Uncertainty Estimates for Atomic Structure Calculations

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Uncertainty Estimates for Theoretical Atomic and Molecular Data

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Sources of uncertainty are reviewed for calculated atomic and molecular data that are important for plasma modeling: atomic and molecular structure and cross sections for electron-atom, electron-molecule, and heavy particle collisions. We concentrate on model uncertainties due to approximations to the fundamental many-body quantum mechanical equations and we aim to provide guidelines to estimate uncertainties as a routine part of computations of data for structure and scattering.

PACS numbers: 34.20.Cf (Interatomic potentials and forces), 34.70.+e (Charge transfer), 34.80.Bm (Elastic scattering), 34.80.Dp (Atomic excitation and ionization), 34.80.Gs (Molecular excitation and ionization), 34.80.Ht (Dissociation and dissociative attachment), 52.20.Fs (Electron collisions), 52.20.Hv (Atomic, molecular, ion, and heavy particle collisions)

Uncertainties

ICAMDATA, Vilnius, Lithuania Sept.2010
(AIP Conference Proceedings No.1344)

Role of Accuracy Estimates in Atomic and Molecular Theory

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Abstract. The various roles that theoretical work plays in the evolution of physics are reviewed, and classified. The need for properly justified uncertainty estimates to accompany theoretical atomic and molecular data is discussed. A new set of guidelines is described for the conditions under which uncertainty estimates should be included in published work.

Keywords: uncertainty estimates, error analysis, atomic and molecular theory
PACS: 01.30.-y

INTRODUCTION

The purpose of this paper is to discuss the need for uncertainty estimates in physics papers whose main purpose is to present the results of theoretical calculations for physical processes. The discussion will be placed in the context of the overall evolution of physics, and the progressive maturing of particular subfields of physics. It will also be placed in the context of the development of computational power, and the ability of researchers to make meaningful uncertainty estimates for their calculations.

There is another context for the discussion that particularly affects the authors of

PHYSICAL REVIEW A
covering atomic, molecular, and optical physics and quantum information

Phys. Rev. A 83, 040001 (2011)

Editorial: Uncertainty Estimates

The purpose of this Editorial is to discuss the importance of including uncertainty estimates in papers involving theoretical calculations of physical quantities.

It is not unusual for manuscripts on theoretical work to be submitted without uncertainty estimates for numerical results. In contrast, papers presenting the results of laboratory measurements would usually not be considered acceptable for publication in *Physical Review A* without a detailed discussion of the uncertainties involved in the measurements. For example, a graphical presentation of data is always accompanied by error bars for the data points. The determination of these error bars is often the most difficult part of the measurement. Without them, it is impossible to tell whether or not bumps and irregularities in the data are real physical effects, or artifacts of the measurement. Even papers reporting the observation of entirely new phenomena need to contain enough information to convince the reader that the effect being reported is real. The standards become much more rigorous for papers claiming high accuracy.

The question is to what extent can the same high standards be applied to papers reporting the results of theoretical calculations. It is all too often the case that the numerical results are presented without uncertainty estimates. Authors sometimes say that it is difficult to arrive at error estimates. Should this be considered an adequate reason for omitting them? In order to answer this question, we need to consider the goals and objectives of the theoretical (or computational) work being done. Theoretical papers can be broadly classified as follows:

1. Development of new theoretical techniques or formalisms.
2. Development of approximation methods, where the comparison with experiment, or other theory, itself provides an assessment of the error in the method of calculation.
3. Explanation of previously unexplained phenomena, where a semiquantitative agreement with experiment is already significant.
4. Proposals for new experimental arrangements or configurations, such as optical lattices.
5. Quantitative comparisons with experiment for the purpose of (a) verifying that all significant physical effects have been taken into account, and/or (b)

There are many cases where it is indeed not practical to give a meaningful error estimate for a theoretical calculation; for example, in scattering processes involving complex systems. The comparison with experiment itself provides a test of our theoretical understanding. However, there is a broad class of papers where estimates of theoretical uncertainties can and should be made. Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances:

1. If the authors claim high accuracy, or improvements on the accuracy of previous work.
2. If the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements.
3. If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

These guidelines have been used on a case-by-case basis for the past two years. Authors have adapted well to this, resulting in papers of greater interest and significance for our readers.

