High accuracy calculations for atoms and atomic tests of fundamental laws

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- Why do we still need to develop atomic theory?

- Theory of atoms with several valence electrons.

- Tests of the theory (spectra, expectation values, transition amplitudes).

- Parity non-conservation (PNC) in atoms and tests of the standard model.

- Anapole moments of the nuclei and weak nuclear forces.

- Search for the time-variation of the fundamental constants.

What limits the accuracy of atomic theory?

- Typical atom (ion) is a many-electron system with several electrons in open shells.

- Correlation corrections to the transition frequences and allowed $E1$-transition amplitudes are typically $\sim$10%; for the hyperfine structure (HFS) and PNC interactions — $\sim$30%.

- QED corrections to the frequences are $\sim$0.1% and $\sim$1% for the PNC amplitudes and for HFS.

- Nuclear charge radii are known to a one percent accuracy; magnetic moment destributions (for HFS) and neutron destributions (for PNC) are known to a few percent accuracy.

What accuracy of the theory we need?

- Atomic frequences are known from the experiment to 7-9 digits; sometimes – upto 12-15 digits. For systems like H and He the theory is competitive. That is why QED is the best tested theory. For a typical atom the theory gives 1-0.1% accuracy at best.

- We need theory to extract nuclear charge radii, magnetic, quadrupole, and *anapole* moments from the spectroscopic experiments. Therefore, the accuracy to which we know these characteristisc is often limited by atomic theory.

- PNC effects in heavy atoms are of the size of $10^{-8} - 10^{-5}$ and are known from the experiment with the accuracy of $1 - 0.3\%$. Theoretical accuracy is $3 - 0.5\%$. That allows to test standard model on the level of radiative corrections.

Method of effective operators for valence electrons (CI+MBPT)

In quantum mechanics the many-electron system is described by the following equations:

$$\begin{array}{lcccl} \text{spectrum} & : & H\Psi_n & = & E_n\Psi_n, \\ \text{observables} & : & A_{m,n} & = & \langle\Psi_m|A|\Psi_n\rangle, \end{array} \qquad (1)$$

where H is all-electron Hamiltonian and Ψ is all-electron wave function.

Instead of solving (1) we use many-body perturbation theory (MBPT) to form effective operators for valence electrons and use configuration-interaction (CI) to solve the valence equation:

$$\begin{aligned} H_{\text{eff}}(E_n)\Phi_n &= E_n\Phi_n, \\ A_{m,n} &= \langle\Phi_m|A_{\text{eff}}|\Phi_n\rangle. \end{aligned} \qquad (2)$$

CI+MBPT formalism

We devide all-electron space into valence subspace and complimentary subspace and introduce corresponding projectors P and $Q = 1 - P$.

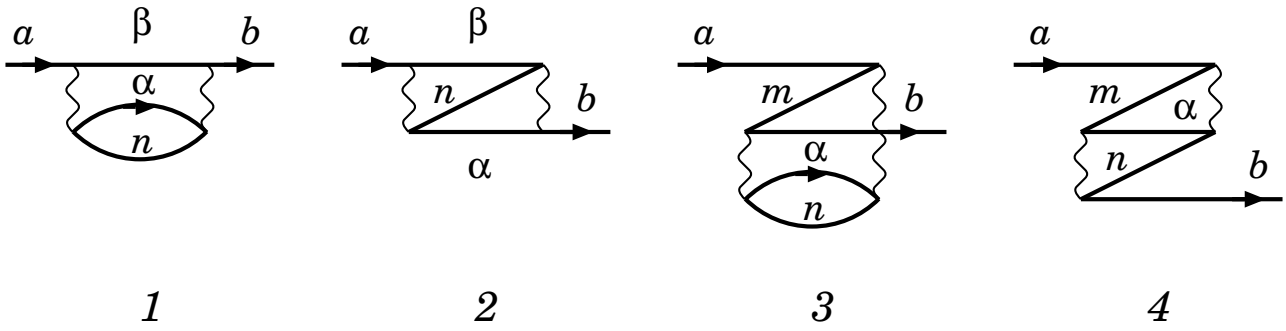
All-electron Schrödinger equation is equivalent to the system:

