## Precise Atomic Spectra and Neutral Weak Charges



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Precision Tests with Neutral-Current Coherent Interactions with Nuclei, May 23-27, 2022, Mainz

## Outline

- Objective of the study
- General approach to atomic calculations
- Coupled-cluster theory ansaetz
- Atomic parity violation and neutral weak charge
- Sum-over-states vs. linear response approaches
- Accuracy test
- Results and Summary


## Multi-electron atomic systems

Electromagnetic interaction (long-range):

- Mediated by photon (massless)
- Strength scales ~ Z
- Parity is a good quantum number
- Requires many-body methods to solve


In typical approach Hamiltonian: $\boldsymbol{H}_{\boldsymbol{a t}}\left(\boldsymbol{M}_{\boldsymbol{N}}, \boldsymbol{R}_{\boldsymbol{N}}, \boldsymbol{r}_{\boldsymbol{e}}\right)=\boldsymbol{H}_{\boldsymbol{n u c}} \oplus \boldsymbol{H}_{\boldsymbol{a t}}$

Non-relativistic: $\boldsymbol{H}_{a t}^{N R}=\sum_{i}\left[\frac{p_{i}^{2}}{2 m_{e}}+V_{N}\left(\boldsymbol{r}_{i}\right)\right]+\frac{1}{2} \sum_{i, j} \frac{1}{\left|\vec{r}_{i}-\vec{r}_{j}\right|}$
Relativistic: $H_{a t}^{R e l}=\sum_{i}\left[c \vec{\alpha}_{i} \cdot \vec{p}_{i}+\beta_{i} m_{e} c^{2}+V_{N}\left(r_{i}\right)\right]+\frac{1}{2} \sum_{i, j} \frac{1}{\left|\vec{r}_{i}-\vec{r}_{j}\right|}$

## General approaches to atomic calculations

In precision studies: $\boldsymbol{H}_{\boldsymbol{a t}}=\boldsymbol{H}_{a t}^{D C}+\boldsymbol{H}_{a t}^{B r e i t}+\boldsymbol{H}_{a t}^{l o-Q E D}($ model $)$

Atomic Hamiltonian: $\boldsymbol{H}_{\boldsymbol{a t}}=\boldsymbol{F}+\boldsymbol{G}$

EOM: $\boldsymbol{H}_{\boldsymbol{a t}}\left|\Psi_{\mathbf{0}}\right\rangle=\boldsymbol{E}_{\mathbf{0}}\left|\Psi_{0}\right\rangle$

Perturbative approach: $\boldsymbol{H}_{\boldsymbol{a t}}=\boldsymbol{H}_{\boldsymbol{M F}}+\lambda \boldsymbol{V}_{\text {res }}$

$$
\begin{aligned}
& \left|\Psi_{0}\right\rangle=\left|\Phi_{0}^{(0)}\right\rangle+\lambda\left|\Phi_{0}^{(1)}\right\rangle+\lambda^{2}\left|\Phi_{0}^{(2)}\right\rangle+\lambda^{3}\left|\Phi_{0}^{(3)}\right\rangle+\cdots \\
& E_{0}=E_{0}^{(0)}+\lambda E_{0}^{(1)}+\lambda^{2} E_{0}^{(2)}+\cdots
\end{aligned}
$$

## All-order atomic calculations

$\left|\Psi_{0}\right\rangle=\left|\Phi_{0}^{(0)}\right\rangle+\lambda_{1}\left|\Phi_{0}^{(1)}\right\rangle+\lambda_{1}^{2}\left|\Phi_{0}^{(2)}\right\rangle+\lambda_{1}^{2}\left|\Phi_{0}^{(3)}\right\rangle+\cdots$
Fock space P-space --------------------------s-space
i.e. $\quad\left|\Phi_{0}^{(n)}\right\rangle=\sum_{k \neq 0}^{N}\left|\Phi_{k}^{(0)}\right\rangle C_{0 k}^{(n)}$