The Editors

Published 29 April 2011
DOI: 10.1103/PhysRevA.83.040001
PACS number(s): 01.30.Ww

General Considerations

- Estimation of theoretical uncertainties is said to be "difficult," but the results are too important to be ignored. New technologies are needed.
- Uncertainty estimates are <u>estimates</u>, not rigorous error bounds.
- Uncertainties come from both
  - computational uncertainties,
  - knowledge and/or completeness of underlying theory.
- Uncertainty estimates for atomic structure are the best developed so far.
- Begin with $g-2$, the highest-precision comparison ever made between theory and experiment.
- Continue with one- and two-electron atoms where both computational accuracy and underlying theory play a role.
- Finish with many-electron atoms where computational accuracy is the main concern.

Most Precise Prediction of the Standard Model

Anomalous Magnetic Moment $g-2$

$$-\frac{\mu}{\mu_B} = 1 + C_2\left(\frac{\alpha}{\pi}\right) + C_4\left(\frac{\alpha}{\pi}\right)^2 + C_6\left(\frac{\alpha}{\pi}\right)^3 + C_8\left(\frac{\alpha}{\pi}\right)^4 + C_{10}\left(\frac{\alpha}{\pi}\right)^5 + \cdots$$
$$+ a_{\text{hadronic}} + a_{\text{weak}}$$

where $\mu_B = \dfrac{e\hbar}{2m}$ is the Bohr magneton, and

$\alpha = \dfrac{1}{4\pi\epsilon_0}\dfrac{e^2}{\hbar c} \simeq \dfrac{1}{137}$ is the fine structure constant.

Dirac	1			
QED	C_2	$=$	$1/2$	exact
	C_4	$=$	$-0.328\,478\,444\,002\,55(33)$	
	C_6	$=$	$1.181\,234\,016\,815(11)$	
	C_8	$=$	$-1.909\,7(20)$	
	C_{10}	$=$	$9.16(57)$	Kinoshita et al.
Hadronic	a_{hadronic}	$=$	$1.677(16)\times 10^{-12}$	
Weak	a_{weak}	$=$	small	

T. Aoyama et al. PRD **91**, 033006 (2015).

Kinoshita et al. PRD 91, 033006 (2015)