$$\Psi = P\Psi + Q\Psi \equiv \Phi + \chi,$$
$$H_{\text{eff}}(E)\Phi = E\Phi,$$

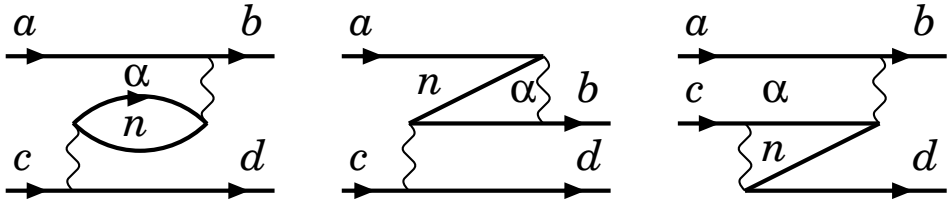
where

$$\begin{aligned} H_{\text{eff}}(E) &\equiv PHP + \Sigma(E), \\ \Sigma(E) &\equiv PHQ\, R_Q(E)\, QHP, \\ R_Q(E) &\equiv (E - QHQ)^{-1}. \end{aligned}$$

Linked diagrams for self-energy operator Σ



1 2 3 4



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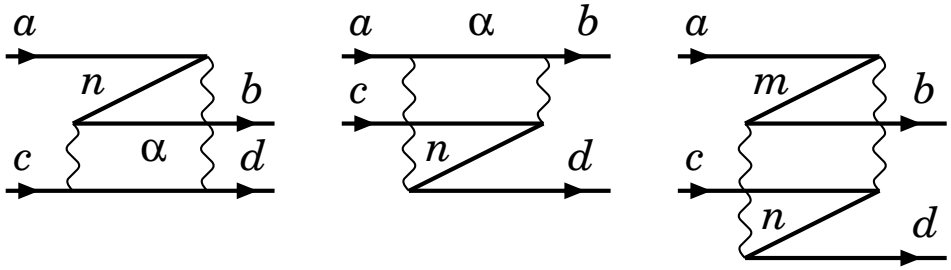
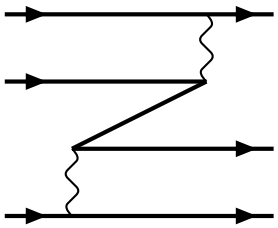
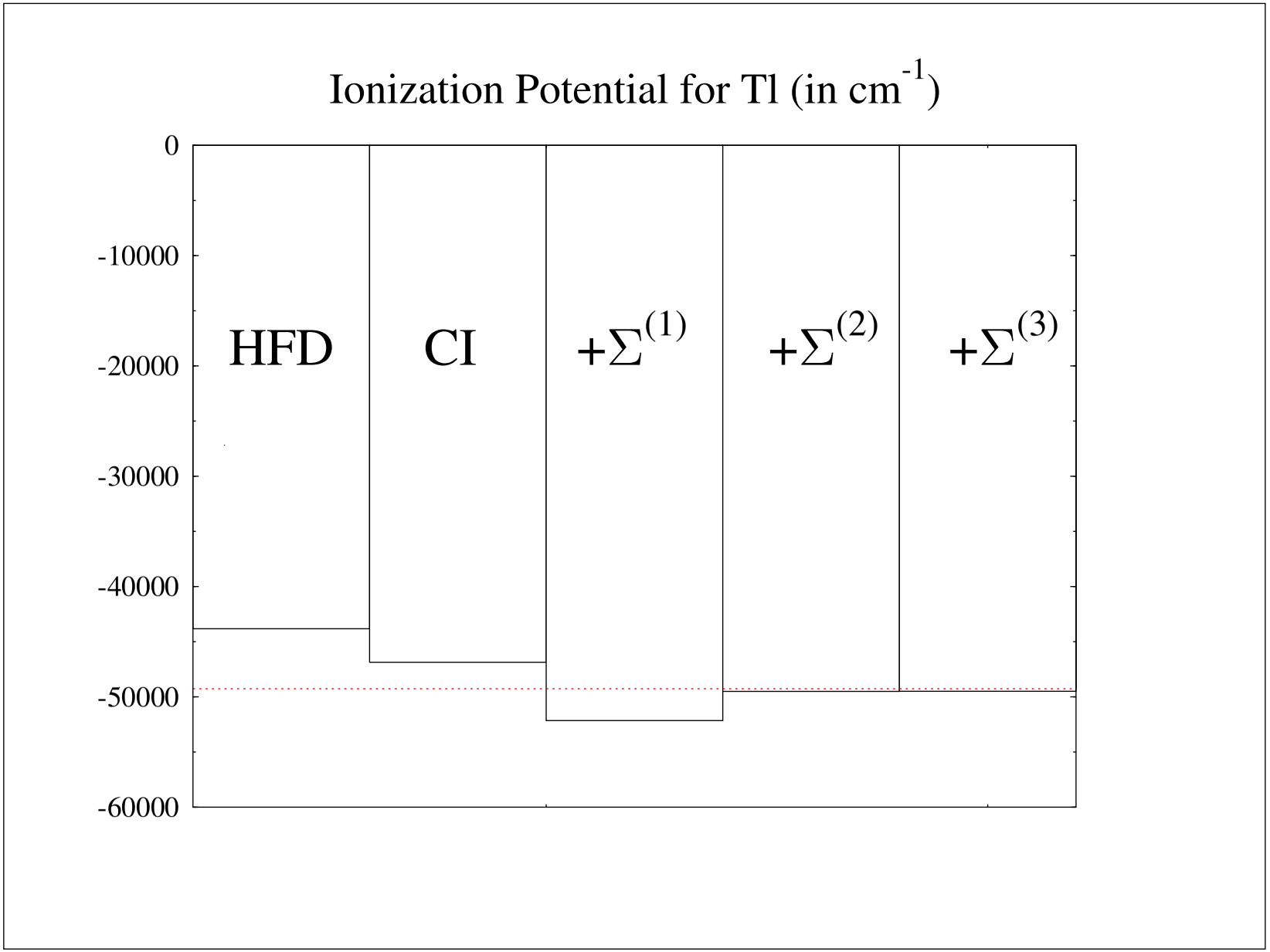
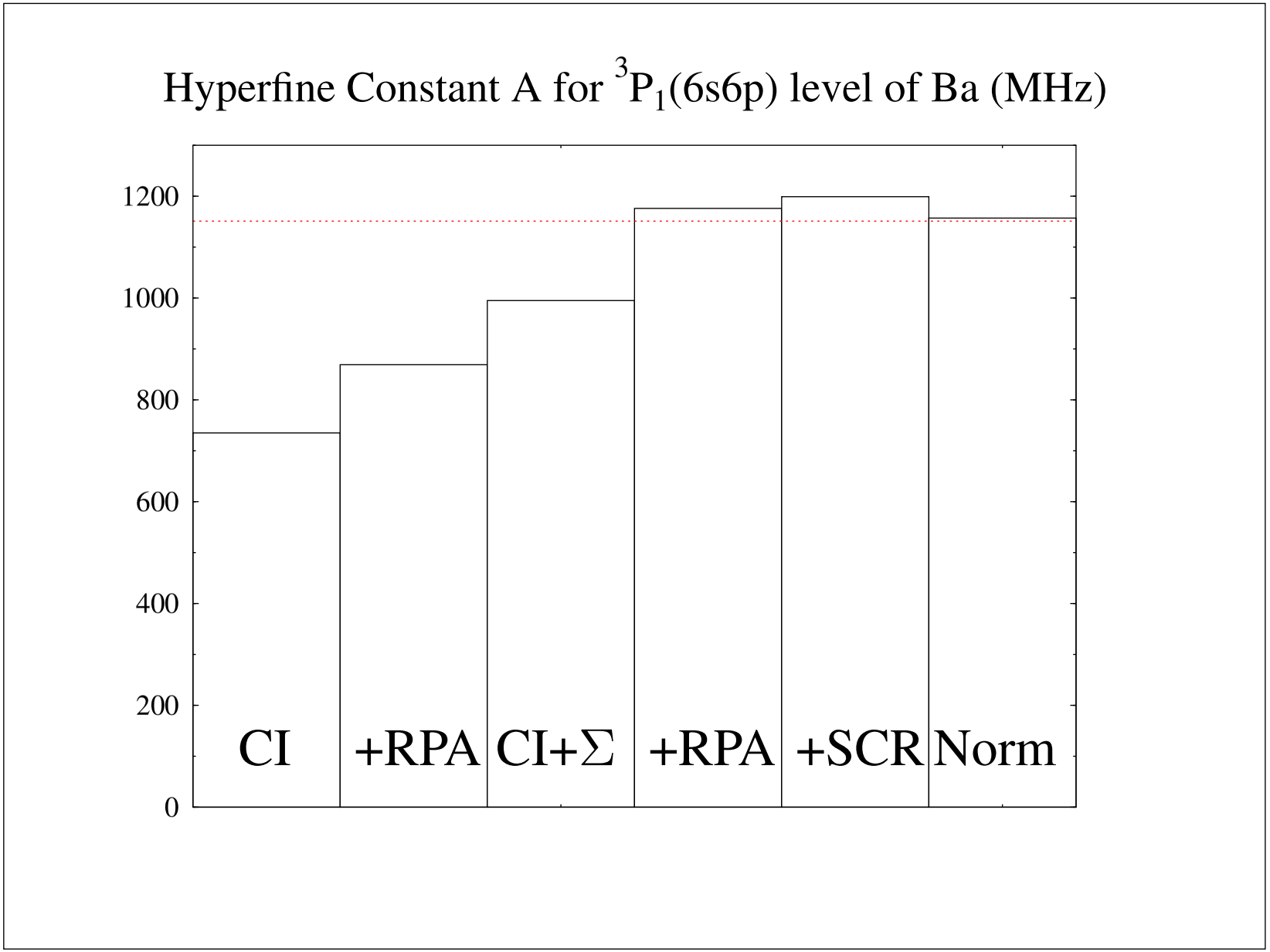
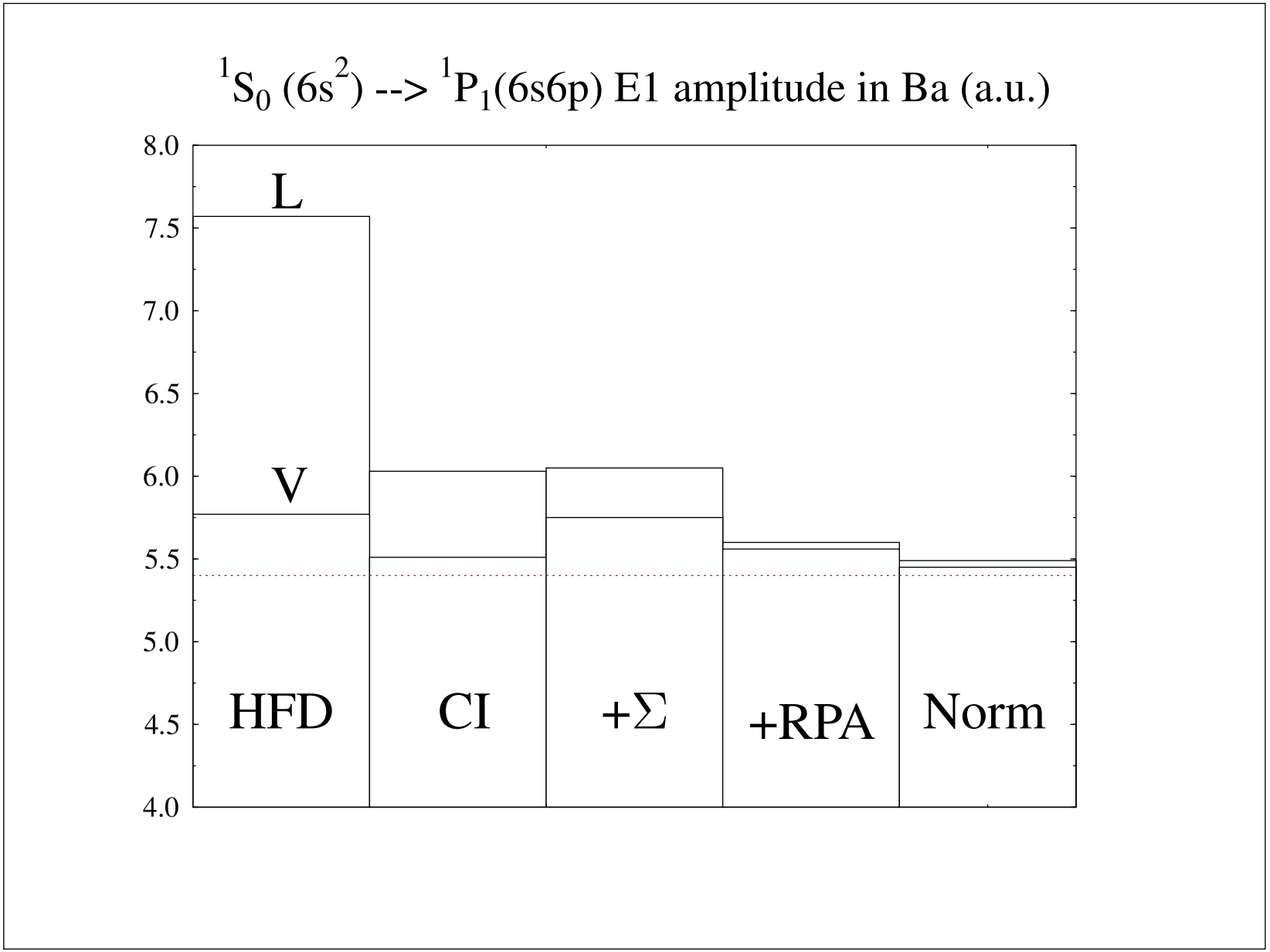


