12	0.13	1.24	-103.61
$4p\ ^2P_{1/2}$	−0.08	4.05	3.80	0.01	∼ 0.0	−0.05	3.81
$4p\ ^2P_{3/2}$	∼ 0.0	4.17	3.87	0.01	−0.01	−0.04	3.87
$5s\ ^2S_{1/2}$	−19.34	−24.76	−24.53	−0.02	0.03	0.29	-24.52
$5p\ ^2P_{1/2}$	−0.03	1.45	1.35	∼ 0.0	−0.01	−0.02	1.34
$5p\ ^2P_{3/2}$	∼ 0.0	1.48	1.37	0.01	∼ 0.0	−0.01	1.38
$6s\ ^2S_{1/2}$	−7.86	−9.73	−9.67	−0.01	0.01	0.11	-9.67
			K^{NMS} values (in GHz amu)				
$4s\ ^2S_{1/2}$	941.13	559.22	545.45	−1.12	−1.79	−2.06	542.54
$4p\ ^2P_{1/2}$	488.53	351.99	345.57	−1.45	−1.81	−1.69	342.31
$4p\ ^2P_{3/2}$	488.87	351.69	345.41	−1.17	−1.43	−1.40	342.81
$5s\ ^2S_{1/2}$	324.53	226.78	222.47	0.37	0.21	0.15	223.05
$5p\ ^2P_{1/2}$	214.14	166.99	164.33	−0.24	−0.35	−0.31	163.74
$5p\ ^2P_{3/2}$	213.61	166.88	164.23	−0.15	−0.23	−0.21	163.85
$6s\ ^2S_{1/2}$	162.52	123.50	121.20	0.04	−0.02	−0.04	121.22
			K^{SMS} values (in GHz amu)				
$4s\ ^2S_{1/2}$	−388.76	−12.72	−25.05	−0.53	0.48	0.31	-25.10
$4p\ ^2P_{1/2}$	−115.54	−5.34	−5.33	−0.14	0.22	−0.06	-5.25
$4p\ ^2P_{3/2}$	−116.33	−8.95	−9.48	−0.13	0.11	−0.06	-9.50
$5s\ ^2S_{1/2}$	−94.60	6.05	9.04	−0.15	0.13	0.06	9.02
$5p\ ^2P_{1/2}$	−40.19	−2.98	−0.33	−0.07	0.08	−0.03	-0.32
$5p\ ^2P_{3/2}$	−40.49	−4.13	−1.78	−0.05	0.04	−0.15	-1.79
$6s\ ^2S_{1/2}$	−37.49	3.34	5.80	−0.07	0.06	0.02	5.79