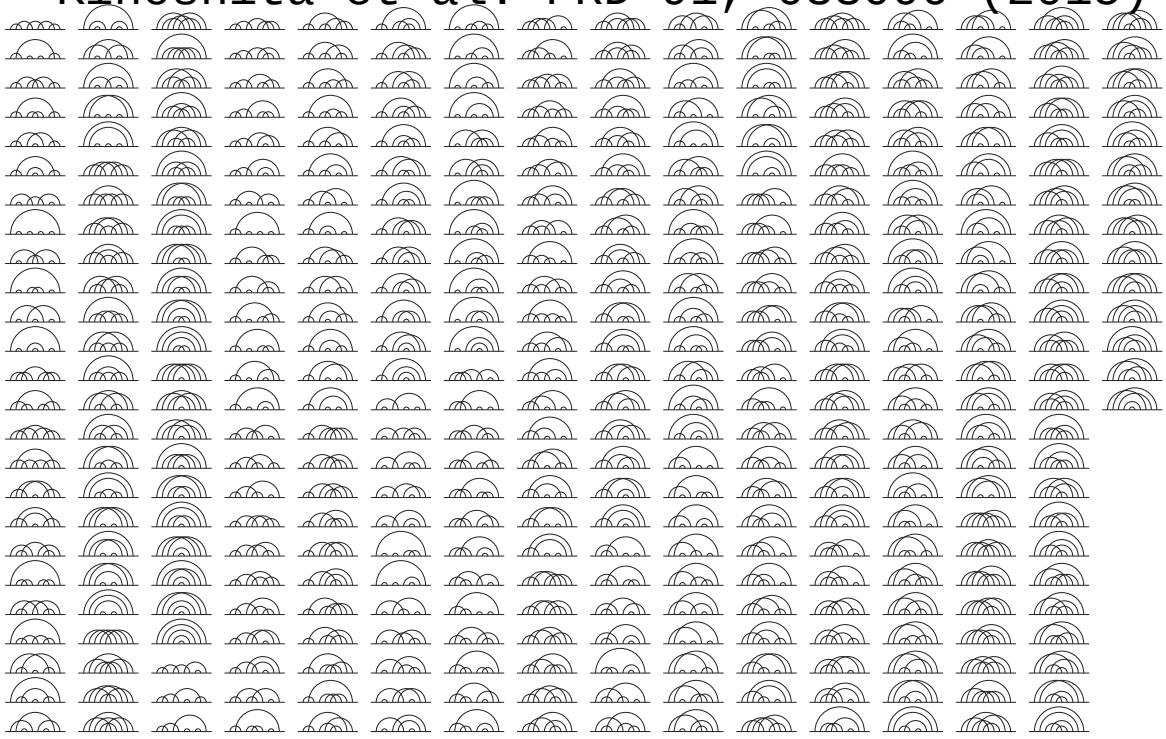

FIG. 1: Overview of 389 diagrams which represents 6354 vertex diagrams of Set V. The horizontal solid lines represent the electron propagators in a constant weak magnetic field. Semi-circles stand for photon propagators. The left-most figures are denoted as X001–X025 from the top to the bottom. The top figure in the second column from the left is denoted X026, and so on.

To Test QED, an Independent Value of α Is Needed

$$\alpha = \frac{1}{4\pi\epsilon_0}\frac{e^2}{\hbar c} \quad \text{and} \quad R_\infty = \frac{1}{(4\pi\epsilon_0)^2}\frac{e^4 m_e}{2\hbar^3 c}$$

Then

$$\alpha^2 = \frac{2R_\infty}{c}\,\frac{h}{M_{\text{Rb}}}\,\frac{M_{\text{Rb}}}{M_p}\,\frac{M_p}{m_e}$$

Key measurement:

$$\frac{h}{M_{\text{Rb}}} = 2c^2\frac{f_{\text{recoil}}}{f^2} \quad \text{from atom recoil velocity from 1000 photons}$$

R. Bouchendira et al., PRL **106**, 080801 (2011).

Results of Comparison

		Exp't.	Theory	
$\alpha^{-1} =$	137.035 999 173(33)(8)	[0.24 ppb]	[0.06 ppb]	from $g-2$
	137.035 999 173(34)	[0.25 ppb]		from photon recoil

(G. Gabrielse, ICAP presentation, Seoul, 2016).

Consequence: electrons have no internal structure!

Hydrogenic Atoms

- Uncertainties here limit what can be achieved for more complex systems.
- For hydrogen, the Schrödinger (or Dirac) equation can be solved exactly, and so uncertainties come from QED corrections and the effects of finite nuclear size and structure.
- Relativistic corrections can be expressed as an expansion in powers of $(\alpha Z)^2$, and summed to infinity by solving the Dirac equation.
- QED effects (self energy and vacuum polarization) can be written as a dual expansion in powers of αZ and α, but cannot be summed to infinity.

$$E_{\text{Total}} = E_{\text{NR}} + \Delta E_{\text{rel.}} + \Delta E_{\text{QED}}$$

where E_{NR} is the nonrelativistic energy, and (in atomic units)

$$\begin{aligned} \Delta E_{\text{rel.}} &= (\alpha Z)^2 E^{(2)}_{\text{rel.}} + (\alpha Z)^4 E^{(4)}_{\text{rel.}} + \cdots \\ \Delta E_{\text{QED}} &= \alpha^3 Z^4 \left[\ln(\alpha Z) E^{(3,1)}_{\text{QED}} + E^{(3,0)}_{\text{QED}} + O(\alpha Z)^2 + O(\alpha/\pi) \right] \end{aligned}$$

- QED Terms are known in their entirety up to $O(\alpha^5 Z^6)$, and so the uncertainty is of $O(\alpha^6 Z^7)$ (at least in the low-Z region), or a few kHz for hydrogen 2s state [K. Pachucki and U. D. Jentschura, Phys. Rev. Lett. **91**,113005 (2003)].
- The proton size discrepancy of 0.84 fm (muonic) – 0.87 fm (electronic) also corresponds to an energy discrepancy of 3 kHz for the 2s state.

