

Atomic-Physics Tests of QED & the Standard Model

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Abstract

A brief review of tests of strong-field QED in many-electron atoms and of atomic parity-nonconservation (PNC) induced by Z_0 exchange is given, with emphasis on the role of precise atomic many-body calculations.

Outline

(1970's) "Strong-Field" Lamb-shift corrections for K-shell electrons in heavy atoms were tested to about 2%.

(Dirac Hartree-Fock level atomic theory)

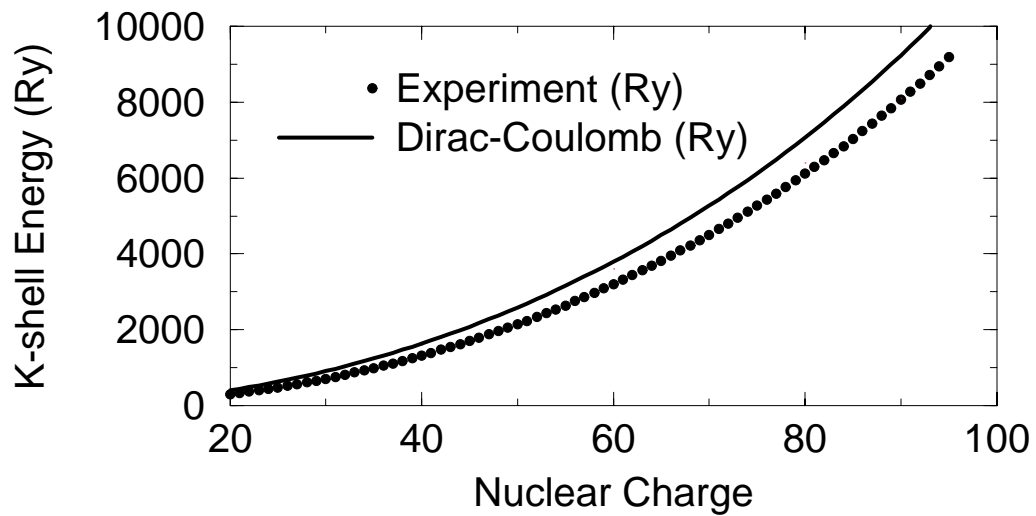
(1980's) QED corrections for valence electrons in highly-charged Li-like, Na-like, and Cu-like ions were tested to about 5%.

(Third-order relativistic MBPT)

(1990's) Amplitudes for parity-forbidden transitions in Cs, Tl, Bi, and Pb were measured to better than 1%. Comparisons with precise theory in Cs gave a test of the standard-model at the 1% level and the first measurement of a nuclear anapole moment.

(All-order relativistic MBPT)

K-shell Binding Energies



Dirac-Coulomb $1s$ energy

$$\epsilon_{1s} = \frac{2Z^2}{1 + \sqrt{1 - \alpha^2 Z^2}} \text{ Ry}$$

Electron-Electron Interaction

Dirac Hartree-Fock Approximation:

One-electron orbitals ϕ_a satisfy Dirac equations

$$(H_{\text{Dirac}} + V_{\text{HF}})\phi_a = \epsilon_a\phi_a$$

$$V_{\text{HF}} \phi_a(\mathbf{r}) = \sum_b \int \frac{d^3r'}{|\mathbf{r} - \mathbf{r}'|} \phi_b^\dagger(\mathbf{r}') \phi_b(\mathbf{r}') \phi_a(\mathbf{r}) \\ - \sum_b \int \frac{d^3r'}{|\mathbf{r} - \mathbf{r}'|} \phi_b^\dagger(\mathbf{r}') \phi_a(\mathbf{r}') \phi_b(\mathbf{r})$$

Equations solved self-consistently.

$-\epsilon_a =$ “frozen-core” binding energy.

Smaller Corrections

Relaxation Energy:

$$\begin{aligned} E_{1s} &= E_{\text{ion}} - E_{\text{atom}} \\ &= -\epsilon_{1s} + \Delta_{1s} \end{aligned}$$

Breit Interaction:

$$b_{12} = \frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 + \boldsymbol{\alpha}_1 \cdot \hat{\boldsymbol{r}}_{12} \boldsymbol{\alpha}_2 \cdot \hat{\boldsymbol{r}}_{12}}{2r_{12}}$$

Hg 1s binding energy (Ry)	
Coulomb	7064.38
HF correction	-911.90
Relaxation	-7.01
Relaxed Breit	-22.29
Breit Retardation	0.45
Nuclear size	-4.03
Structure	6119.59
Expt.	6108.44