In terms of level of excitations $\rightarrow$ Configuration Interaction (CI)

$$
\Rightarrow\left|\Psi_{0}\right\rangle=\left|\Phi_{0}^{(0)}\right\rangle+C_{I}^{(\infty)}\left|\Phi_{I}^{(0)}\right\rangle+C_{I I}^{(\infty)}\left|\Phi_{I I}^{(0)}\right\rangle+\cdots
$$

Further: $\left|\Phi_{k}^{(0)}\right\rangle \equiv\left|\Phi_{a b c \ldots \ldots}^{p q r \ldots}\right\rangle=a_{p}^{+} a_{q}^{+} a_{r}^{+} \ldots a_{a} a_{b} a_{c}\left|\Phi_{0}^{(0)}\right\rangle$
Coupled-cluster (CC) method:

$$
\begin{aligned}
\Rightarrow\left|\Psi_{0}\right\rangle & =\left|\Phi_{0}^{(0)}\right\rangle+T_{I}\left|\Phi_{0}^{(0)}\right\rangle+\left(T_{I I}+\frac{1}{2} T_{I}^{2}\right)\left|\Phi_{0}^{(0)}\right\rangle+\cdots+T_{N}\left|\boldsymbol{\Phi}_{0}^{(0)}\right\rangle \\
& =e^{T}\left|\Phi_{0}^{(0)}\right\rangle \quad \text { where } \mathrm{T}=\mathrm{T}_{\mathrm{I}}+\mathrm{T}_{\mathrm{II}}+\cdots+T_{N}
\end{aligned}
$$

## Calculating properties using standard CC theory

Property: $\langle 0\rangle_{f i}=\frac{\left\langle\Psi_{f}\right| O\left|\Psi_{i}\right\rangle}{\sqrt{\left\langle\Psi_{f} \mid \Psi_{f}\right\rangle\left\langle\Psi_{i} \mid \Psi_{i}\right\rangle}}$
Also, here: $\mathbf{0}=\boldsymbol{O}^{N R}+\boldsymbol{O}^{\text {Rel }}+\boldsymbol{O}^{\text {QED }}($ model $)$
In RCC theory: $\langle 0\rangle_{f i}=\frac{\left\langle\Phi_{f}\right| e^{T_{f}^{+}} O e^{T_{i}}\left|\Phi_{i}\right\rangle}{\sqrt{\left\langle\Phi_{f}\right| e^{T_{f}^{+}} e^{T_{f}}\left|\Phi_{f}\right\rangle\left\langle\Phi_{i}\right| e^{T_{i}^{+}} e^{T_{i}}\left|\Phi_{i}\right\rangle}}$

## Points to be noted:

- Possesses two non-terminating series.
- Unmanageable with two-body operators like SMS operator. It does not satisfy the Hellmann-Feynman theorem.
But any property can be evaluated.


## Atomic parity violation and neutral weak charge

$C_{1 u}=-\frac{1}{2}+\frac{4}{3} \sin ^{2}\left(\theta_{W}\right) \approx-0.19$
$C_{1 d}=\frac{1}{2}-\frac{2}{3} \sin ^{2}\left(\theta_{W}\right) \approx 0.35$
$C_{2 u}=-\frac{1}{2}+2 \sin ^{2}\left(\theta_{W}\right) \approx-0.04$
$C_{2 d}=\frac{1}{2}-2 \sin ^{2}\left(\theta_{W}\right) \approx 0.04$.

where $\theta_{\mathrm{w}}$ is the Weinberg angle.

NSI: $C_{1 q}=2 g_{A}^{e} g_{V}^{q}$

NSD: $C_{2 q}=2 g_{V}^{e} g_{A}^{q}$

Standard Model (SM) scenario:


In NSI interaction, couplings are added coherently:

$$
\begin{aligned}
Q_{W}^{S M}= & (2 Z+N) C_{1 u}+(Z+2 N) C_{1 d} \\
& =-N+Z\left(1-4 \operatorname{Sin}^{2} \theta_{W}\right)
\end{aligned}
$$