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High-Z Hydrogenic Ions

- There has been considerable progress in summing the αZ binding energy corrections to infinity [A. Gumberidze et al., Hyperfine Interact. **199**, 59 (2011)]. For U^{91+}, the Lamb shift is
  464.26 ± 0.5 eV theory
  460.2 ± 4.6 eV experiment.

- For excited s-states, the Lamb shifts and uncertainties scale approximately as $1/n^3$ with n and Z^6 with Z. These uncertainties place a fundamental limit on the accuracy of atomic structure computations.

Heliumlike Atoms and Ions

- The Schrödinger equation cannot be solved exactly, and so approximation methods must be used. This provides a great testing ground for uncertainty estimates. For example, for the ground state of helium, the correlation energy is the difference between:

$$\begin{aligned} \text{Hartree-Fock energy} &= -2.87\ldots \\ \text{exact nonrelativistic energy} &= -2.903724\ldots \end{aligned}$$

  The difference of 0.03 a.u. $\simeq$ 0.8 eV is the actual error in the H.F. approximation.

- For comparison, $k_B T \simeq 0.026$ eV at room temperature. All of chemistry is buried in the correlation energy!

Methods of Theoretical Atomic Physics.

Method	Typical Accuracy for the Energy
Many Body Perturbation Theory	$\geq 10^{-6}$ a.u.
Configuration Interaction	10^{-6} – 10^{-8} a.u.
Explicitly Correlated Gaussians[a]	$\sim 10^{-10}$ a.u.
Hylleraas Coordinates (He)[b,c]	$\leq 10^{-35}$ – 10^{-40} a.u.
Hylleraas Coordinates (Li)[d]	$\sim 10^{-15}$ a.u.

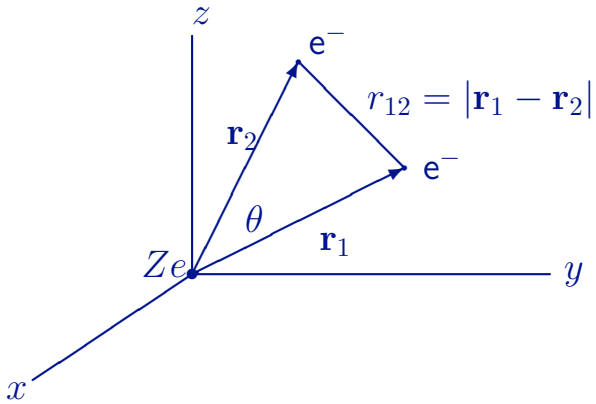
[a] S. Bubin and Adamowicz J. Chem. Phys. **136**, 134305 (2012).

[b] C. Schwartz, Int. J. Mod. Phys. E–Nucl. Phys. **15**, 877 (2006).

[c] H. Nakashima, H. Nakatsuji, J. Chem. Phys. **127**, 224104 (2007).

[d] Present work: L.M. Wang et al., Phys. Rev. A **85**, 052513 (2012) .

Nonrelativistic Eigenvalues



Hylleraas coordinates

(Hylleraas, 1929)

The Hamiltonian in atomic units is

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}$$

Expand

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{i,j,k} a_{ijk}\, r_1^i\, r_2^j\, r_{12}^k\, e^{-\alpha r_1 - \beta r_2}\, \mathcal{Y}_{l_1 l_2 L}^M(\hat{\mathbf{r}}_\mathbf{1}, \hat{\mathbf{r}}_\mathbf{2}) \pm \text{exchange}$$

where $i + j + k \leq \Omega$ (Pekeris shell).

Diagonalize H in the

$$\phi_{ijk} = r_1^i\, r_2^j\, r_{12}^k\, e^{-\alpha r_1 - \beta r_2}\, \mathcal{Y}_{l_1 l_2 L}^M(\hat{\mathbf{r}}_\mathbf{1}, \hat{\mathbf{r}}_\mathbf{2}) \pm \text{exchange}$$

basis set.

Convergence study for the ground state of helium [1].