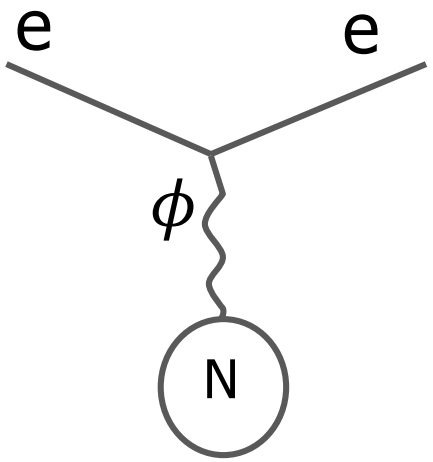
IS constants of K from EVE approach

State	DHF	RCCSD	RCCSDT	+Basis	+Breit	+QED	Total
			F values (in MHz/fm^{-2})				
$4s\ ^2S_{1/2}$	−73.08	−103.95	−104.01	−0.09	0.22	1.23	-103.88
$4p\ ^2P_{1/2}$	−0.08	4.48	4.70	0.01	−0.01	−0.05	4.70
$4p\ ^2P_{3/2}$	∼ 0.0	4.54	4.75	0.01	−0.01	−0.05	4.75
$5s\ ^2S_{1/2}$	−19.34	−24.48	−24.53	−0.01	∼ 0.0	0.28	-24.54
$5p\ ^2P_{1/2}$	−0.03	1.56	1.64	∼ 0.0	∼ 0.0	−0.02	1.64
$5p\ ^2P_{3/2}$	∼ 0.0	1.58	1.66	∼ 0.0	∼ 0.0	−0.02	1.66
$6s\ ^2S_{1/2}$	−7.86	−9.64	−9.66	−0.01	∼ 0.0	0.11	-9.67
			K^{NMS} values (in GHz amu)				
$4s\ ^2S_{1/2}$	941.13	594.22	553.75	1.12	−0.44	−0.38	554.43
$4p\ ^2P_{1/2}$	488.53	357.97	339.14	0.49	−0.08	0.04	339.55
$4p\ ^2P_{3/2}$	486.87	356.79	338.19	0.48	0.01	0.02	338.68
$5s\ ^2S_{1/2}$	324.53	235.11	224.69	0.43	0.09	−0.09	225.21
$5p\ ^2P_{1/2}$	214.14	169.33	162.88	0.13	−0.03	0.01	162.98
$5p\ ^2P_{3/2}$	213.61	168.98	162.63	0.13	−0.01	∼ 0.0	162.75
$6s\ ^2S_{1/2}$	162.52	126.73	122.64	0.09	∼ 0.0	−0.03	122.73
			K^{SMS} values (in GHz amu)				
$4s\ ^2S_{1/2}$	−388.76	−57.87	−106.84	0.22	0.21	0.37	-106.41
$4p\ ^2P_{1/2}$	−115.54	−21.44	−42.02	0.32	∼ 0.0	−0.06	-41.70
$4p\ ^2P_{3/2}$	−116.33	−20.52	−41.05	0.31	−0.02	−0.05	-40.74
$5s\ ^2S_{1/2}$	−94.60	−4.90	−11.42	0.02	0.15	0.07	-11.25
$5p\ ^2P_{1/2}$	−40.19	−8.68	−12.93	0.10	0.01	−0.02	-12.82
$5p\ ^2P_{3/2}$	−40.49	−8.36	−12.63	0.10	0.02	−0.01	-12.51
$6s\ ^2S_{1/2}$	−37.49	−0.99	−2.97	0.01	0.06	0.03	-2.90

New IS interaction from BSM physics

In addition to photons, there could be other intermediate particles between electrons and nucleus in an atom.





A new spin-1 light boson:

$$V(r) = (-1)^{1+s} \sum_n y_e y_n \frac{e^{-\frac{m_\phi c r}{\hbar}}}{4\pi r}$$

where m_ϕ and s are the mass and spin of the new boson, respectively, y_e is the electron coupling coefficient and y_n is the neutron coupling coefficient.

It could contribute to the IS shifts in isotopes, but will be of the order-of second-order effects (non-linear King's plot).

Inferring BSM Physics from King's Plot

King's plot for the first-order IS:

$$\frac{\nu_b^{AA'}}{\mu_{AA'}} \simeq \frac{F_b}{F_a}\frac{\nu_a^{AA'}}{\mu_{AA'}} + \left(K_b^{MS} - \frac{F_b}{F_a} K_a^{MS}\right)$$

Inclusion of higher-order field shift (FS):

$$E_i^{AA'} \simeq \mu_{AA'} K_i^{MS} + \boldsymbol{F_i \delta\langle r_{rms}^2\rangle} + G_i^{(2)} \left(\boldsymbol{\delta\langle r_{rms}^2\rangle}\right)^2 + \boldsymbol{G_i^{(4)} \delta\langle r_{rms}^4\rangle}$$

This will lead to:

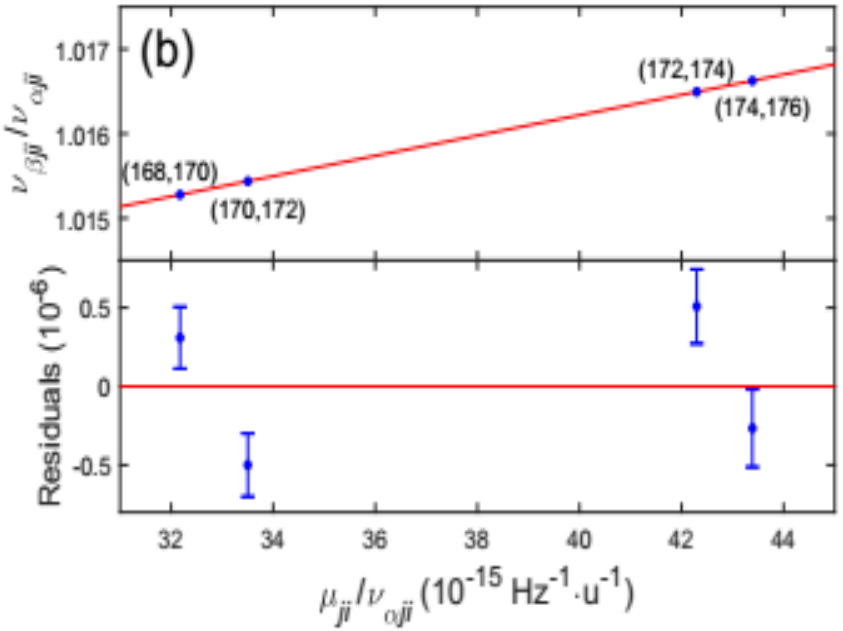
$$\frac{\nu_b^{AA'}}{\mu_{AA'}} \cong \frac{\nu_a^{AA'}}{\mu_{AA'}} + \left(K_b^{MS} - \frac{F_b}{F_a} K_a^{MS}\right) + \left(G_b^{(2)} - \frac{F_b}{F_a} G_a^{(2)}\right)\frac{\boldsymbol{\delta\langle r_{rms}^2\rangle^2}}{\mu_{AA'}}$$