Inclusion of radiative corrections:

$$
Q_{W} \approx Q_{W}^{S M}-0.008 S
$$

## Probing BSM physics from APV



## Beyond SM scenario:

$$
\begin{aligned}
& C_{1 u}=-\frac{1}{2}+\frac{4}{3} \sin ^{2}\left(\theta_{W}\right) \approx-0.19 \\
& C_{1 d}=\frac{1}{2}-\frac{2}{3} \sin ^{2}\left(\theta_{W}\right) \approx 0.25 \\
& C_{2 u}=-\frac{1}{2}+2 \sin ^{2}\left(\theta_{W}\right) \approx-0.04 \\
& C_{2 d}=\frac{1}{2}-2 \sin ^{2}\left(\theta_{W}\right) \approx 0.04 .
\end{aligned}
$$

Thus, we can have: $Q_{W}=Q_{W}^{S M}+\Delta \mathbf{Q}_{W}=Q_{W}^{S M}+\Delta Q_{W}^{R a d}+\Delta Q_{W}^{B S M}$
New physics:
PHYSICAL REVIEW D 82, 036008 (2010)

$$
\begin{aligned}
& Q_{W}=376 g_{A V}^{e u}+422 g_{A V}^{e d} \\
& \Delta Q_{W}\left(Z_{x}\right) \simeq 0.4(Z+2 N) \frac{M_{Z_{0}}^{2}}{M_{Z_{x}}^{2}} \\
& \Delta \operatorname{Sin}^{2} \Theta_{W}(\mu) \simeq-0.43 \epsilon \delta \frac{M_{Z_{0}}}{M_{Z_{d}}} \\
& \quad \text { Phys. Rev. D 103, L111303(2021) }
\end{aligned}
$$

## Additional interaction Hamiltonian

## Weak interaction (short-range)

- Mediated by $\mathrm{Z}_{0}$ bosons (heavy mass)
- Strength scales $\sim Z^{3}$
- Mixes spectra of different parities
- Nucleus gets nuclear weak charge ( $Q_{w}$ )

$$
\mathrm{e}
$$

บi.

Periodic Table of Elements


$$
\begin{aligned}
H_{P N C} & =H_{P N C}^{N S I}+H_{P N C}^{N S D} \\
& =\frac{G_{F}}{\sqrt{2}}\left[-\frac{Q_{W}}{2} \gamma_{5}+\kappa \vec{\alpha} \cdot \vec{I}\right] \rho_{n}\left(r_{e}\right) \\
& \simeq Q_{W} G_{F} H_{w}
\end{aligned}
$$

$\Rightarrow$ Sensitive to electronic wave functions in nuclear region.

## Precise measurement in ${ }^{133} \mathrm{Cs}(\sim 0.35 \%)$


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

NSI amplitude:
$\operatorname{Im}\left(\frac{E 1_{P N C}^{N S I}}{\beta}\right)=-1.5935(56) \mathrm{mV} / \mathrm{cm}$
NSD amplitude:

$$
\operatorname{Im}\left(\frac{E 1_{P N C}^{N S D}}{\beta}\right)=-0.077(11) \mathrm{mV} / \mathrm{cm}
$$

where $\beta$ is the Stark induced vector polarizability.

$$
\begin{gathered}
\operatorname{Im}\left(\frac{\boldsymbol{E} 1_{P N C}^{N S I}}{\boldsymbol{\beta}}\right)^{\text {expt }}=\boldsymbol{Q}_{W} \times\left(\frac{\boldsymbol{E} 1_{P N C}^{N S I}}{\boldsymbol{Q}_{W}}\right)^{\text {theory }} \times\left(\frac{\mathbf{1}}{\boldsymbol{\beta}}\right)^{\text {expt/theory }} \\
\leq 0.5 \% \\
\leq 0.5 \% \\
\leq 0.5 \%
\end{gathered}
$$

## Challenges in the calculation



Total Hamiltonian:

$$
\begin{gathered}
H=H_{a t}+H_{P N C}^{N S I}=H_{a t}+G_{F} H_{w} \\
\left(\frac{E 1_{P N C}^{N S I}}{Q_{W}}\right)^{\text {theory }}=\frac{\left\langle\Psi_{f}\right| D\left|\Psi_{i}\right\rangle}{\sqrt{\left\langle\Psi_{f} \mid \Psi_{f}\right\rangle\left\langle\Psi_{i} \mid \Psi_{i}\right\rangle}}
\end{gathered}
$$

However, $[\boldsymbol{H}, \boldsymbol{P}] \neq \mathbf{0}$

Do not treat parity as a good quantum number:

* Result obtained in one step, but amount of computation cost will multiply.
* Will be difficult to estimate accuracy of the result.