Estimated accuracy ≈ 0.1 Ry ≈ 1 eV

Theory vs. Experiment

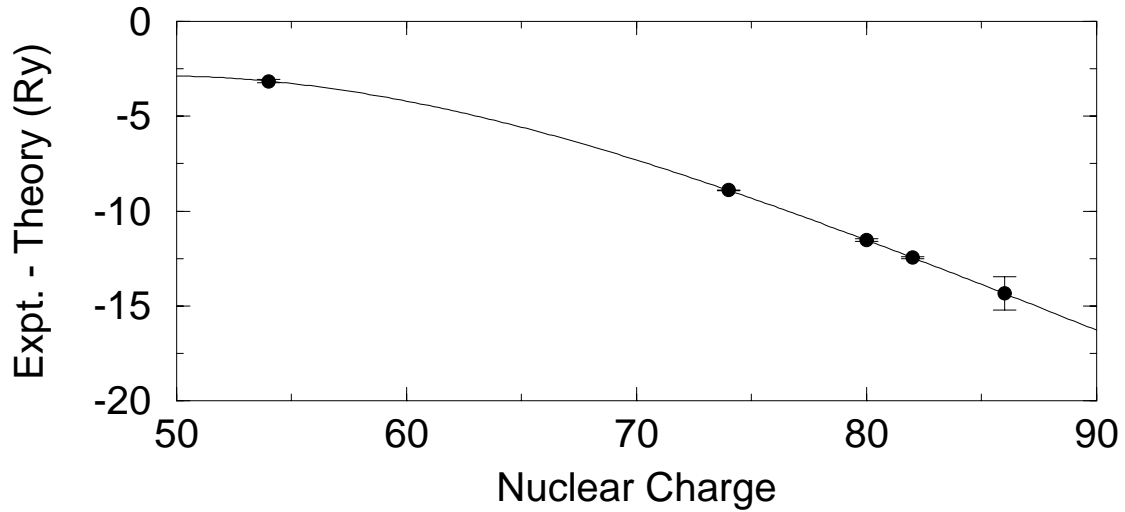


Figure 1: Difference between experimental and theoretical K-shell energies as a function of Z .

K-electron Self-Energy

$$\Delta E_{1s} = \frac{\alpha}{\pi} (\alpha Z)^4 F(Z\alpha) mc^2$$

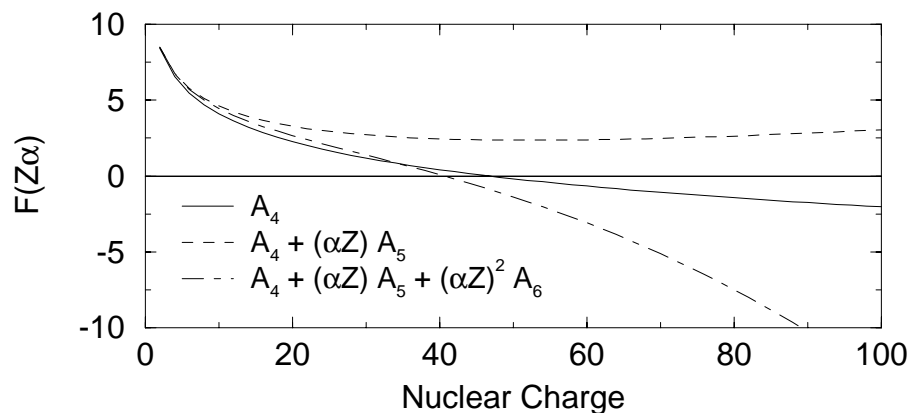
$$F(Z\alpha) = A_4 + \alpha Z A_5 + (\alpha Z)^2 A_6 + \dots$$

where,

$$A_4 = \frac{4}{3} \left[\ln(Z\alpha)^{-2} + \frac{5}{6} - 2.9841285 \right]$$

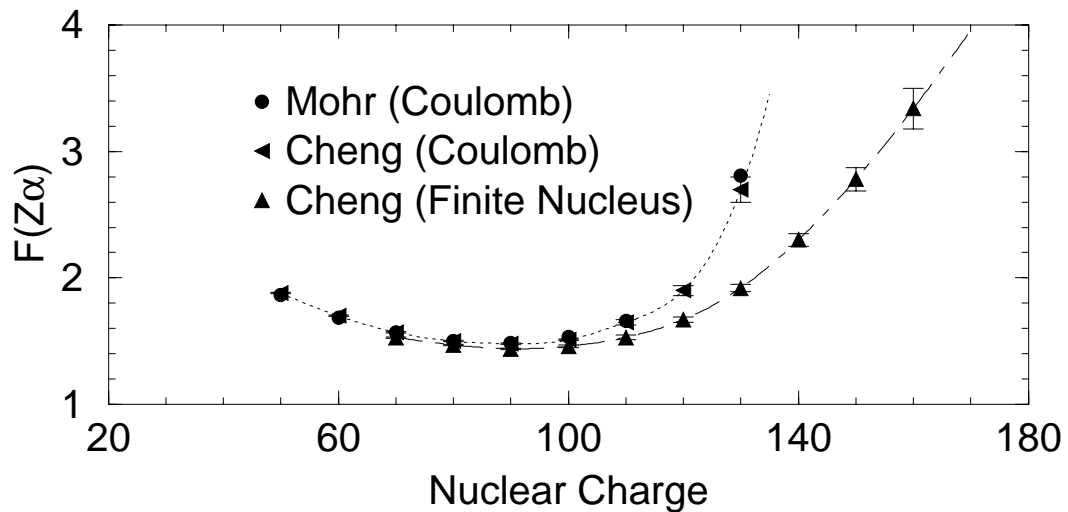
$$A_5 = 3\pi \left[1 + \frac{11}{128} - \frac{1}{2} \ln 2 \right]$$

$$A_6 = \left[7 \ln 2 - \frac{63}{80} \right] \ln(Z\alpha)^{-2} - \frac{3}{4} \ln^2(Z\alpha)^{-2} - 33.2$$