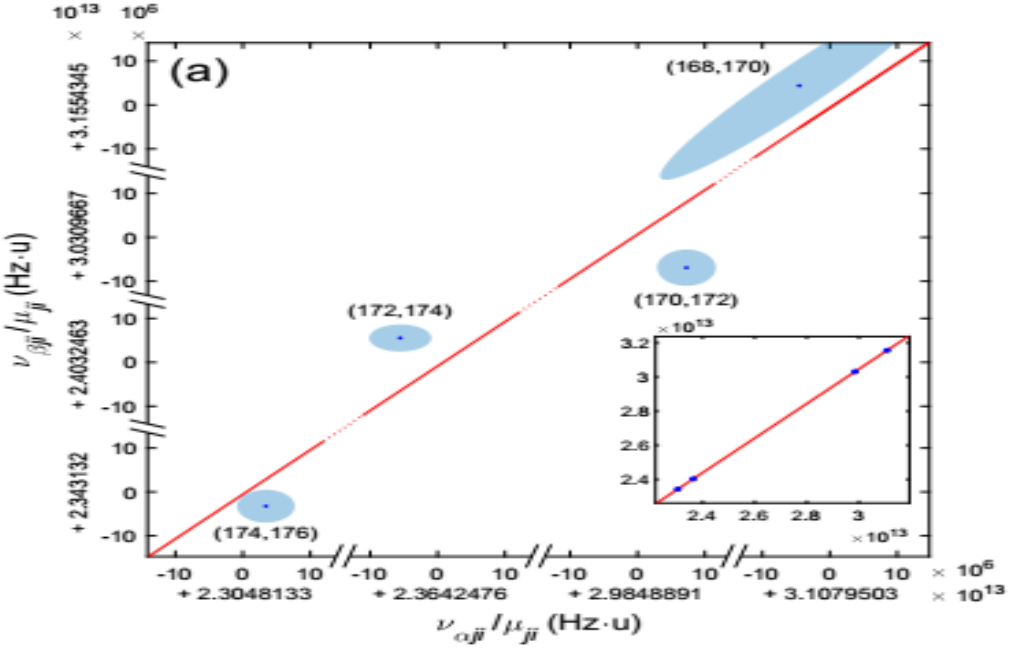
$$+ \left(G_b^{(4)} - \frac{F_b}{F_a} G_a^{(4)}\right)\frac{\boldsymbol{\delta\langle r_{rms}^4\rangle}}{\mu_{AA'}} + \left(\boldsymbol{\nu_b^{NP}} - \frac{F_b}{F_a}\boldsymbol{\nu_a^{NP}}\right)\frac{\mathbf{1}}{\mu_{AA'}}$$

Editors' Suggestion | Featured in Physics

Evidence for Nonlinear Isotope Shift in Yb^+ Search for New Boson

Ian Counts,[1,*] Joonseok Hur,[1,*] Diana P. L. Aude Craik,[1] Honggi Jeon,[2] Calvin Leung,[1] Julian C. Berengut,[3] Amy Geddes,[3] Akio Kawasaki,[4] Wonho Jhe,[2] and Vladan Vuletić[1,†]





Isotope pair (j,i)	μ_{ji} (10^{-6}u^{-1})	$\nu_{\alpha ji}$ (kHz) $\alpha: {}^2S_{1/2} \rightarrow {}^2D_{5/2}$	$\nu_{\beta ji}$ (kHz) $\beta: {}^2S_{1/2} \rightarrow {}^2D_{3/2}$	$\delta\langle r^2\rangle_{ji}$ (fm^2) CI	MBPT	Reference [34]
(168, 170)	70.113 698(46)	2 179 098.93(21)	2 212 391.85(37)	-0.156	-0.149	-0.1561(3)
(170, 172)	68.506 890 50(63)	2 044 854.78(34)	2 076 421.58(39)	-0.146	-0.140	-0.1479(1)
(172, 174)	66.958 651 95(64)	1 583 068.42(36)	1 609 181.47(22)	-0.115	-0.110	-0.1207(1)
(174, 176)	65.474 078 21(65)	1 509 055.29(28)	1 534 144.06(24)	-0.110	-0.105	-0.1159(1)
(170, 174)		3 627 922.95(50)	3 685 601.95(33)			