## A perturbative approach (NSI)

Here: $\quad H=H_{a t}+G_{F} H_{w}$ with $G_{F} \approx 2.2 \times \mathbf{1 0}^{-14}$ a.u.

## Since electromagnetic interactions dominates strongly:

$$
\left|\Psi_{n}(n, J)\right\rangle=\left|\Psi_{n}^{(0)}(n, J, \pi)\right\rangle+G_{F}\left|\Psi_{n}^{(1)}\left(n, J, \pi^{\prime}\right)\right\rangle+O\left(G_{F}^{2}\right)
$$

And $O\left(G_{F}^{2}\right) \approx 10^{-28}, \quad\left|\Psi_{n}(n, J)\right\rangle \approx\left|\Psi_{n}^{(0)}(n, J, \pi)\right\rangle+G_{F}\left|\Psi_{n}^{(1)}\left(n, J, \pi^{\prime}\right)\right\rangle$
Thus: $\left(\frac{E 1_{P N C}^{\text {NSI }}}{Q_{W}}\right)^{\text {theory }}=\frac{\left\langle\Psi_{f}\right| \boldsymbol{D}\left|\Psi_{i}\right\rangle}{\sqrt{\left.\left|\Psi_{f}\right| \Psi_{f}\right\rangle\left\langle\Psi_{i} \mid \Psi_{i}\right\rangle}} \simeq \frac{\left[\left\langle\Psi_{f}^{(0)}\right| D\left|\Psi_{i}^{(1)}\right\rangle+\left\langle\Psi_{f}^{(1)}\right| D\left|\Psi_{i}^{(0)}\right\rangle\right]}{\sqrt{\left\langle\Psi_{f}^{(0)} \mid \Psi_{f}^{(0)}\right\rangle\left\langle\Psi_{i}^{(0)} \mid \Psi_{i}^{(0)}\right\rangle}}$
$>$ 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: $\left|\Psi_{n}^{(1)}\right\rangle=\sum_{I \neq n}\left|\Psi_{I}^{(0)}\right\rangle \frac{\left\langle\Psi_{I}^{(0)}\right| H_{w}\left|\Psi_{n}^{(0)}\right\rangle}{E_{n}^{(0)}-E_{I}^{(0)}}$

## Which leads to:

$$
E 1_{P N C}^{N S I} \simeq \sum_{I \neq i} \frac{\left\langle\Psi_{f}^{(0)}\right| D\left|\Psi_{I}^{(0)}\right\rangle\left\langle\Psi_{I}^{(0)}\right| H_{w}\left|\Psi_{i}^{(0)}\right\rangle}{E_{i}^{(0)}-E_{I}^{(0)}}+\sum_{f \neq i} \frac{\left\langle\Psi_{f}^{(0)}\right| H_{w}\left|\Psi_{I}^{(0)}\right\rangle\left\langle\Psi_{I}^{(0)}\right| D\left|\Psi_{i}^{(0)}\right\rangle}{E_{f}^{(0)}-E_{I}^{(0)}}
$$

where $Q_{W}$ is absorbed in defining unit of the $E 1_{P N C}^{N S I}$ amplitude.

