Combination of experiment and theory

Measurement: $E1_{PNC}$ with another forbidden amplitude such as $M1$, $E2$ or $E1_{Stark}$

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

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

→ Our approach

$$= \frac{G_F}{N}\left[\sum_{I\neq i}\frac{\left\langle\Psi_f^{(0)}\middle|D\middle|\Psi_I^{(0)}\right\rangle\left\langle\Psi_I^{(0)}\middle|H_{PNC}^{NSI}\middle|\Psi_i^{(0)}\right\rangle}{E_i^{(0)}-E_I^{(0)}} + \sum_{I\neq f}\frac{\left\langle\Psi_f^{(0)}\middle|H_{PNC}^{NSI}\middle|\Psi_I^{(0)}\right\rangle\left\langle\Psi_I^{(0)}\middle|D\middle|\Psi_i^{(0)}\right\rangle}{E_f^{(0)}-E_I^{(0)}}\right]$$

→ Others

$$= Q_W\, X^{Theory} \rightarrow < 0.5\%$$

Combination: **Nuclear weak charge "Q_W".**

Calculation for ^{133}Cs in 10^{-11} $(-Q_W/N)iea_0$

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

= Core (n<6) + Main (n=6-9) + Tail

- -0.002(2) + 0.893(7) + 0.018(5) → 1%
  [Blundell et al, Phys. Rev. Lett. **65**, 1411 (1990)]
- -0.0020 + 0.8823(17) + 0.0195 → 0.27 %
  [Porsev et al, Phys. Rev. Lett. **102**, 181601 (2009)]
- +0.0018(8) + 0.8823(17) + 0.0238(35) → 0.5 %
  [Dzuba et al, Phys. Rev. Lett. **109**, 203003 (2012)]

The main objective of the present work is to address the issue of large differences in the core-contribution.

Commonly used many-body methods

Random phase approximation (RPA):

$$\left|\Psi_n^{(0)}\right\rangle \rightarrow |\Phi_n\rangle \qquad \text{and} \qquad \left|\Psi_n^{(1)}\right\rangle \rightarrow \Omega_{I,CP}^{(\infty,1)}|\Phi_n\rangle = \Omega_{RPA}^{(1)}|\Phi_n\rangle$$

Configuration interaction (CI) method:

$$\left|\Psi_n^{(0)}\right\rangle = C_0|\Phi_n\rangle + C_I\,|\Phi_I\rangle + C_{II}\,|\Phi_{II}\rangle + \cdots$$

Coupled-cluster (CC) method (all-order perturbation):

$$\begin{aligned}\left|\Psi_n^{(0)}\right\rangle &= C_0|\Phi_n\rangle + C_I\,|\Phi_I\rangle + C_{II}\,|\Phi_{II}\rangle + \cdots \\ &= |\Phi_n\rangle + T_I^{(0)}\,|\Phi_n\rangle + T_{II}^{(0)}\,|\Phi_n\rangle + \frac{1}{2}\,T_I^{(0)^2}|\Phi_n\rangle + \cdots \\ &= e^{T_I^{(0)}+T_{II}^{(0)}+\cdots}\,|\Phi_n\rangle = e^{T^{(0)}}\,|\Phi_n\rangle\end{aligned}$$

First-order perturbed RCC method

$$H = H_{at} + G_F H_{PNC}^{NSI} \quad \text{and} \quad |\Psi_n\rangle \simeq |\Psi_n^{(0)}\rangle + G_F\,|\Psi_n^{(1)}\rangle$$

First-order eqn.: $(H_{at} - E_n^{(0)})|\Psi_n^{(1)}\rangle = (E_n^{(1)} - H_{PNC}^{NSI})\,|\Psi_n^{(0)}\rangle$

$$\Rightarrow \quad \left|\Psi_n^{(1)}\right\rangle = e^{T^{(0)}}\left(1 + T^{(1)}\right)|\Phi_n\rangle$$

It yields: $E1_{PNC}^{NSI} = \langle\Phi_f|e^{T^{(0)+}} D e^{T^{(0)}} T^{(1)}|\Phi_i\rangle$

$$+\langle\Phi_f|T^{(1)+} e^{T^{(0)+}} D e^{T^{(0)}}|\Phi_i\rangle$$

Advantages:

1. Treats "Core", "Main" and "Tail" contributions on an equal footing unlike the "Sum-over-states" approach; thus enables to estimate errors consistently.
2. Incorporates all physical effects including double-core-polarization (DCP) effects implicitly to all orders in correlation effects at a given level of particle-hole excitation.

