

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) interpolating or extrapolating known experimental data.
6. Provision of benchmark results intended as reference data or standards of comparison with other less accurate methods.

It is primarily papers in the last two categories 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.

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

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