Non-Perturbative $1s$ Self-Energy

- Brown et al. 1959 – $Z = 80$ (incorrect numerics)
- Desiderio 1971 – Coulomb (70 – 90)
- Mohr 1972 – Coulomb (10 – 100)
- Cheng 1976 – Nuclear Size
- Soff et al. 1982 – Nuclear Size
- Blundell & Snyderman 1991
- Lindgren et al. 1993



Test of Lowest-Order QED

QED = Self-Energy + Vacuum Polarization
 Vacuum-Polarization \approx Uehling Potential

“Experimental” vs. Theoretical QED

Atom	Expt.	Theory	Diff.	QED
Xe	2540.28(8)	2543.43	-3.15(8)	-3.22
W	5110.42(2)	5119.03	-8.61(2)	-8.73
Hg	6108.44(6)	6119.59	-11.15(6)	-11.36
Pb	6468.71(5)	6480.83	-12.11(5)	-12.35
Rn	7232.73(89)	7247.07	-14.34(89)	-14.51

“Experimental” radiative corrections are systematically smaller than lowest-order QED predictions by 2%.

$$\begin{aligned} \text{Diff./QED} &= 0.98 \pm 0.01 \text{ (excluding Rn)} \\ &= 0.98 \pm 0.03 \text{ (including Rn)} \end{aligned}$$

We therefore have a 2% test of strong-field QED. The systematic differences are possibly explained by higher-order QED diagrams.

Many-Electron Hamiltonian

The *no-pair* Hamiltonian¹ is a many-electron generalization of the Dirac Hamiltonian derived from the field-theoretic Hamiltonian of QED:

$$H = H_0 + V$$

$$H_0 = \sum_i \epsilon_i a_i^\dagger a_i$$

$$V = \frac{1}{2} \sum_{ijkl} v_{ijkl} a_i^\dagger a_j^\dagger a_l a_k - \sum_{ij} \Delta_{ij} a_i^\dagger a_j$$

1. the sums are restricted to electron states only,
2. v_{ijkl} is a two-particle matrix element of the sum of the Coulomb and Breit interactions,
3. Δ_{ij} compensates for including average $e - e$ potential in h_0 .

¹BROWN, G.E. & RAVENHALL, D.G. 1951 *Proc. R. Soc. London, Ser. A* **208**, 552-559.

QED Tests for Copper-like Ions

Largest atom having a “complete” isoelectronic sequence.

Structure:

$$(1s)^2(2s)^2(2p)^6(3s)^2(3p)^6(3d)^{10} + \text{valence}$$

Outline of MBPT calculations:

$$E^{(0)} = \sum_a \epsilon_a + \epsilon_v$$

$$E^{(1)} = E_c^{(1)} = -1/2 \sum_a (V_{\text{HF}})_{aa}$$

$$E^{(2)} = E_c^{(2)} + E_v^{(2)}$$

$$E^{(3)} = E_c^{(3)} + E_v^{(3)} \dots$$

$$E_v^{(2)} = \sum_{amn} \frac{\tilde{v}_{mnav} v_{avmn}}{\epsilon_m + \epsilon_n - \epsilon_v - \epsilon_a} - \sum_{abm} \frac{\tilde{v}_{abmv} v_{mvab}}{\epsilon_m + \epsilon_v - \epsilon_a - \epsilon_b}$$

$$E_v^{(3)} = \sum_{mabcd} \frac{\tilde{v}_{abvm} v_{cdab} v_{mvcd}}{(\epsilon_{ab} - \epsilon_{vm})(\epsilon_{cd} - \epsilon_{mv})} + 17 \text{ more terms}$$

Energies of Cu-like Sn ($Z=50$) (a.u.)