Preliminary Calculations using AR-RCC in the Yb^+ ion

NMS (GHz amu)

	6S1/2	5D3/2	5D5/2
DHF	3755.62	5847.74	5524.06
RCCSD	1335.43	1074.63	1085.54
RCCSD-T	1372.24	1065.39	1080.01
RCCSDTv	1510.01	972.52	1040.80
+Breit	2.13	6.01	6.10
Final	1512(100)	979(50)	1047(50)
Scaling	1615.52	1237.91	1215.35

SMS (GHz amu)

DHF	-2331.98	-4479.18	-4198.62
RCCSD	446.43	-653.61	-687.37
RCCSD-T	-85.06	-1002.32	-1002.67
RCCSDTv	551.19	-811.97	-850.59
+Breit	5.11	-12.24	-10.01
Final	556.30	-824.21	-860.60

FS (MHz/fm^2)

DHF	-11327.28	-0.0002	~0.0
RCCSD	-14811.36	1664.98	1444.95
RCCSD-T	-14610.25	1663.95	1439.48
RCCSDTv	-15077.50	1526.21	1295.46
+Breit	51.59	10.83	14.06
Final	-15025.91(450)	1537.04(50)	1309.52(50)

G^(2) (MHz/fm^4)

DHF	30.33	~0.0	~0.0
RCCSD	39.66	-4.44	-3.86
RCCSD-T	39.12	-4.44	-3.84
RCCSDTv	40.18	-4.10	-3.48
+Breit	-0.15	-0.06	-0.06
Final	40.03	-4.16	-3.54

G^(4) from fitting (MHz/fm^4)

DHF	10.93	~0.0	0.0
RCCSD	13.86	-1.78	-1.70
+Breit	-0.05	-0.01	~0.0
Final	13.81(20)	-1.79(22)	-1.70(20)

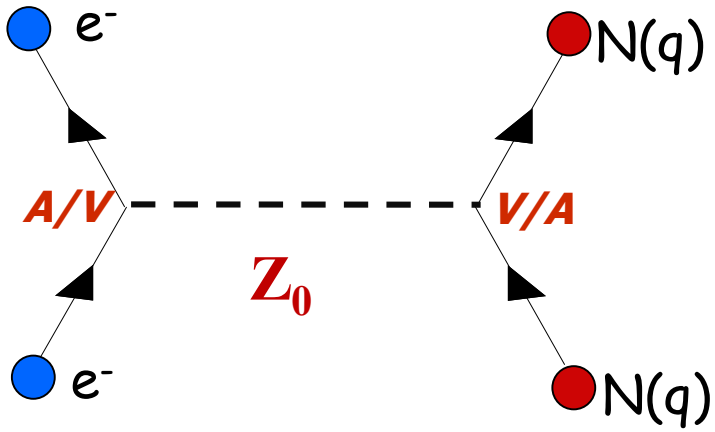
Summary and Outlook

- Developed all-order relativistic many-body methods for accurate calculations of atomic properties..
- We have developed RCC methods in the FF, EVE and AR frameworks to estimate isotope shifts.
- Nuclear charge radii of indium, aluminum, potassium etc. isotopes were investigated using our RCC methods.

- ➢ Intend to extend these studies in other elements of periodic table to understand roles of electron correlation effects in them.
- ➢ Planning to develop codes further to study the effects of non-linear effects and infer new physics from Isotope Shifts.
- ➢ Developing new many-body methods to study these effects.

Weak interaction Hamiltonian(s)

Strength: $\sim 10^{-14}$



Atomic Hamiltonian:

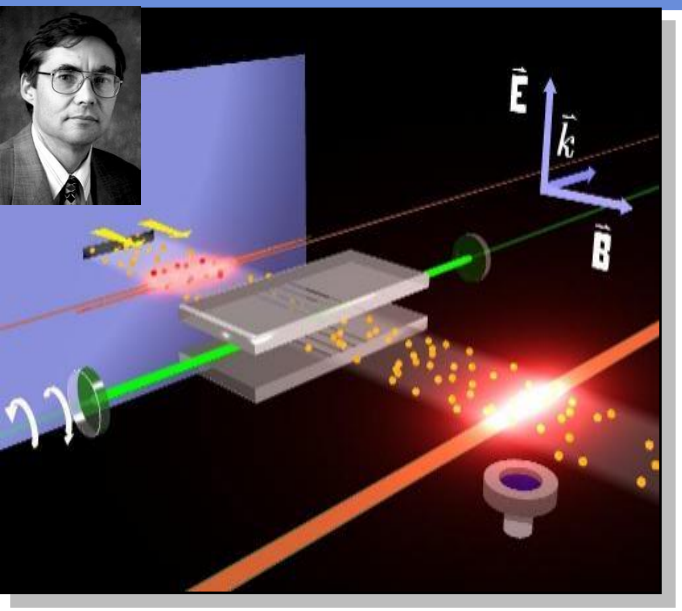
$$H_{PNC} = H_{PNC}^{NSI} + H_{PNC}^{NSD}$$

