Uncertainty Estimates for Theoretical Papers

Gordon W.F. Drake
University of Windsor, Canada
and Editor

- Role of Accuracy Estimates in Atomic and Molecular Theory : Drake G. W. F. in *7th International Conference on Atomic and Molecular Data and Their Applications* - ICAMDATA, Vilnius, LITHUANIA SEP 21-24, 2010, AIP Conference Proceedings 1344, pp.116-121
- EDITORIAL in Phys. Rev. A **83**, 040001 (2011).

Outline

- Background and rationale
- Policy statement
- Implementation
- Recent examples

Background

- Part of an overall goal to keep ***Physical Review A*** in step with the user community.
- Policy to reject a larger fraction of papers without external review (about 20%). Papers must contain new physics.
- What about extensive tabulations of data? They are very useful to plasma physicists and astrophysicists, but the ICAMDATA meeting presented many talks about the need for a ***critical evaluation*** of the data.
- The authors themselves are in the best position to do a critical evaluation. This is now a condition in order to meet the acceptance criterion of "new physics."

Evolution of Physics

- The hallmark of good physics is that theory and experiment progress hand-in-hand.
- In a new field, the role of theory is to provide a qualitative explanation of experimental observations.
- As the field matures, the focus shifts to high precision comparisons between theory and experiment. Small deviations reveal new physics. Uncertainty estimates become crucial.
- The focus also shifts to the applications in other areas of science and technology (astrophysics, plasma physics, lasers, the lighting industry …)

Emergence of Data Bases

A large part of the motivation to construct huge data bases of atomic and molecular data to make the results of AMO physics available to a broad base of users – the consumer market.

- The Virtual Atomic and Molecular Data Centre (VAMDC): Marie-Lise Dubernet
- Database and related activities in Japan: Izumi Marakami
- NIST Atomic Databases: Alexander Kramida
- Vienna VALD3 and VAMDC databases for astrophysics: Nikolai Piskunov
- The ADAS project for fusion research: Hugh Summers
- Database for plasma physics in Korea: Jung-Sik Yoon
- IAEA Atomic and Molecular Data Unit: Bastiaan Braams

Needs for Expert Evaluation of Data

- A new profession of ***Expert Evaluator*** is emerging to assess the accuracy of the data found in the literature.
- In most cases, the authors themselves (and referees) are the best and most knowledgeable people to perform this task.
- Perhaps the journals have a role to play in expecting a higher standard for the assessment of the accuracy of the data they publish.

Policy Statement on Uncertainty Estimates

- 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 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:

Classification of Theoretical Papers

- Development of new theoretical techniques or formalisms.
- Development of new approximation methods, where the comparison with experiment, or other theory, itself provides an assessment of the error in the method of calculation.
- Explanation of previously unexplained phenomena, where a semiquantitative agreement with experiment is already significant.
- Proposals for new experimental arrangements or configurations, such as optical lattices or BEC's.
- Quantitative comparisons with experiment for the purpose of (a) verifying that all significant physical effects have been taken into account, and/or (b) interpolating or extrapolating known experimental data.
- Provision of benchmark results intended as reference data or standards of comparison with other less accurate methods.

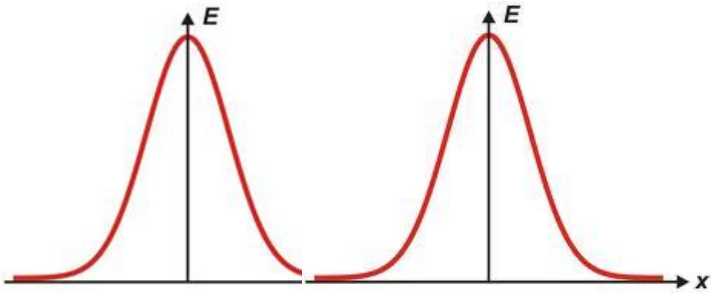
It is primarily papers in the last category that require a careful assessment of the theoretical uncertainties. The uncertainties can arise from two sources:

(a) the degree to which the numerical results accurately represent the predictions of an underlying theoretical formalism, for example, convergence with the size of a basis set, or the step size in a numerical integration, and

(b) physical effects not included in the calculation from the beginning, such as electron correlation and relativistic corrections.

It is of course never possible to state precisely what the error is without in fact doing a larger calculation and obtaining the higher accuracy. However, the same is true for the uncertainties in experimental data. The aim is to estimate the uncertainty, not to state the exact amount of the error or provide a rigorous bound.

Bimodal Distribution for Theoretical Uncertainties



For example

Total = nonrelativistic value ± relativistic corrections

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. Our policy is intended to cover cases where theoretical uncertainty estimates are practical, without placing undue restrictions in cases where the policy would be inappropriate.

The following policy statement on uncertainty estimates focuses on the goals and objectives for the work being done, rather than the particular method being used.

Summary Statement

Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances:

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

Current Procedure: Memo to Authors

Dear Dr. ……,

We have received your submission of the above manuscript to Physical Review A. Before we seek external review, we ask that you please take note of the attached memo regarding the need for uncertainty estimates for theoretical papers. Please add uncertainties to the numerical values in your tables, and a corresponding discussion of these uncertainties in the text.

Yours sincerely,

Impact

- 50 papers affected in the past year.
- Authors have responded well in most cases. No papers withdrawn.
- New procedures are being implemented in standard software packages (GRASP, Desclaux code, RMBPT, CI etc.) to retain information needed for uncertainty estimates.

Recent Example

M. S. Safronova and U. I. Safronova

"Blackbody radiation shift, multipole polarizabilities, oscillator strengths, lifetimes, hyperfine constants, and excitation energies in Ca^+", Phys. Rev. A **83**, 012503 (2011).

Some Recent Examples

1. Theoretical study on mechanisms of anomalous fine structure in the magnesium isoelectronic sequence
2. Sub-meV accuracy in first-principles computations of the ionization potentials and electron affinities of the atoms H to Ne
3. Hyperfine structure and (e-,e+)-pair annihilation in the muonium-positronium MuPs and positronium hydrides
4. Spectral representation of the three-body Coulomb problem. I. Nonautoionizing doubly excited states of high angular momentum in helium

5. Molecular polarizability in quantum defect theory: Polar molecules
6. Relativistic many-body calculation of energies, lifetimes, hyperfine constants, multipole polarizabilities, and blackbody radiation shift in ^{137}Ba II
7. Calculation of transition probabilities and ac Stark shifts in two-photon laser transitions of antiprotonic helium
8. Ground state of the polar alkali-metal-atom–strontium molecules: Potential energy curve and permanent dipole moment

9. High-accuracy calculation of energies, hyperfine constants, multipole polarizabilities, and blackbody radiation shift in $^{87}Sr^{+}$
10. Peculiarities of spectroscopic properties of W^{24+}
11. Real-space calculations of atomic and molecular polarizabilities using asymptotically correct exchange-correlation potentials
12. Multipole effects in atom-surface Interactions: A theoretical study with an application to He-alpha-quartz
13. Multiconfiguration Dirac-Hartree-Fock calculations of the electric dipole moment of radium induced by the nuclear Schiff moment
14. Theoretical studies of spectroscopic properties of the Cm^{4+} and Am^{3+} ions

In Conclusion:

- The aim is not to be excessively rigid, or to make unreasonable demands. The aim is just to expect a realistic assessment of the accuracy in theoretical calculations when a field has reached a high degree of maturity, and it is perfectly possible to do so.
- The journals have a lot of influence in encouraging authors to give properly justified uncertainty estimates.