## Accuracy test:

- $\left\langle\Psi_{I}\right| D\left|\Psi_{J}\right\rangle \rightarrow$ comparing calculated E 1 matrix elements with expt values.
- $\left\langle\Psi_{I}\right| H_{W}\left|\Psi_{J}\right\rangle \rightarrow\left\langle\Psi_{I}\right| H_{h y f}\left|\Psi_{J}\right\rangle \approx \sqrt{\left\langle\Psi_{I}\right| H_{h y f}\left|\Psi_{I}\right\rangle\left\langle\Psi_{J}\right| H_{h y f}\left|\Psi_{J}\right\rangle} \quad$ (expt values).
- $E_{I}^{(0)}-E_{J}^{(0)} \rightarrow$ comparing calculated excitation energies with expt values.


## Calculations for Cs and Shortcomings

$$
E 1_{P N C}^{N S I}(6 S \rightarrow 7 S)=\sum_{n p_{1 / 2}} \frac{\langle 7 S| D\left|n p_{1 / 2}\right\rangle\left\langle n p_{1 / 2}\right| H_{W}|6 S\rangle}{E_{6 S}^{(0)}-E_{n P_{1 / 2}}^{(0)}}
$$

$$
+\sum_{n p_{1 / 2}} \frac{\langle 7 S| H_{W}\left|n p_{1 / 2}\right\rangle\left\langle n p_{1 / 2}\right| D|6 S\rangle}{E_{7 S}^{(0)}-E_{n p_{1 / 2}}^{(0)}}
$$

$=$ Core $(\mathrm{n}<6)+$ Main $(\mathrm{n}=6-9)+$ 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.


## Linear response approach using RCC theory

$$
\begin{aligned}
& \boldsymbol{H}_{a t}\left|\Psi_{n}^{(\mathbf{0})}\right\rangle=\boldsymbol{E}_{n}^{(\mathbf{0})}\left|\Psi_{n}^{(\mathbf{0})}\right\rangle \quad \text { and } \\
& \left(\boldsymbol{H}_{a t}-\boldsymbol{E}_{n}^{(\mathbf{0})}\right)\left|\boldsymbol{\Psi}_{n}^{(\mathbf{1})}\right\rangle=\left(\boldsymbol{E}_{n}^{(1)}-\boldsymbol{H}_{\boldsymbol{w}}\right)\left|\boldsymbol{\Psi}_{n}^{(\mathbf{0})}\right\rangle \quad \text { with } E_{n}^{(1)} \approx 0
\end{aligned}
$$

In (R)CC ansatz: $\quad\left|\Psi_{n}\right\rangle=e^{S}\left|\widetilde{\Phi}_{n}\right\rangle=e^{T}\left|\Phi_{n}\right\rangle$
By expanding: $\quad \boldsymbol{T}=\boldsymbol{T}^{(0)}+\boldsymbol{G}_{\boldsymbol{F}} \boldsymbol{T}^{(\mathbf{1})}+\boldsymbol{O}\left(\boldsymbol{G}_{\boldsymbol{F}}^{2}\right)$
$\Rightarrow \quad\left|\Psi_{n}^{(0)}\right\rangle=e^{T^{(0)}}\left|\Phi_{n}\right\rangle \quad$ and $\quad\left|\Psi_{n}^{(1)}\right\rangle=e^{T^{(0)}}\left(\mathbf{1}+\boldsymbol{T}^{(1)}\right)\left|\Phi_{n}\right\rangle$
$\Rightarrow E 1_{P N C}^{N S I}=\left\langle\Phi_{f}\right| \boldsymbol{e}^{T^{(0)+}} \boldsymbol{D} e^{T^{(0)}} \boldsymbol{T}^{(1)}\left|\Phi_{i}\right\rangle+\left\langle\Phi_{f}\right| T^{(1)+} e^{T^{(0)+}} \boldsymbol{D} e^{T^{(0)}}\left|\Phi_{i}\right\rangle$
Using singles and doubles RCC theory ( $\times \mathbf{1 0}^{\mathbf{- 1 1}}\left(-Q_{w} / N\right)$ iea $a_{0}$ ):