$$= \frac{G_F}{\sqrt{2}}\left[-\frac{Q_W}{2}\gamma_5 + \kappa\,\vec{\alpha}\cdot\vec{I}\right]\rho_n(r)$$

where $G_F \approx 2.219 \times 10^{-14}\ au$ is the Fermi constant, $\vec{I}$ is the nuclear spin, α and γ_5 are the Dirac matrices and $\rho_n(r)$ is the nuclear density.

The dimensionless constants Q_W and κ characterize the strengths of the NSI and NSD interactions respectively.

Precise measurement in ^{133}Cs (~0.35%)



C. S. Wood et al, Science 275, 1759 (1997).

NSI amplitude:

$$Im\left(\frac{E1_{PNC}^{NSI}}{\beta}\right) = -1.5935(56)\ mV/cm$$

NSD amplitude:

$$Im\left(\frac{E1_{PNC}^{NSD}}{\beta}\right) = -0.077(11)\ mV/cm$$

$\leq 0.5\%$ $\leq 0.5\%$ $\leq 0.5\%$

$$Im\left(\frac{E1_{PNC}^{NSI}}{\beta}\right)^{expt} = Q_W \times \left(\frac{E1_{PNC}^{NSI}}{Q_W}\right)^{theory} \times \left(\frac{1}{\beta}\right)^{expt/theory}$$

Till today 3 groups have reported calculations within 0.5% but their final results differ by about 1%. The measurement may have an issue.

A perturbative approach (NSI)

Here: $H = H_{at} + G_F H_w$ with $G_F \approx 2.2 \times 10^{-14}\ a.u.$

Since electromagnetic interactions dominates strongly:

$$|\Psi_n(n,J)\rangle = \left|\Psi_n^{(0)}(n,J,\pi)\right\rangle + G_F \left|\Psi_n^{(1)}(n,J,\pi')\right\rangle + O\left(G_F^2\right)$$

And $O\left(G_F^2\right) \approx 10^{-28}$, $|\Psi_n(n,J)\rangle \approx \left|\Psi_n^{(0)}(n,J,\pi)\right\rangle + G_F \left|\Psi_n^{(1)}(n,J,\pi')\right\rangle$

Thus: $$\left(\frac{E1_{PNC}^{NSI}}{Q_W}\right)^{theory} = \frac{\langle \Psi_f | D | \Psi_i \rangle}{\sqrt{\langle \Psi_f | \Psi_f \rangle \langle \Psi_i | \Psi_i \rangle}} \simeq \frac{\left[\left\langle \Psi_f^{(0)} \middle| D \middle| \Psi_i^{(1)} \right\rangle + \left\langle \Psi_f^{(1)} \middle| D \middle| \Psi_i^{(0)} \right\rangle\right]}{\sqrt{\left\langle \Psi_f^{(0)} \middle| \Psi_f^{(0)} \right\rangle \left\langle \Psi_i^{(0)} \middle| \Psi_i^{(0)} \right\rangle}}$$

- **Requirements are:**
  - Determination of the zeroth- and first-order wave functions.
  - Equal treatment of both the wave functions using a single theory.

Sum-over-states approach and accuracy test

In sum-over-states approach: $\left|\Psi_n^{(1)}\right\rangle = \sum_{I\neq n} |\Psi_I^{(0)}\rangle \frac{\left\langle \Psi_I^{(0)}\middle| H_w \middle|\Psi_n^{(0)}\right\rangle}{E_n^{(0)} - E_I^{(0)}}$

Which leads to:

$$E1_{PNC}^{NSI} \simeq \sum_{I\neq i} \frac{\left\langle \Psi_f^{(0)}\middle| D \middle|\Psi_I^{(0)}\right\rangle \left\langle \Psi_I^{(0)}\middle| H_w \middle|\Psi_i^{(0)}\right\rangle}{E_i^{(0)} - E_I^{(0)}} + \sum_{f\neq i} \frac{\left\langle \Psi_f^{(0)}\middle| H_w \middle|\Psi_I^{(0)}\right\rangle \left\langle \Psi_I^{(0)}\middle| D \middle|\Psi_i^{(0)}\right\rangle}{E_f^{(0)} - E_I^{(0)}}$$

where Q_W is absorbed in defining unit of the $E1_{PNC}^{NSI}$ amplitude.