Term	$4s_{1/2}$	$4p_{1/2}$	$4p_{3/2}$
$E^{(0)}$	-23.56930	-21.91682	-21.48453
$E^{(2)}$	-0.06009	-0.06000	-0.05583
$E^{(3)}$	0.00406	0.00383	0.00355
$B^{(1)}$	0.01493	0.02117	0.01478
$B^{(2)}$	-0.00433	-0.00451	-0.00449
$B^{(3)}$	0.00017	0.00027	0.00019
Recoil	0.00009	0.00005	0.00005
E_{Tot}	-23.61488	-21.95601	-21.52627

	$p_{3/2} - p_{1/2}$	$p_{3/2} - s_{1/2}$
E_{Tot}	0.4297(2)	2.0886(3)
E_{Expt}	0.4303(3)	2.0807(1)

Tests of QED in Cu-like Ions

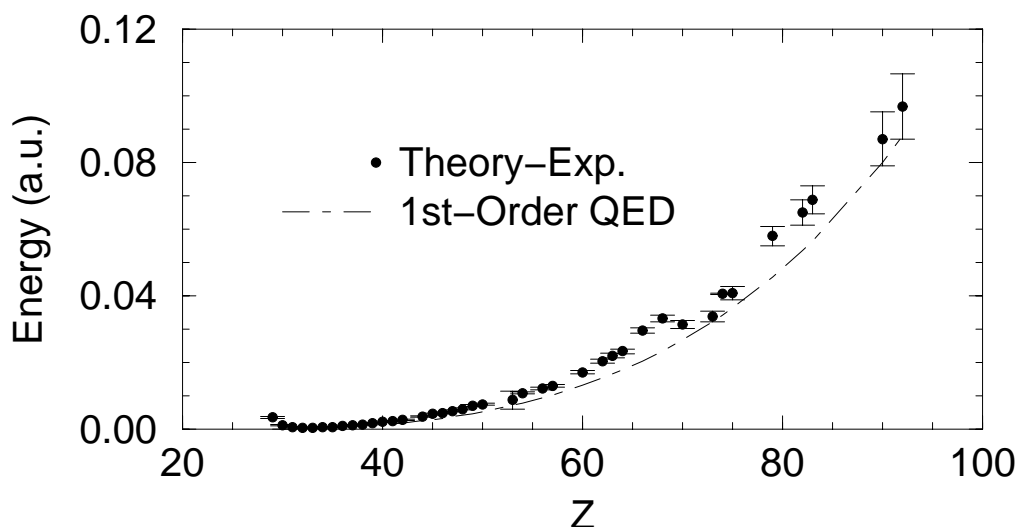


Figure 2: Comparison of “experimental” and theoretical values of the $4p_{3/2} - 4s_{1/2}$ Lamb-shift in copper-like ions.

Conclusion: QED corrections evaluated in a HF potential agree with the “experimental” Lamb-shift to $\sim 5\%$ for high- Z Cu-like ions. Alternatively, assuming the QED corrections are precise, this is a $1:10^5$ test of MBPT calculations for highly-charged Cu-like ions.

Atomic Tests of the Standard Model

$$H^{(1)} = \frac{G}{\sqrt{2}} (\bar{\psi}_e \gamma_\mu \gamma_5 \psi_e) \sum_i [c_{1p} (\bar{\psi}_{pi} \gamma^\mu \psi_{pi}) + c_{1n} (\bar{\psi}_{ni} \gamma^\mu \psi_{ni})]$$

$$H^{(2)} = \frac{G}{\sqrt{2}} (\bar{\psi}_e \gamma_\mu \psi_e) \sum_i [c_{2p} (\bar{\psi}_{pi} \gamma^\mu \gamma_5 \psi_{pi}) + c_{2n} (\bar{\psi}_{ni} \gamma^\mu \gamma_5 \psi_{ni})]$$

$$c_{1p} = \frac{1}{2} (1 - 4 \sin^2 \theta_W) \approx 0.038,$$

$$c_{1n} = -\frac{1}{2},$$

$$c_{2p} = \frac{1}{2} g_A (1 - 4 \sin^2 \theta_W) \approx 0.047,$$

$$c_{2n} = -\frac{1}{2} g_A (1 - 4 \sin^2 \theta_W) \approx -0.047.$$

$g_A \approx 1.25$ for the partially conserved axial current
 $\sin^2 \theta_W = 0.23124(24)$ is Weinberg's angle.

Nonrelativistic Nucleon Reduction

$$H_{\text{eff}}^{(1)} = \frac{G}{2\sqrt{2}} \gamma_5 Q_w \rho(r)$$

$$H_{\text{eff}}^{(2)} = -\frac{G}{\sqrt{2}} \frac{\kappa - 1/2}{I(I+1)} \boldsymbol{\alpha} \cdot \mathbf{I} [c_{2p} \rho_{pv}(r) + c_{2n} \rho_{nv}(r)]$$

$$H_{\text{eff}}^{(a)} = \frac{G}{\sqrt{2}} K_a \frac{\kappa}{I(I+1)} \boldsymbol{\alpha} \cdot \mathbf{I} \rho_v(r)$$

$$Q_w = [2Z c_{1p} + 2N c_{1n}] = -N + Z (1 - 4 \sin^2 \theta_W)$$



Nuclear Anapole

Single-Double Equations

$$\Psi_v = \Psi_{\text{DHF}} + \delta\Psi$$

$$\delta\Psi = \left\{ \begin{aligned} &\sum_{am} \rho_{ma} a_m^\dagger a_a + \frac{1}{2} \sum_{abmn} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a \\ &+ \sum_{m \neq v} \rho_{mv} a_m^\dagger a_v + \sum_{bmn} \rho_{mnbv} a_m^\dagger a_n^\dagger a_b a_v \end{aligned} \right\} \Psi_{\text{DHF}}$$