Ω	N	$E(\Omega)$	$R(\Omega)$
8	269	–2.903 724 377 029 560 058 400	
9	347	–2.903 724 377 033 543 320 480	
10	443	–2.903 724 377 034 047 783 838	7.90
11	549	–2.903 724 377 034 104 634 696	8.87
12	676	–2.903 724 377 034 116 928 328	4.62
13	814	–2.903 724 377 034 119 224 401	5.35
14	976	–2.903 724 377 034 119 539 797	7.28
15	1150	–2.903 724 377 034 119 585 888	6.84
16	1351	–2.903 724 377 034 119 596 137	4.50
17	1565	–2.903 724 377 034 119 597 856	5.96
18	1809	–2.903 724 377 034 119 598 206	4.90
19	2067	–2.903 724 377 034 119 598 286	4.44
20	2358	–2.903 724 377 034 119 598 305	4.02
Extrapolation	∞	–2.903 724 377 034 119 598 311(1)	
Korobov [2]	5200	–2.903 724 377 034 119 598 311 158 7	
Korobov extrap.	∞	–2.903 724 377 034 119 598 311 159 4(4)	
Schwartz [3]	10259	–2.903 724 377 034 119 598 311 159 245 194 404 4400	
Schwartz extrap.	∞	–2.903 724 377 034 119 598 311 159 245 194 404 446	
Goldman [4]	8066	–2.903 724 377 034 119 593 82	
Bürgers *et al.* [5]	24 497	–2.903 724 377 034 119 589(5)	
Baker *et al.* [6]	476	–2.903 724 377 034 118 4	

[1] G.W.F. Drake, M.M. Cassar, and R.A. Nistor, Phys. Rev. A **65**, 054501 (2002).
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[6] J.D. Baker, D.E. Freund, R.N. Hill, J.D. Morgan III, Phys. Rev. A **41**, 1247 (1990).

Relativistic Corrections

Nonrelativistic Energy: $1/Z$ Expansion

$$E_{\mathsf{NR}} = E_{\mathsf{NR}}^{(0)} Z^2 + E_{\mathsf{NR}}^{(1)} Z + \underline{E_{\mathsf{NR}}^{(2)}} + \cdots$$

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Relativistic Corrections: $(\alpha Z)^2$ and $1/Z$ Expansions

$$\begin{aligned} E_{\mathsf{rel}} &= E_{\mathsf{rel}}^{(2,4)} \alpha^2 Z^4 + E_{\mathsf{rel}}^{(4,6)} + \cdots \\ &+ \underline{E_{\mathsf{rel}}^{(2,3)} \alpha^2 Z^3} + \cdots \end{aligned}$$

Cross-over point: $E_{\mathsf{NR}}^{(2)} \simeq E_{\mathsf{rel}}^{(2,3)} \alpha^2 Z^3$ when $\alpha^2 Z^3 \simeq 1$, or $Z \simeq 1/\alpha^{2/3} \simeq 27$

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Cross-over point: $E_{\mathsf{NR}}^{(2)} \simeq E_{\mathsf{rel}}^{(2,3)} \alpha^2 Z^3$ when $\alpha^2 Z^3 \simeq 1$, or $Z \simeq \alpha^{2/3} \simeq 27$

Two Strategies

- $Z < 27$: start from the nonrelativistic Schrödinger equation and treat relativistic effects as a perturbation. Uncertainty dominated by relativistic (and QED) corrections.
- $Z \geq 27$: start from the Dirac equation and treat electron correlation effects as a perturbation. Uncertainty dominated by electron correlation corrections.

Current Status for Helium

- Nonrelativistic Energy: Essentially exact
- Relativistic and QED Corrections:
  - α^2 Breit interaction: essentially exact
  - α^3 QED terms: essentially exact
  - α^4 Douglas and Kroll terms: essentially exact but complicated operators [recently completed by Yerokhin and Pachucki PRA 81, 022507 (2010)].
  - α^5 QED terms: can be estimated from the known hydrogenic terms.
- Final uncertainty: $\pm$36 MHz for the ground state ionization energy of helium. This scales roughly as $1/n^3$ with n and Z^5 with Z.

High-Z Heliumlike Ions

- Start from the Dirac equation and use all-orders methods to sum relativistic and QED effects to infinity.
- Dominant source of uncertainty comes from the combined effects of electron correlation and relativistic effects: leading order $(\alpha Z)^4$.
- Final uncertainty for $n = 2$ is approximately $(Z/10)^4$ cm^{-1} or $\pm$0.9 eV for U^{90+}.
- This is an order of magnitude larger than the one-electron QED uncertainty.