Accuracy test:

- $\langle \Psi_I | D | \Psi_J \rangle$ → comparing calculated E1 matrix elements with expt values.
- $\langle \Psi_I | H_W | \Psi_J \rangle \rightarrow \langle \Psi_I | H_{hyf} | \Psi_J \rangle \approx \sqrt{\langle \Psi_I | H_{hyf} | \Psi_I \rangle \langle \Psi_J | H_{hyf} | \Psi_J \rangle}$ (expt values).
- $E_I^{(0)} - E_J^{(0)}$ → comparing calculated excitation energies with expt values.

Calculations for Cs and Shortcomings

$$E1_{PNC}^{NSI}(6S \rightarrow 7S) = \sum_{np_{1/2}} \frac{\langle 7S|D|np_{1/2}\rangle\langle np_{1/2}|H_W|6S\rangle}{E_{6S}^{(0)} - E_{nP_{1/2}}^{(0)}}$$

$$+ \sum_{np_{1/2}} \frac{\langle 7S|H_W|np_{1/2}\rangle\langle np_{1/2}|D|6S\rangle}{E_{7S}^{(0)} - E_{np_{1/2}}^{(0)}}$$

$$= \text{Core (n<6)} + \text{Main (n=6-9)} + \text{Tail}$$

Limitations:

- Core, Main and Tail contributions cannot be treated on equal footing.
- Correlations among the Core and Valence electrons not treated aptly.
- Correlations among weak and electromagnetic ints. are not on same level. So it misses double-core-polarization (DCP) effects.

Discrepancies from high-accuracy calculations

$$E1_{PNC}^{NSI} = \sum_n \frac{\left\langle 7S_{1/2}^{(0)} \middle| D \middle| nP_{1/2}^{(0)} \right\rangle \left\langle nP_{1/2}^{(0)} \middle| H_w \middle| 6S_{1/2}^{(0)} \right\rangle}{E_{6S_{1/2}}^{(0)} - E_{nP_{1/2}}^{(0)}} + \sum_n \frac{\left\langle 7S_{1/2}^{(0)} \middle| H_w \middle| nP_{1/2}^{(0)} \right\rangle \left\langle nP_{1/2}^{(0)} \middle| D \middle| 6S_{1/2}^{(0)} \right\rangle}{E_{7S_{1/2}}^{(0)} - E_{nP_{1/2}}^{(0)}}$$

$$= Core(n<6) + \underbrace{Main(n=6-9) + Tail(n\geq 10)}_{Valence}$$

Contribution to the $E1_{PV}^{NSI}$ amplitude of the 7S-6S transition in ^{133}Cs in $10^{-11} i\left(-\frac{Q_w}{N}\right) e a_0$

Reference	Core	Main	Tail	Total	Method
Porsev et al. PRL 2009, PRD 2010	-0.0020	0.8823	0.0195	**0.8998**	CCSDvT, sum-over-states, Blend of methods
Dzuba et al. PRL 2012	0.0018	0.8711	0.0238	**0.8967**	TDHF+BO (original)
	0.0018	0.8823	0.0238	0.9079	Borrowed from Porsev et al.
Sahoo et al. PRD 2021	-0.0018	0.8594*	0.0391	**0.8967**	RCCSDT
Tan et al. PRA 2022	_	_	_	**0.8903**	Parity-mixed RPA

* Contribution from the $9P_{1/2}$ state included in Tail

Equivalent expressions

$$E1_{PNC}^{NSI} = \left\langle \Psi_f^{(0)} | D | \Psi_i^{(1)} \right\rangle + \left\langle \Psi_f^{(1)} | D | \Psi_i^{(0)} \right\rangle$$

$$= \sum_{k \neq i} \left\langle \Psi_f^{(0)} \middle| D \middle| \Psi_k^{(0)} \right\rangle \frac{\left\langle \Psi_k^{(0)} | H_w | \Psi_i^{(0)} \right\rangle}{E_i^{(0)} - E_k^{(0)}} + \sum_{k \neq f} \frac{\left\langle \Psi_f^{(0)} \middle| H_w \middle| \Psi_k^{(0)} \right\rangle}{E_f^{(0)} - E_k^{(0)}} \left\langle \Psi_k^{(0)} | D | \Psi_i^{(0)} \right\rangle$$