4 5 6




Ionization Potential for Tl (in cm-1)
0
-10000
-20000
-30000
-40000
-50000
-60000
HFD
CI
+Σ(1)
+Σ(2)
+Σ(3)


Hyperfine Constant A for $^3P_1(6s6p)$ level of Ba (MHz)
1200
1000
800
600
400
200
0
CI
+RPA
CI+Σ
+RPA
+SCR
Norm


$^1S_0$ ($6s^2$) --> $^1P_1$(6s6p) E1 amplitude in Ba (a.u.)
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
L
V
HFD
CI
+Σ
+RPA
Norm

$E1_{\mathrm{PNC}}$ amplitude for $6p_{1/2} \to 6p_{3/2}$ transition in ^{205}Tl ($i \cdot 10^{-10}(-Q_w/N)$ a.u.).

CI	-6.408
H_{eff} & RPA	-0.725
A_σ	$+0.241$
A_{sbt}	$+0.180$
A_{tp}	-0.082
SR	-0.006
Subtotal	-6.81
Normalization	$+0.14$
Total	-6.67

$M1$ amplitude (10^{-3} a.u.)	
CI+MBPT-II	4.145
MBPT-III(1e)	4.149

$\mathcal{R} = 10^8 \times \mathrm{Im}\frac{E1_{\mathrm{PNC}}}{M1}$ $\left(Q_w = Q_w^{\mathrm{SM}} = -116.8\right)$
$-15.2(4)$

Experimental and theoretical values of $\mathcal{R} = 10^8 \times \frac{\mathrm{Im}E1_{\mathrm{PNC}}}{M1}$ for $6p_{1/2} \to 6p_{3/2}$ transition in ^{205}Tl

Experiment

Oxford	Edwards *et al* (1995)	−15.68 (45)
	Majumder & Tsai (1999)[1]	−15.00 (45)
Seattle	Vetter *et al* (1995)	−14.68 (17)

Theory[2]

(Standard model value $Q_W = -116.8$ assumed)

Novosibirsk	Dzuba *et al* (1987)	−15.0 (5)
Notre Dame	Liu *et al* (1996)	−16.0 (10)
Gatchina	Kozlov *et al* (1997)	−14.9 (6)
Gatchina-ND	Kozlov *et al* (2001)	−15.1 (4)

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[1] scaling of Oxford result

[2] includes QED radiative correction (-0.7)%
(Kuchiev & Flambaum (02);
Milstein, Sushkov, & Terekhov (02))

Astrophysical search for α-variation

Suppose that the fine structure constant α can vary in space-time. Then, for a distant quasar all atomic frequences will be shifted:

$$\begin{aligned} \omega_i &= \omega_{i,0} + q_i x + \ldots, \\ x &\equiv (\alpha/\alpha_0)^2 - 1, \end{aligned}$$

where $\alpha_0 = 1/137\ldots$ and $\omega_{i,0}$ are the laboratory values.