$$E_C = E_C^{\text{DHF}} + \delta E_C$$

$$E_v = E_v^{\text{DHF}} + \delta E_v$$

Later, we will discuss triples

Core Excitation Equations

$$\begin{aligned}
 (\epsilon_a - \epsilon_m)\rho_{ma} &= \sum_{bn} \tilde{v}_{mban}\rho_{nb} \\
 &+ \sum_{bnr} v_{mbnr}\tilde{\rho}_{nrab} - \sum_{bcn} v_{bcan}\tilde{\rho}_{mncb}
 \end{aligned}$$

$$\begin{aligned}
 (\epsilon_a + \epsilon_b - \epsilon_m - \epsilon_n)\rho_{mnab} &= v_{mnab} \\
 &+ \sum_{cd} v_{cdab}\rho_{mncd} + \sum_{rs} v_{mnr s}\rho_{rsab} \\
 &+ \left[\sum_r v_{mnr b}\rho_{ra} - \sum_c v_{cnab}\rho_{mc} + \sum_{rc} \tilde{v}_{cnrb}\tilde{\rho}_{mrac} \right] \\
 &+ [a \leftrightarrow b \quad m \leftrightarrow n]
 \end{aligned}$$

$$\delta E_C = \frac{1}{2} \sum_{abmn} v_{abmn}\tilde{\rho}_{mnab}$$

$\approx 15,000,000$ ρ_{mnab} coefficients for Cs ($\ell = 6$).

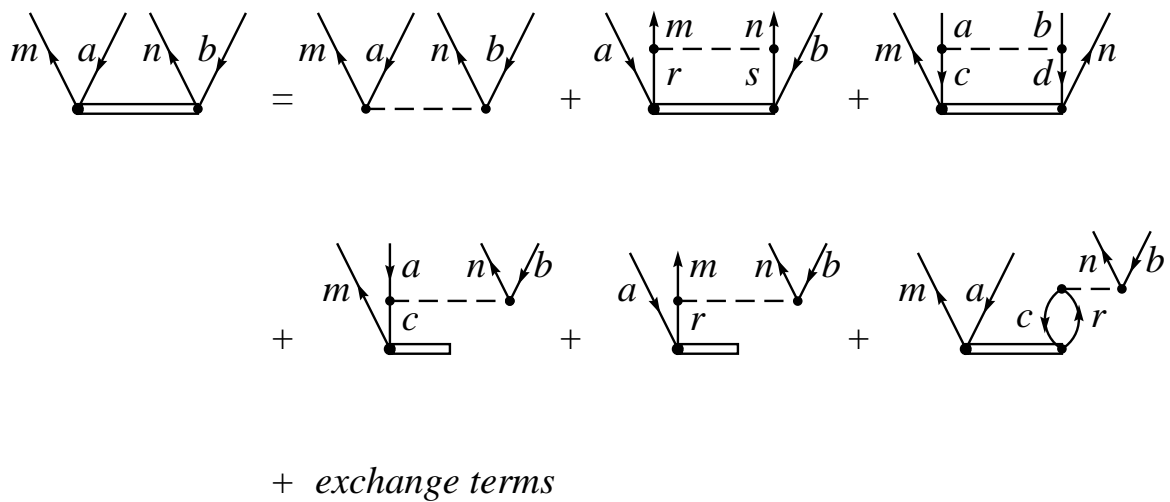
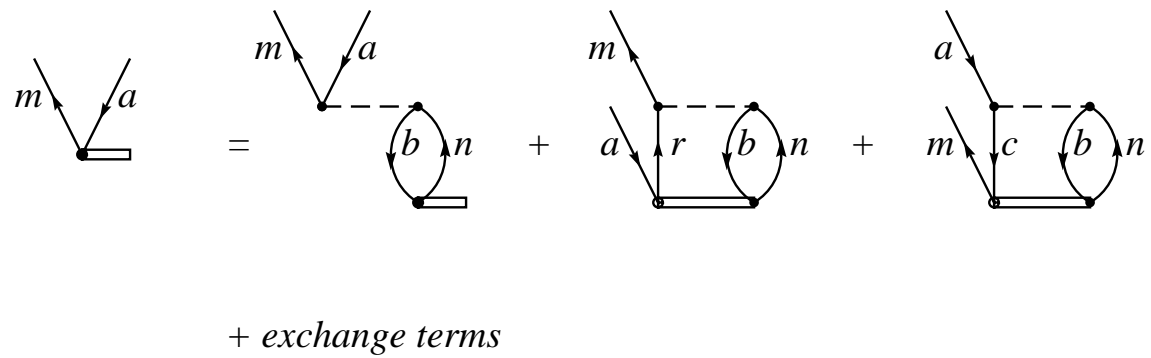


Figure 3: Many-body diagrams for the core SD equations.