By using $\omega = E_f^{(0)} - E_i^{(0)}$, we can write:

$$|\tilde{\Psi}_i^{(1)}\rangle = \sum_{k \neq f} |\Psi_k^{(0)}\rangle \frac{\langle \Psi_k^{(0)} | D | \Psi_i^{(0)} \rangle}{(E_i^{(0)} - E_k^{(0)} + \omega)}$$

and

$$|\tilde{\Psi}_f^{(1)}\rangle = \sum_{k \neq i} |\Psi_k^{(0)}\rangle \frac{\langle \Psi_k^{(0)} | D | \Psi_f^{(0)} \rangle}{(E_f^{(0)} - E_k^{(0)} - \omega)}$$

$$E1_{PV}^{NSI} = \left\langle \Psi_f^{(0)} | D | \Psi_i^{(1)} \right\rangle + \left\langle \Psi_f^{(1)} | D | \Psi_i^{(0)} \right\rangle$$

$$= \left\langle \tilde{\Psi}_f^{(1)} | H_w | \Psi_i^{(0)} \right\rangle + \left\langle \Psi_f^{(0)} | H_w | \tilde{\Psi}_i^{(1)} \right\rangle$$

$$= \left\langle \Psi_f^{(0)} | D | \Psi_i^{(1)} \right\rangle + \left\langle \Psi_f^{(0)} | H_w | \tilde{\Psi}_i^{(1)} \right\rangle$$

$$= \left\langle \tilde{\Psi}_f^{(1)} | H_w | \Psi_i^{(0)} \right\rangle + \left\langle \Psi_f^{(1)} | D | \Psi_i^{(0)} \right\rangle$$

All are equivalent in an exact theory.

Differences due to approximations

$$E1_{PNC}^{NSI} = \left\langle \Psi_f^{(0)} \middle| D \middle| \Psi_i^{(1)} \right\rangle + \left\langle \Psi_f^{(1)} \middle| D \middle| \Psi_i^{(0)} \right\rangle \quad \rightarrow \textbf{RCC method}$$

$$\sim \left\langle \Phi_f^{(0)} \middle| D \middle| \Phi_i^{(\infty,1)} \right\rangle + \left\langle \Phi_f^{(\infty,1)} \middle| D \middle| \Phi_i^{(0)} \right\rangle \quad \rightarrow \textbf{CPDF method}$$

$$\sim \left\langle \Phi_f^{(0)} \middle| H_{NSI}^{PNC} \middle| \Phi_i^{(\infty,1)} \right\rangle + \left\langle \Phi_f^{(\infty,1)} \middle| H_{NSI}^{PNC} \middle| \Phi_i^{(0)} \right\rangle \quad \rightarrow \textbf{RPA}$$

$$\sim \left\langle \Phi_f^{(0)} \middle| H_{NSI}^{PNC} \middle| \Phi_i^{(\infty,1)} \right\rangle + \left\langle \Phi_f^{(0)} \middle| D \middle| \Phi_i^{(\infty,1)} \right\rangle \quad \rightarrow \textbf{TDHF method}$$

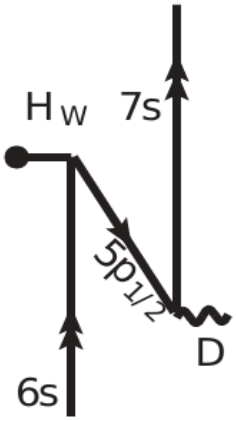
CPDF and RPA methods:

- Includes only a set of single excitations with all-order perturbation in residual interactions (core-polarization effects).
- Misses out pair-correlation contributions.
- Does not include correlations among the D and H_{PNC}^{NSI} operators.

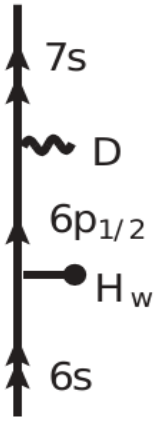
Diagrammatic representation

At the DHF level:

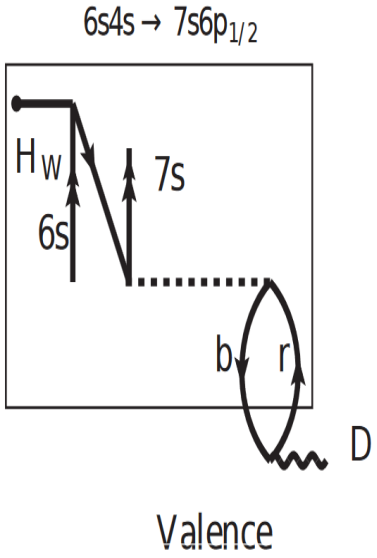
- **The intermediate state is a single atomic state.**
- **We can segregate Core and Valence contribution uniquely.**