1. $6 s^{2} S_{1 / 2} \rightarrow 5 d^{2} D_{3 / 2}$ transition in ${ }^{137} \mathrm{Ba}^{+}: \mathbf{2 . 4 6 ( 2 )}$ ( $\sim 1 \%$ ) Phys. Rev. Lett. 96, 163003 (2006)
2. $7 s^{2} S_{1 / 2} \rightarrow 6 d^{2} D_{3 / 2}$ transition in ${ }^{226}$ Ra' $^{+}: 46.4$ ( $\sim 1 \%$ ) Phys. Rev. A 78, 050501(R) (2008)
3. $6 s^{2} S_{1 / 2} \rightarrow 5 d^{2} D_{3 / 2}$ transition in ${ }^{171} \mathrm{Yb}^{+}: 8.5(5)(\sim 5 \%)$ Phys. Rev. A 84, 010502(R) (2011)

TABLE III. The "core", "main," and "tail" contributions to the $E 1_{\mathrm{PV}}$ amplitude [in units of $-i\left(Q_{W} / N\right) e a_{0} \times 10^{-11}$ ] using the DiracCoulomb Hamiltonian in the DHF, RCCSD, and RCCSDT methods. The "main" contribution is determined using the $n p^{2} P_{1 / 2}$ intermediate states with $n=6,7$, and 8 . Contributions from Breit and QED interactions are quoted separately. Contributions from "extra," the neutral weak interactions among electrons $(e-e)$, and the NSKIN effect are also mentioned. The final results (final) from different works show significant differences.

| Method | Core | Main | Tail | Breit | QED | Extra | $e-e$ | $\delta E 1_{\text {PV }}^{\text {NS }}$ | Final |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| DHF | -0.0017 | 0.7264 | 0.0137 |  |  |  |  |  |  |
| RCCSD | -0.0019 | 0.8623 | 0.0357 |  |  |  |  |  |  |
| RCCSDT | -0.0018 | 0.8594 | $0.0391^{\mathrm{a}}$ | -0.0055 | -0.0028 | 0.0026 | $0.0003^{\mathrm{b}}$ | $-0.00377(39)$ | $0.8893(27)$ |
|  |  |  |  |  |  | $-0.0018(5)^{\mathrm{b}}$ | $0.8977(40)$ |  |  |
| Ref. [23] | $0.0018(8)$ | $0.8823(17)^{\mathrm{a}, \mathrm{b}}$ | $0.0238(35)$ | $-0.0055(1)^{\mathrm{b}}$ | $-0.0029(3)^{\mathrm{b}}$ |  |  |  |  |
| Ref. [22] | -0.0020 | $0.8823(17)^{\mathrm{a}}$ | 0.0195 | $-0.0054^{\mathrm{b}}$ | $-0.0024^{\mathrm{b}}$ | -0.00006 | $0.0003^{\mathrm{b}}$ | $-0.0017^{\mathrm{b}}$ | $0.8906(24)$ |
| Ref. [47] |  | 0.9078 |  | -0.0055 | 0.0036 |  |  | -0.0018 | $0.904(1 \pm 0.5)$ |
| Ref. [48] | $-0.002(2)$ | $0.893(7)^{\mathrm{a}}$ | $0.018(5)$ | $-0.002(2)$ |  |  |  | -0.0006 | $0.907(9)$ |
| Ref. [49] |  | 0.908 |  |  |  |  |  |  | $0.91(1)$ |

${ }^{\text {a }}$ Contains additional contribution from the $9 p^{2} P_{1 / 2}$ state.
${ }^{\mathrm{b}}$ Taken from previous calculation [51].
[This work] B. K. Sahoo, B. P. Das and H. Spiesberger, Phys. Rev. D 103, 111303(L) (2021).
[22] S. G. Porsev, K. Beloy and A. Derevianko, Phys. Rev. Lett. 102, 181601 (2009).
[23] V. A. Dzuba, J. C. Berengut, V. V. Flambaum and B. Roberts, Phys. Rev. Lett. 109, 203003 (2012).
[48] S. A. Blundell, W. R. Johnson and J. Sapirstein, Phys. Rev. Lett. 65, 1411 (1990).
[23] V. A. Dzuba, V. V. Flambaum and O. P. Sushkov, Phys. Lett. A 141, 147 (1989.