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Precision determination of weak charge of ^{133}Cs from atomic parity violation

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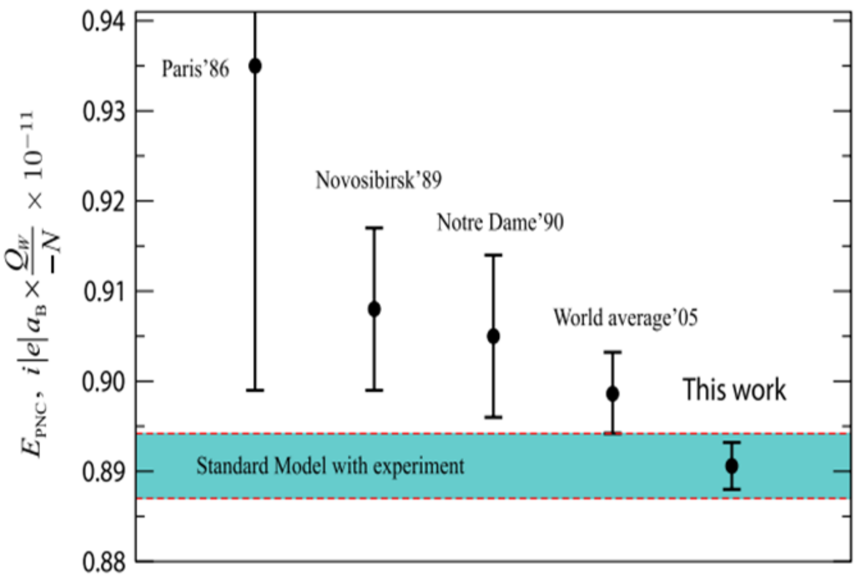

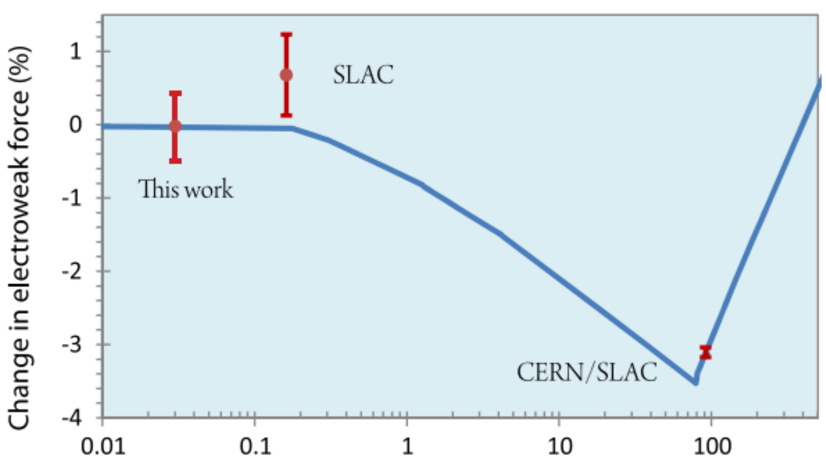

Approximation	E_{PNC}	Δ
"Main" term:		
SD	0.8952	
CC	0.8800	−0.0152
vT (no vT in MEs; pure)	0.8911	0.0111
vT (no vT in MEs; scaled)	0.8915	0.0004
vT (no vT in MEs; scaled, E_{corr})	0.8885	−0.0030
vT (scaled, E_{corr})	0.8856	−0.0029
Line-dressing	0.8825	−0.0031
Vertex dressing	0.8823	−0.0002
Final main (n = 6–9)	0.8823(17)	
Tail:		
$n \geq 10$		0.0195
Core contribution		−0.0020
Basis extrapolation		−0.000 06
Total	0.8998(24)	
Complementary corrections:		
Breit[a]		−0.0054
QED[b]		−0.0024
Neutron skin [c]		−0.0017
e-e weak interaction[d]		0.0003
Sum of corrections		−0.0092
Final E_{PNC}	0.8906(24)	

Revisiting Parity Nonconservation in Cesium

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TABLE I. Partial contributions to the E_{PNC} [in $10^{-11}i(-Q_W/N)$ a.u.] for Cs in different approximations.