Valence Equations

$$\begin{aligned}
 (\epsilon_v - \epsilon_m + \delta E_v) \rho_{mv} &= \sum_{bn} \tilde{v}_{mbvn} \rho_{nb} \\
 &+ \sum_{bnr} v_{mbnr} \tilde{\rho}_{nrub} - \sum_{bcn} v_{bcvn} \tilde{\rho}_{mnb}
 \end{aligned}$$

$$\begin{aligned}
 (\epsilon_v + \epsilon_b - \epsilon_m - \epsilon_n + \delta E_v) \rho_{mnvb} &= v_{mnvb} \\
 &+ \sum_{cd} v_{cdvb} \rho_{mncd} + \sum_{rs} v_{mnrsv} \rho_{rsvb} \\
 &+ \left[\sum_r v_{mnrsv} \rho_{rv} - \sum_c v_{cnvb} \rho_{mc} + \sum_{rc} \tilde{v}_{cnrb} \tilde{\rho}_{mrv} \right] \\
 &+ [v \leftrightarrow b \quad m \leftrightarrow n]
 \end{aligned}$$

$$\begin{aligned}
 \delta E_v &= \sum_{ma} \tilde{v}_{vavm} \rho_{ma} + \sum_{mab} v_{abvm} \tilde{\rho}_{mvab} \\
 &+ \sum_{mna} v_{vbmna} \tilde{\rho}_{mnvb}
 \end{aligned}$$

$\approx 1,000,000$ ρ_{mnvb} coefficients for each state (Cs)

Perturbation Expansion of the Energy

- δE_C agrees with MBPT through third order.
- δE_v agrees with MBPT through second order.
- $\delta E_v^{(3)}$ **disagrees** with $E_v^{(3)}$ from MBPT.

Add triple excitations to wave function

$$\frac{1}{6} \sum_{abmnr} \rho_{mnr} v_{ab} a_m^\dagger a_n^\dagger a_r^\dagger a_v a_b a_a \Psi_{\text{HF}}$$

$$E_{v \text{ extra}} = \frac{1}{2} \sum_{mnab} \tilde{v}_{abmn} \rho_{mnr} v_{ab}$$

- $\delta E_v^{(3)} + E_{v \text{ extra}}^{(3)}$ gives the **entire** third-order valence correlation energy

$$E_v^{(3)} = \delta E_v^{(3)} + E_{v \text{ extra}}^{(3)}$$

Table 1: Na $3s$ and $3p$ states (a.u.)

Term	$3s_{1/2}$	$3p_{1/2}$	$3p_{3/2}$
$\delta E_v^{(3)}$	-3.446[-4]	-1.454[-4]	-1.449[-4]
$E_{v \text{ extra}}^{(3)}$	-0.418[-4]	-0.070[-4]	-0.072[-4]
$E_v^{(3)}$	-3.865[-4]	-1.525[-4]	-1.521[-4]