## Leading-order non-RPA Core Correlations

$$
\text { PHYS. REV. D 105, } 018302 \text { (2022) }
$$

| Method | Approach | Core | Virtual | Reference |
| :---: | :---: | :---: | :---: | :---: |
| HF | $a b$ initio | -0.00174 |  | [1] |
| RPA | $a b$ initio | 0.00170 |  | [1] |
| RPA | Scaled | 0.00259 |  | [1] |
| $\mathrm{BO}+\mathrm{RPA}$ | $a b$ initio | 0.00181 |  | [1] |
| $\mathrm{BO}+\mathrm{RPA}$ | Scaled | 0.00181 |  | [1] |
| HF | $a b$ initio | -0.0017 | 0.7401 | [2] |
| RCCSD | $a b$ initio | -0.0019 | 0.9006 | [2] |
| RCCSDT | $a b$ initio | -0.0018 | 0.9011 | [2] |
| Lower order |  | -0.0020 |  | [3] |
| RCCSDT | sum-over |  | 0.9073 | [3] |
| RCCSDT | sum-over + scaled |  | 0.9018 | [3] |
| HF | $a b$ initio | -0.00174 |  | [4] |
| RPA | Scaled | 0.00259 |  | [4] |
| $\mathrm{BO}+\mathrm{RPA}$ | $a b$ initio | 0.00170 | 0.8949 | [4] |
| $\mathrm{BO}+\mathrm{RPA}$ | Scaled | 0.00182 | 0.8920 | [4] |
| Earlier reported Core contributions |  |  |  |  |
| RCCSD | $a b$ initio | -0.002 |  | [8] |
| RCCSD | $a b$ initio | -0.002 |  | [9] |
| RCCSD | $a b$ initio | -0.0019 |  | [10] |
| Lower order |  | -0.002(2) |  | [13] |



## New physics constraints from atomic parity violation in ${ }^{133} \mathrm{Cs}$

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TABLE I. Comparison of the calculated energies (in $\mathrm{cm}^{-1}$ ) and $A_{\text {hyf }}$ values (in MHz) from the present work with the NIST data and experimental results. Since the uncertainties of the experimental (Expt) results are below the significant digits, they are not quoted here.

| Method | $6 S$ | $6 P_{1 / 2}$ | $7 S$ | $7 P_{1 / 2}$ | $8 P_{1 / 2}$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Energy values |  |  |  |  |  |
| This work | $31357(50)$ | $20243(20)$ | $12861(15)$ | $9641(10)$ | $5697(10)$ |
| Expt [31] | 31406.47 | 20229.21 | 12871.94 | 9642.12 | 5698.63 |
| $A_{\text {hyf }}$ values |  |  |  |  |  |
| This work | $2306(10)$ | $291(2)$ | $547(2)$ | $94(1)$ | $42(1)$ |
| Expt | $2298.16^{\mathrm{a}}$ | $291.91^{\mathrm{b}}$ | $545.82^{\mathrm{c}}$ | $94.40^{\mathrm{d}}$ | $42.97^{\mathrm{c}}$ |

## PHYS. REV. D 105, 018302 (2022)

TABLE VI. Comparison of contributions from the Breit and QED interactions to the $E 1_{\mathrm{PV}}$ amplitude [in $-i\left(Q_{W} / N\right) e a_{0} \times$ $\left.10^{-11}\right]$ ) of the $6 s^{2} S_{1 / 2}-7 s^{2} S_{1 / 2}$ transition in ${ }^{133} \mathrm{Cs}$ from various methods employed in different works.

| Breit | QED | Method | Reference |
| :--- | :---: | :--- | :---: |
| $-0.0055(5)$ | $-0.0028(3)$ | RCCSDT | $[2]$ |
|  | $-0.0029(3)$ | Correlation potential | $[26]$ |
| -0.0054 |  | RMP(3) | $[17]$ |
| -0.0045 | $-0.27(3) \%$ | Local DHF potential | $[31]$ |
| -0.004 |  | Optimal energy | $[19]$ |
|  | $-0.33(4) \%$ | Radiative potential | $[33]$ |
| -0.0055 |  | Correlation potential | $[34]$ |