Approximation	Core	Main	Tail	Total
RPA[a]	0.0026	0.8705	0.0192	0.8923
BO($\hat{\Sigma}^{(2)}$)[b]	0.0015	0.8641	0.0272	0.8928
BO($\lambda\hat{\Sigma}^{(2)}$)[c]	0.0018	0.8709	0.0244	0.8971
BO($\hat{\Sigma}^{(\infty)}$)[d]	0.0018	0.8711	0.0238	0.8967
BO($\lambda\hat{\Sigma}^{(\infty)}$)[e]	0.0018	0.8678	0.0242	0.8938
Ref. [10][f]	−0.0020	0.8823	0.0195	0.8998

[a]Core polarization but no correlations beyond it.
[b]Brueckner orbitals (BO) calculated with the second-order $\hat{\Sigma}$.
[c]BO calculated with rescaled second-order $\hat{\Sigma}$.
[d]BO calculated with the all-order $\hat{\Sigma}$.
[e]BO calculated with rescaled all-order $\hat{\Sigma}$.
[f]DHF for the core term; coupled cluster for the main term.

TABLE IV. All significant contributions to the E_{PNC} [in $10^{-11}i(-Q_W/N)$ a.u.] for Cs.

Contribution	Value	Source
Core ($n < 6$)	0.0018 (8)	This work
Main ($n = 6$–9)	0.8823 (17)	Ref. [10]
Tail ($n > 9$)	0.0238 (35)	This work
Subtotal	0.9079 (40)	This work
Breit	−0.0055 (1)	Refs. [5,6]
QED	−0.0029 (3)	Ref. [7]
Neutron skin	−0.0018 (5)	Ref. [5]
Total	0.8977 (40)	This work

Calculation for ^{133}Cs in 10^{-11} $(-Q_W/N)iea_0$

RCC term	RLCCSD	RCCSD	RCCSDT
Core contributions			
$\overline{D}T_1^{(1)}$	−0.0534	−0.0410	−0.0410
$T_1^{(1)\dagger}\overline{D}$	0.0519	0.0392	0.0392
Others	−0.0001	−0.0001	~ 0.0
Total	−0.0016	−0.0019	−0.0018
Valence (Main+Tail) contributions			
$\overline{D}S_{1i}^{(1)}$	−0.1663	−0.1913	−0.1874
$S_{1f}^{(1)\dagger}\overline{D}$	2.0603	1.8064	1.7925
$S_{1f}^{(0)\dagger}\overline{D}S_{1i}^{(1)}$	−0.3045	−0.2336	−0.2288
$S_{1f}^{(1)\dagger}\overline{D}S_{1i}^{(0)}$	−0.5529	−0.4218	−0.4147
$\overline{D}S_{2i}^{(1)}$	−0.0357	−0.0263	−0.0257
$S_{2f}^{(1)\dagger}\overline{D}$	0.0006	0.0009	0.0004
$T_2^{(0)\dagger}DS_{3i}^{(1)}$			−0.0019
$S_{3f}^{(1)\dagger}DT_2^{(0)}$			−0.0007
$T_2^{(1)\dagger}\overline{D}S_{3i}^{(0)}$			−0.0004
$S_{3f}^{(0)\dagger}\overline{D}T_2^{(1)}$			−0.0006
$S_{2f}^{(0)\dagger}\overline{D}S_{3i}^{(1)}$			−0.0006
$S_{3f}^{(1)\dagger}\overline{D}S_{2i}^{(0)}$			0.0007
Others	−0.0608	−0.0363	−0.0343
Total	0.9407	0.8980	0.8985
Breit			−0.0055(5)
QED			−0.0028(3)
Extra			0.0026
$e-e$ PNC correction [40]			0.0003
Final			0.8914(27)

Method	Core	Main	Tail	Extra
This work (*ab initio* values)				
DHF	−0.0017	0.7264	0.0137	
RCCSD	−0.0019	0.8623	0.0357	
RCCSDT	−0.0018	0.8594	0.0391	0.0026
Ref. [16]†	−0.002(2)	0.893(7)	0.018(5)	
Ref. [13]†	−0.0020	0.8823(17)	0.0195	
Ref. [14]†	0.0018(8)	~~0.8678~~ 0.8823(17)‡	0.0238(35)	

† Contains additional contribution from the $9p\ ^2P_{1/2}$ state.

