Uncertainty Estimates for Atomic Structure Calculations

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Atomic structure calculations play a key role not only in plasma diagnostics and astrophysical calculations, but also in fundamental tests of quantum electrodynamics (QED) and elementary particle interactions. The accuracies that can be achieved for one-, two-, and three-electron systems place fundamental limits on what can be achieved for many-electron atoms. The talk will present a brief survey of uncertainty estimates for effects arising from both higher-order physical effects not included in the calculations (such as relativistic and/or QED corrections), and approximate solutions to the few-body Schroedinger (or Dirac) equation. For two- and three-electron atoms or ions, extremely accurate solutions can be obtained by use of explicitly correlated wave functions in Hylleraas coordinates. The results are essentially exact for all practical purposes in the nonrelativistic limit. However, this is not the case for many-electron atoms. Here, the generally applicable, but less accurate methods of atomic physics must be used, such as the Hartree-Fock approximation and its extensions to include electron correlation effects (configuration interaction and many-body perturbation theory). The low-Z and high-Z regions of nuclear charge must be considered separately. Here, uncertainty estimates are much more difficult, but important progress has been made in recent years in quantifying the computational uncertainties [1].

The requirement of uncertainty estimates for theoretical calculations, as appropriate, is now part of the acceptance criteria for papers published in *Physical Review A* [2]. The journal policies and their impacts on the field will be briefly discussed.

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[1] H-K. Chung et al., J. Phys. D-Appl. Phys. **49**, 363002 (2016).

[2] The Editors, Phys. Rev. A **83**, 040001 (2011).