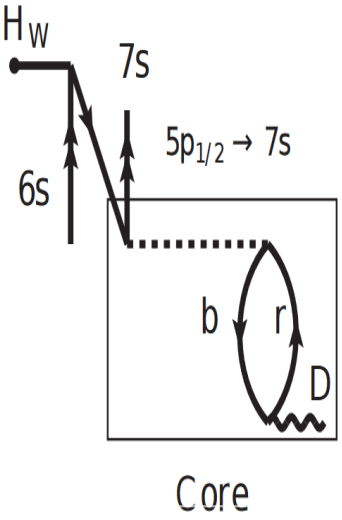
Core



Valence



Valence



Core

After including correlation effect:

- **One cannot uniquely split correlation correction in the Core and Valence contributions.**
- **Depending upon choice of perturbation the definition of Core and Valence contribution changes.**

Reproducing Dzuba et al's results (J Chem Phys A 127, 7518 (2023))

Table: $E1_{PV}^{NSI}$ for the $7S - 6S$ transition in ^{133}Cs across different many body methods

Method	$\langle 7S^{PV}\|D\|6S\rangle$	$\langle 7S\|D\|6S^{PV}\rangle$	Sum	Method	$\langle 7S^{PV}\|D\|6S\rangle$	$\langle 7S\|D\|6S^{PV}\rangle$	Sum
Ours				Core		Roberts et al. PRD 2022	
DHF	−0.02638	0.02465	−0.00173	HF	−0.02645	0.02472	−0.00174
CPDF	−0.04298	0.04099	−0.00199	HF+δV_w^{∞}	−0.04319	0.04119	−0.00201
RPA	−0.03536	0.03564	0.00028				
CPDF-RPA*	−0.05794	0.05963	0.00169	HF+δV_w^{∞} + δV_d^{∞}	−0.05822	0.05992	0.00170
Method	$\langle 7S^{PV}\|D\|6S\rangle$	$\langle 7S\|D\|6S^{PV}\rangle$	**Sum**		$\langle 7S^{PV}\|D\|6S\rangle$	$\langle 7S\|D\|6S^{PV}\rangle$	**Sum**
Ours				Total		Martensson et al. J. Phys. 1985	
DHF	1.01168	−0.27418	0.73750	DHF	1.010	−0.274	0.736
CPDF	1.26664	−0.34409	0.92255	CPDF	1.267	−0.344	0.924
RPA	1.02557	−0.31617	0.70940	RPA	1.023	−0.316	0.707
CPDF-RPA*	1.27910	−0.39150	0.88760	CPDF-RPA*	1.279	−0.391	0.888
CPDF-RPA			0.88590	CPDF-RPA			0.886

e-q couplings and Masses of extra Z-bosons

Phys. Rev. D 103, 111303(L) (2021)

Measurement + calculations: $\boldsymbol{Q_W^{Z,N} = -73.71(26)_{ex}(23)_{th}}$

In the SM: $\boldsymbol{Q_W^{SM} = -73.23(1)}$ with $\sin^2\bar{\theta}_W(2.4\,MeV) = 0.23857(5)$

From the difference: $\boldsymbol{\sin^2\bar{\theta}_W(2.4\,MeV) = 0.2408(16)}$

By using the relation: $376C_{1u} + 422C_{1d} = 73.71(35)$

$\boldsymbol{C_{1u} = -0.1877(9)}$ for $C_{1d} = 0.3419$ and

$\boldsymbol{C_{1d} = 3429(8)}$ for $C_{1u} = -0.1888.$

Mass of a dark-boson: $\boldsymbol{\delta\epsilon\frac{M_Z}{M_{Z_d}} \simeq -0.0051(37).}$

Mass of an extra boson: $\boldsymbol{M_{Z_x} \geq 2.36\,TeV.}$

Summary & Outlook

- Our RCC method treats the ``Core", ``Main" and ``Tail" contributions to $E1_{PNC}$ on an equal footing.
- It also accounts for DCP contributions implicitly.
- Though our calculation shows ``Core" contribution is agreeing with Porsev et al (2009 & 2010); it neglects a lot of physical effects that Dzuba et al and we consider.
- It estimates uncertainties to ``Core", ``Main" and ``Tail" in a consistent manner.

- We are developing RCC methods to remove non-terminating series in the calculations.
- The method has to be extended for NSD interactions.
- It is also necessary to calculate β using a similar approach.

Open Questions

- Is there an ultimate atomic theory for accurate calculations?
- Why results from different approaches of a given theory differ? Can these differences be removed/suppressed?
- How to estimate uncertainties in many-body calculations?
- What are the implementation differences among nuclear, atomic and molecular many-body methods?

Collaborators and Acknowledgement