The light from the distant objects is red-shifted because of the expansion of the Universe. We can exclude cosmological red shift by taking the ratios of the frequences:

$$\frac{\omega_i}{\omega_k} = \left(\frac{\omega_i}{\omega_k}\right)_0 \left(1 + \left(\frac{q_i\omega_k - q_k\omega_i}{\omega_i\omega_k}\right)_0 x\right).$$

In this way, recent observations for the quasars at distances of $\sim 10^{10}$ light years gave (Murphy *et al* (2003)):

$$\frac{\Delta\alpha}{\alpha} = (-0.57 \pm 0.11) \times 10^{-5}.$$

Atomic calculations of q and mass shift (MS)

To find q_i we make a fully relativistic calculation of atomic frequences for small, but non-zero values of $x = (\alpha/\alpha_0)^2 - 1$:

$$q_i \approx 4\left(\omega_i(x = 1/8) - \omega_i(x = -1/8)\right).$$

The main systematcs can be caused by the possible evolution of the natural abundances. If the nuclear mass is changed by δM, the atomic frequency is changed too:

$$\omega_i = \omega_{i,0} + k_{i,\mathrm{MS}}\,\frac{\delta M}{M^2}.$$

There are two contributions to k_{MS}. Normal mass shift is caused by the substitution of the electron mass m with the reduced mass $\mu = mM/(m + M)$.

Specific mass shift (SMS) is described by the two-electron operator:

$$H_{\rm SMS} = \frac{1}{M} \sum_{i>k} \vec{p}_i \cdot \vec{p}_k,$$

where $\vec{p}_i$ is the momentum of the electron i and M is nuclear mass.

$H_{\rm SMS}$ is added to the many-electron Hamiltonian:

$$H_\lambda = H_0 + \lambda\, M\, H_{\rm SMS}.$$

The eigenvalue problem for this Hamiltonian is solved for $+\lambda$ and for $-\lambda$. Then, $k_{\rm SMS}$ is given by:

$$k_{\rm SMS} \approx \frac{E_{+\lambda} - E_{-\lambda}}{2\lambda}.$$

Coefficients q and $k_{\rm MS}$ for ions used in astrophysical search for α-variation

Ion	Transition	ω_0 cm^{-1}	q cm^{-1}	$k_{\rm MS}$ GHz · amu
Si II	$^2P^o_{1/2} \to {}^2D_{3/2}$	55309	520(30)	1900(300)
	$\to {}^2S_{1/2}$	65500	50(30)	−400(500)
Ti II	$^4F_{3/2} \to {}^4F^o_{3/2}$	30836	530(50)	610(30)
	$\to {}^4F^o_{5/2}$	30959	660(70)	610(30)
Cr II	$^6S_{5/2} \to {}^6P^o_{3/2}$	48399	−1360(150)	−1900(900)
	$\to {}^6P^o_{5/2}$	48491	−1280(150)	−1900(900)
	$\to {}^6P^o_{7/2}$	48632	−1110(150)	−1900(900)
Fe II	$^6D_{9/2} \to {}^6D^o_{9/2}$	38459	1330(150)	1800(400)
	$\to {}^6D^o_{7/2}$	38660	1490(150)	1800(400)
	$\to {}^6F^o_{11/2}$	41968	1460(150)	1900(400)
	$\to {}^6F^o_{9/2}$	42115	1590(150)	1900(400)
	$\to {}^6P^o_{7/2}$	42658	1210(150)	1800(400)
	$\to {}^4F^o_{7/2}$	62066	1100(300)	2000(1000)
	$\to {}^6P^o_{7/2}$	62172	−1300(300)	−2000(1000)
Ni II	$^2D_{5/2} \to {}^2F^o_{7/2}$	57080	−700(250)	−2300(1000)
	$\to {}^2D^o_{5/2}$	57420	−1400(250)	−2300(1000)
	$\to {}^2F^o_{5/2}$	58493	−20(250)	−2300(1000)
Zn II	$^2S_{1/2} \to {}^2P^o_{1/2}$	48481	1584(25)	2110(70)
	$\to {}^2P^o_{3/2}$	49355	2490(25)	2080(70)

How to eliminate MS effect in α-variation search?

Consider two transitions of the same element:

$$\begin{aligned} \omega_i &= \omega_{i,0} + q_i x + k_i \frac{\delta M}{M^2}, \\ \omega_j &= \omega_{j,0} + q_j x + k_j \frac{\delta M}{M^2}, \end{aligned}$$

If we know coefficients k accurately, we can eliminate M-dependance by taking the combination:

$$\begin{aligned} k_j\omega_i - k_i\omega_j &= (k_j\omega_i - k_i\omega_j)_0 \\ &+ (k_j q_i - k_i q_j)x. \end{aligned}$$

High precision atomic calculations are necessary!