Correlation Energy

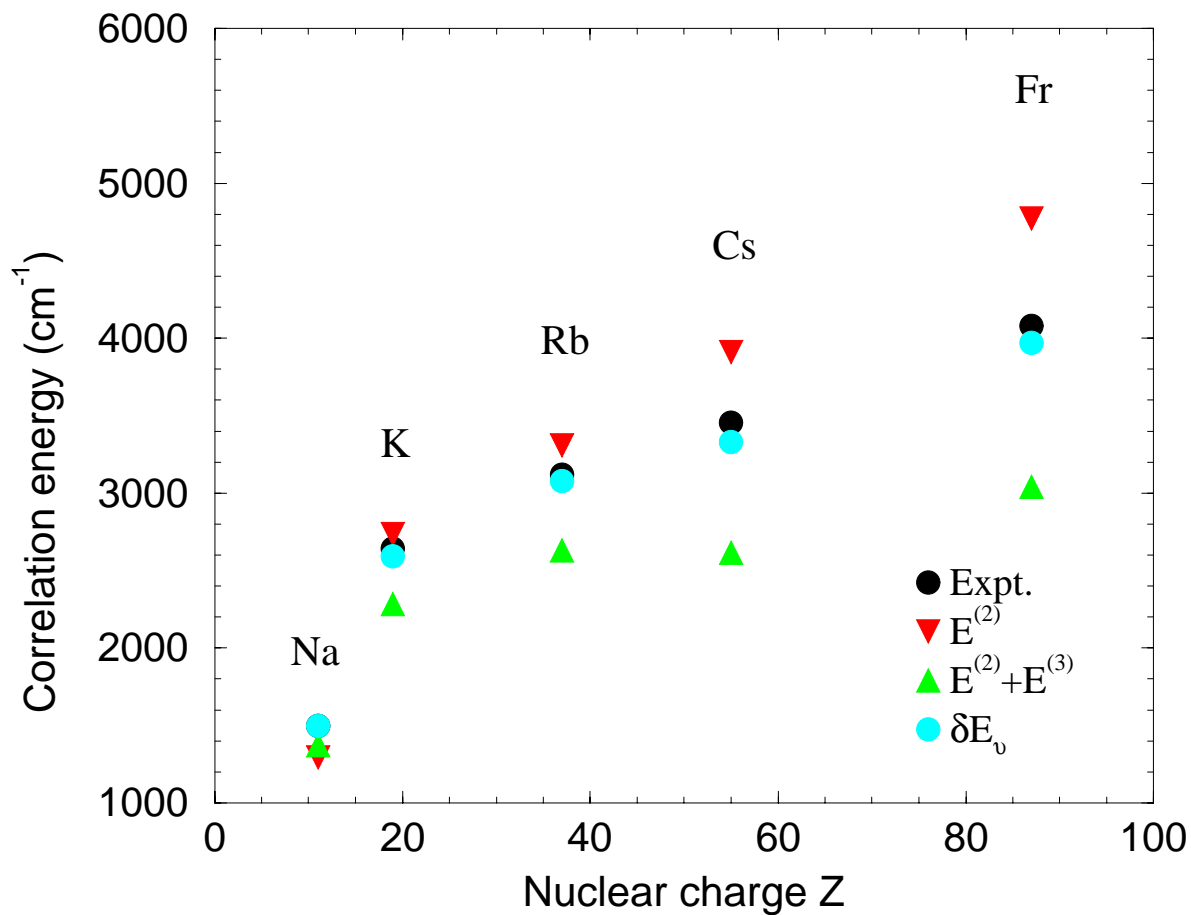


Figure 4: Energy comparisons for alkali-metal atoms.

Higher-order terms

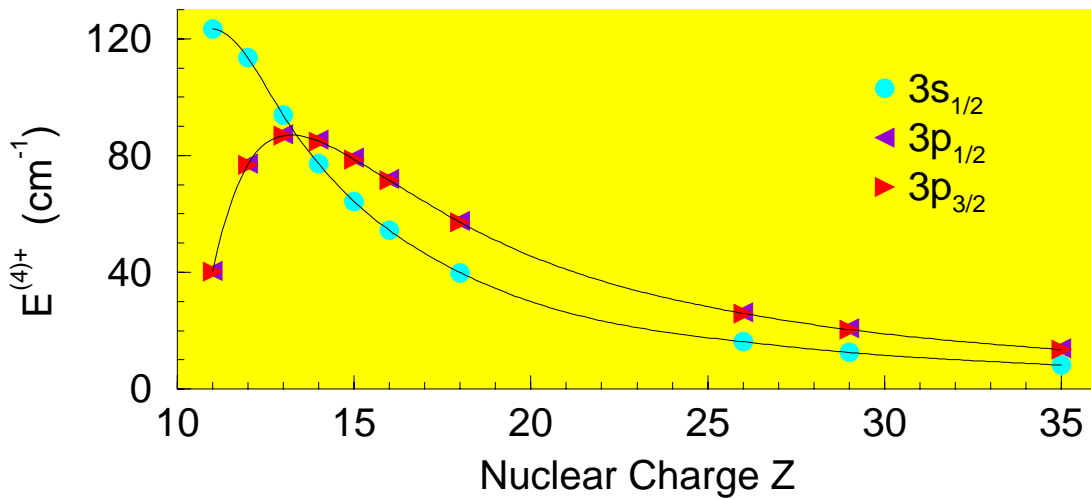


Figure 5: Contributions beyond 3rd-order for Na-like ions.

- $E^{(4)+} < 1\%$ of correlation energy for $Z > 20$

All-order energies

Table 2: Summary for sodium $3s$ and $3p$ states (cm^{-1})

Term	$3s$	$3p_{1/2}$	$3p_{3/2}$
DHF	-39951.6	-24030.4	-24014.1
δE	-1488.8(4)	-463.9	-461.6
$E_{\text{extra}}^{(3)}$	-9.2	-1.5	-1.6
Breit	1.2	1.4	0.1
RM+MP	1.0	0.5	0.5
Theory	-41447.3(4)	-24493.9	-24476.7
Expt.	-41449.4	-24493.3	-24476.1

Results for Heavy Atoms

Table 3: Energies for cesium and francium cm^{-1}

Cs	$6s$	$7s$	$8s$	$9s$
Theory	31262	12801	7060	4479
Expt.	31407	12871	7089	4496
Cs	$6p_{1/2}$	$7p_{1/2}$	$8p_{1/2}$	$9p_{1/2}$
Theory	20204	9621	5687	3760
Expt.	20228	9641	5698	3769
Fr	$7s$	$8s$	$9s$	$10s$
Theory	32735	13051	7148	4522
Expt.	32849	13106	7168	4538
Fr	$7p_{1/2}$	$8p_{1/2}$	$9p_{1/2}$	$10p_{1/2}$
Theory	20583	9712	5724	3782
Expt.	20612	9736	<i>5738</i>	<i>3795</i>

Fine-Structure Intervals

Table 4: Fine-structure (cm^{-1}).