TABLE IX. Progresses in the atomic calculations over the years.

Year	Result	Approach	Reference
1989	0.908(9)	*Ab initio*	Ref. [15]
1990	0.909(4)	Sum-over-states	Ref. [16]
2001	0.901	Scaled optimal energy	Ref. [19]
2002	0.904(5)	*Ab initio*	Ref. [41]
2005	0.904	Ref. [41]+QED corr.	Ref. [20]
2009	0.8906(24)	Sum-over-state	Ref. [13]
2012	0.8977(40)	Ref. [13]+core corr.	Ref. [14]
2020	0.8914(27)	*Ab initio*	This work

Our error estimation is more consistent as we treat all three contributions on an equal-footing in the RCC method.

New value for nuclear weak charge

Combining our results of $E1_{PNC}$ and β with the precisely measured $Im(E1_{PNC}/\beta) = 1.5935(56)$ mV/cm [11], where Im means imaginary part, for the $6s\ ^2S_{1/2} - 7s\ ^2S_{1/2}$ transition in ^{133}Cs, we get $Q_W^{\mathrm{at}} = -73.43(25)_{ex}(23)_{th}$. After taking into account nuclear skin effect [43], we get

$$\begin{aligned} Q_W &= Q_W^{\mathrm{at}} + \Delta Q_W^{N-P} \\ &= -73.43(25)_{ex}(23)_{th} + 0.064 \\ &= -73.37(25)_{ex}(24)_{th} \end{aligned} \tag{45}$$

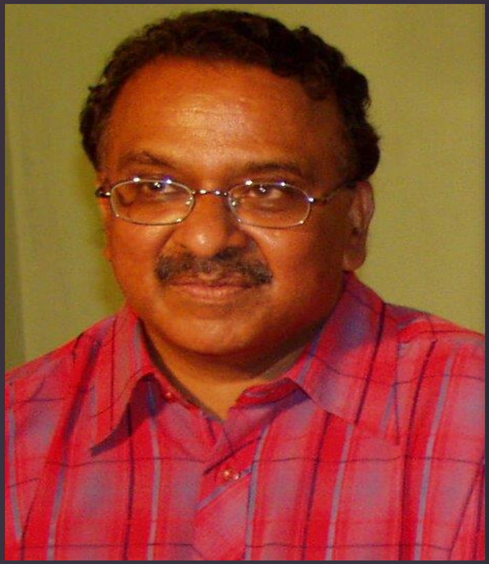
This results in the difference between the value of Q_W obtained from our calculation and the SM value $Q_W^{\mathrm{SM}} = -73.23(1)$ [4] as $\Delta Q_W \equiv Q_W - Q_W^{\mathrm{SM}} = -0.14(35)$.

Summary & Outlook

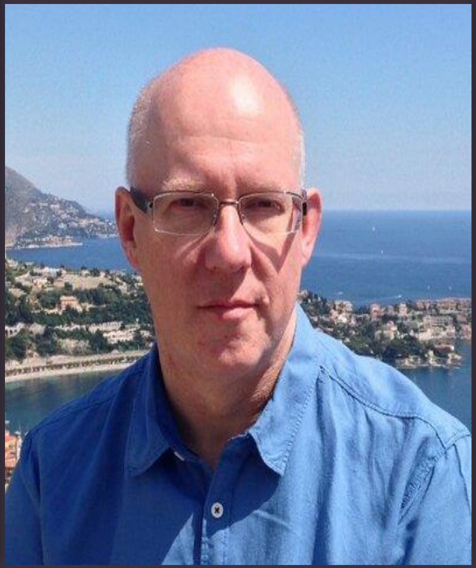
- ❖ Our RCC method treats the ``Core", ``Main" and ``Tail" contributions to $E1_{PNC}$ on an equal footing.
- ❖ It also accounts for DCP contributions implicitly.
- ❖ Our calculation demonstrates ``Core" contribution is agreeing with Porsev et al (2009 & 2010).
- ❖ It estimates uncertainties to ``Core", ``Main" and ``Tail" in a consistent manner and unambiguously.

- ❖ We are developing RCC methods to remove non-terminating series in the calculations.
- ❖ S → D transition or experiments in other systems.
- ❖ A novel technique using optical lattices is proposed.

Acknowledgement



B. P. Das



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Thank You!