## PHYS. REV. D 103, L111303 (2021)

TABLE II. Matrix elements of the operators E1 (in a.u.) and $H_{\mathrm{APV}}^{\mathrm{NSI}}$ [in units of $-i\left(Q_{W} / N\right) \times 10^{-11}$ ], respectively, from our calculations. We also list the precise E1 values inferred from various measurements of lifetimes and Stark shifts of atomic states.

| Transition | E1 amplitude |  | $H_{\text {APV }}^{\text {NSI }}$ amplitude |
| :---: | :---: | :---: | :---: |
|  | This work | Experiment | This work |
| $6 P_{1 / 2} \leftrightarrow 6 S$ | 4.5067(40) | 4.5097(74) [37] | $1.2648(15)$ |
|  |  | $4.4890(65)$ [38] |  |
|  |  | $4.505(2)$ [39] |  |
|  |  | 4.508(4) [40] |  |
| $7 P_{1 / 2} \leftrightarrow 6 S$ | 0.2805(20) | 0.2825 (20) [41] | 0.7210 (15) |
|  |  | 0.2789 (16) [42] |  |
|  |  | $0.27810(45)$ [43] |  |
| $8 P_{1 / 2} \leftrightarrow 6 S$ | 0.0824(10) |  | 0.4783(10) |
| $6 P_{1 / 2} \leftrightarrow 7 S$ | 4.2559(30) | 4.233(22) [44] | $0.6161(15)$ |
|  |  | 4.249(4) [45] |  |
| $7 P_{1 / 2} \leftrightarrow 7 S$ | $10.2915(100)$ | 10.308(15) [46] | 0.3464(10) |
| $8 P_{1 / 2} \leftrightarrow 7 S$ | 0.9623(20) |  | 0.2296(05) |

## BSM physics from Cs PNC study

Measurement + calculations: $Q_{W}^{Z, N}=-73.71(26)_{e x}(23)_{t h}$
In the SM: $\boldsymbol{Q}_{W}^{S M}=-\mathbf{7 3 . 2 3 ( 1 )}$ with $\sin ^{2} \bar{\theta}_{W}(2.4 \mathrm{MeV})=0.23857(5)$

From the difference of nuclear weak charge, we infer:

$$
\sin ^{2} \bar{\theta}_{W}(2.4 \mathrm{MeV})=0.2408(16)
$$

and the isospin conserving oblique parameter: $S=\mathbf{0 . 0 6 0 ( 4 4 )}$
By using the relation: $376 g_{A V}^{e u}+422 g_{A V}^{e d}=73.71(35)$
$\boldsymbol{g}_{A V}^{e u}=\mathbf{- 0 . 1 8 7 7 ( 9 )}$ for $g_{A V}^{e d}=0.3419$ and $g_{A V}^{e d}=\mathbf{3 4 2 9}(8)$ for $g_{A V}^{e u}=-0.1888$.
Mass of a dark-boson: $\delta \epsilon \frac{M_{Z}}{M_{Z_{d}}} \simeq-\mathbf{0 . 0 0 5 1 ( 3 7 )}$.
Mass of an extra boson: $\boldsymbol{M}_{Z_{x}} \geq 2.36 \mathrm{TeV}$.
Phys. Rev. D 103, 111303(L) (2021)

## Summary \& Outlook

Our RCC method treats the "Core", "Main" and "Tail" contributions to $E 1_{P N C}$ on an equal footing.
It also accounts for DCP contributions implicitly.
Our calculation demonstrates "Core" contribution is agreeing with Porsev et al (2009 \& 2010).
It estimates uncertainties to "Core", "Main" and "Tail" in a consistent manner.
$>$ We are developing RCC methods to remove nonterminating series in the calculations.
> The method has to be extended for NSD interactions.
> It is also necessary to calculate $\boldsymbol{\beta}$ using a similar approach.

## Collaborators \& Facility


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