		This work	Expt.
K	$4p_{3/2} - 4p_{1/2}$	57.3	57.7
	$5p_{3/2} - 5p_{1/2}$	18.5	18.8
	$6p_{3/2} - 6p_{1/2}$	8.5	8.4
	$7p_{3/2} - 7p_{1/2}$	4.4	4.5
Rb	$5p_{3/2} - 5p_{1/2}$	236.5	237.6
	$6p_{3/2} - 6p_{1/2}$	76.5	77.5
	$7p_{3/2} - 7p_{1/2}$	34.8	35.1
	$8p_{3/2} - 8p_{1/2}$	18.6	18.9
Cs	$6p_{3/2} - 6p_{1/2}$	552.2	554.1
	$7p_{3/2} - 7p_{1/2}$	178.6	181.0
	$8p_{3/2} - 8p_{1/2}$	81.4	82.6
	$9p_{3/2} - 9p_{1/2}$	43.9	44.7
Fr	$7p_{3/2} - 7p_{1/2}$	1676	1687
	$8p_{3/2} - 8p_{1/2}$	536	545
	$9p_{3/2} - 9p_{1/2}$	244	<i>250</i>
	$10p_{3/2} - 10p_{1/2}$	132	<i>136</i>

Dipole Transitions

Table 5: Matrix Elements for heavy alkali metals (a.u.)

	K	Rb	Cs	Fr
$p_{1/2}-s$	$n = 4$	$n = 5$	$n = 6$	$n = 7$
SD	4.098	4.221	4.478	4.256
Expt.	4.102(5)	4.231(3)	4.489(7)	4.277(8)
$p_{3/2}-s$	$n = 4$	$n = 5$	$n = 6$	$n = 7$
SD	5.794	5.956	6.298	5.851
Expt.	5.800(8)	5.977(4)	6.324(7)	5.898(15)

Application to PNC

$$\begin{aligned} \langle F|ez|I\rangle &= \sum_n \frac{\langle F|ez|n\rangle \langle n|H_W|I\rangle}{E_n - E_I} \\ &+ \sum_n \frac{\langle F|H_W|n\rangle \langle n|ez|I\rangle}{E_n - E_F}, \end{aligned}$$

where $H_W = H_{\text{eff}}^{(1)} + H_{\text{eff}}^{(2)} + H_{\text{eff}}^{(a)}$

$$\langle F|ez|I\rangle = E_{\text{PNC}} [1 + A(F_F, F_I)]$$

For ^{133}Cs ($I = 7/2$), we obtain:

$$E_{\text{PNC}} = 0.906(9) \times 10^{-11} i|e|a_0 Q_w/N$$

$$A(F_F, F_I) = \begin{bmatrix} 0.028 & 0.057 \\ -0.051 & -0.022 \end{bmatrix}$$

Status of PNC Experiments

(a) Optical rotation: $n_+ \neq n_-$ $\phi = E_{\text{PNC}}/M_1$

$6p_{1/2} - 6p_{3/2}$ transition		
Element	Group	$10^8 \times \phi$
Thallium	Oxford	-15.7(5)
Thallium	Seattle	-14.7(2)
Lead	Oxford	-9.8(1)
Lead	Seattle	-9.9(1)
Bismuth	Oxford	-10.1(20)

(b) Stark interference: Add $E(t) = A \cos \omega t$ and detect the heterodyning signal $R = E_{\text{PNC}}/\beta$

$6s_{1/2} - 7s_{1/2}$ (mV/cm)			
Element	Group	R_{4-3}	R_{3-4}
Cesium	Paris (1984)	-1.5(2)	-1.5(2)
Cesium	Boulder (1988)	-1.64(5)	-1.51(5)
Cesium	Boulder (1997)	-1.635(8)	-1.558(8)

Cesium: Theory vs. Experiment

$$\beta = 27.02(8) a_0^3 \quad (1999)$$

(eliminating axial vector + anapole contribution)

$$\Im(E_{\text{PNC}}) = -0.836(4) \times 10^{-11} |e| a_0 \quad (1997)$$

(dividing by theoretical matrix element)

$$Q_w = -71.9(4) \quad (\text{Expt.} + \text{Atomic Theory})$$

$$K = 0.50(7) \quad (\text{Expt.} + \text{Atomic Theory})$$

Marciano & Rosner (with radiative corrections)

$$Q_w = -73.20(13) \quad (\text{Standard Model})$$

$\text{Expt.} - \text{Theory} = 1.3(4)$

Principal source of error is atomic theory.

Conclusions

- I Strong-field QED corrections inner-shell electrons in heavy atoms are tested to 2%.
- II Comparing theoretical and “experimental” values of the Lamb-shift for valence electrons in highly-charged ions provide stringent tests of higher-order MBPT calculations.
- III Tests of the standard-model by comparing experiment and theory show a $\sim 3\sigma$ effect in Q_w .
- IV Modern atomic PNC experiments are underway at Stonybrook, Berkeley, and Seattle. Calculations are needed to aid in extracting quantitative information from such measurements.