Three-electron Atoms

- High precision variational calculations in Hylleraas coordinates are still possible, but the basis sets become much larger (30,000 terms instead of 3000 terms).
- Accuracies are more limited, but spectroscopic accuracy is still possible.
- Only the ground state $1s^2 2s\ ^2S_2$ and a few excited states have been calculated in any detail.

Theoretical contributions to the $1s^2 2s\ ^2S - 1s^2 3s\ ^2S$ transition energy (cm^{-1}) of ^{7}Li [Yan & Drake 2008, Puchalski et al. 2010], and comparison with experiment [Sanchez et al. 2006]. $\mu/M \simeq 7.820 \times 10^{-5}$ is the ratio of the reduced electron mass to the nuclear mass for an atomic mass, and $\alpha \simeq 1/137$ is the fine structure constant.

Contribution	Transition Energy (cm^{-1})
Infinite mass	27 206.492 847 9(5)
μ/M	–2.295 854 362(2)
$\mu/M)^2$	0.000 165 9774
α^2	2.089 120(23)
$\alpha^2\mu/M$	–0.000 003 457(9)
α^3	–0.187 03(26)
$\alpha^3\mu/M$	0.000 009 74(13)
α^4 (Est.)	–0.005 7(6)
α^5 (Est.)	0.000 52(13)
Nucl. size	–0.000 390(10)
Total	27 206.093 7(6)
Exp't.	27 206.094 082(6)

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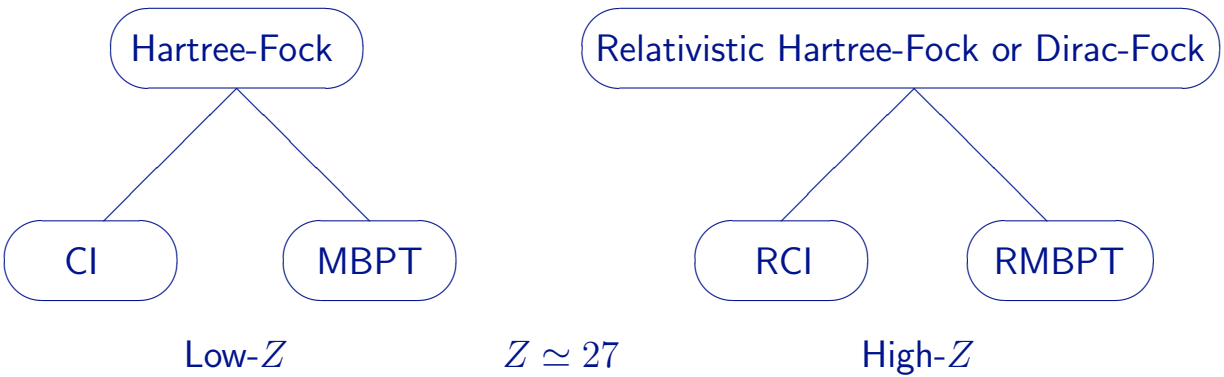
Many-Electron Atoms

- Because of difficulties in calculating integrals in fully correlated Hylleraas coordinates $r_{12}\, r_{23}\, r_{34} \cdots$, no calculations have been done for more than three electrons.
- General methods of atomic structure are needed.



Important progress by
M.S. Safronova et al. Phys. Rev. A **90**, 042513, 052509 (2014), and
B.K. Sahoo et al. Phys. Rev. A **83**, 030503 (2011).

Methods to Estimate Uncertainties

- Study convergence as more configurations (or excitations) are added (SDTQ $\cdots$).
- Compare different methods of calculation.
- Compare with benchmark calculations of higher accuracy, or experimental data.
- Use internal consistency checks, such as length/velocity forms for radiative transitions.
- Estimate order of magnitude for higher-order terms not included in the calculation.

Summary and Outlook

- Estimating uncertainties is indeed "difficult", but it is well worth doing.
- New technologies are emerging to make the estimation of theoretical uncertainties more rigorous and systematic.
- The result greatly increases the interest and significance of theoretical papers if well done.
- The result elevates the importance and significance of the field of theoretical atomic and molecular physics.