High-precision atomic calculations for fundamental physics applications and the development of atomic clocks

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Recent advances in atomic spectroscopy techniques have created a new era of unprecedented precision in the study of atomic phenomena. Atomic physics plays an ever-growing role in fundamental physics studies, including through atomic parity violation and searches for permanent electric dipole moments [1,2], as well as for tests of the CPT theorem and Lorentz symmetry, searches for variation of fundamental constants, and detection of dark matter and dark energy [3].

High precision atomic theory is required both to interpret experimental data in terms of fundamental physics parameters, and to direct experiment by identifying ideal systems for study. Examples include precision tests of the Standard Model at low energy [9], studies of atomic polarisabilities for the development of optical atomic clocks [8], searching for dark matter [4,6], and searching for variation of fundamental constants, including in the extreme gravitational environment around the super-massive black hole at the centre of our galaxy [5].

Motivated by recent measurements of several properties of alkali metal atoms and alkali-like ions, we perform a detailed study of electric dipole (E1) transition amplitudes in K, Ca^+, Rb, Sr^+, Cs, Ba^+, Fr, and Ra^+, which are of interest for studies of atomic parity violation, electric dipole moments, polarisabilities, the development of atomic clocks, and for testing atomic structure theory. Using the all-orders correlation potential method, we perform high-precision calculations of E1 transition amplitudes between the lowest s, p, and d states of the above systems. We perform a robust error analysis, and compare our calculations to 43 amplitudes which have high-precision experimental determinations. We find excellent agreement, with accuracies at the level of 0.1% or better [7].

Half our calculated amplitudes are *within the experimental uncertainties*, demonstrating unprecedented theoretical accuracy for many-body atoms, and setting a new precedent for atomic theory precision. Further, 95% of our calculated amplitudes are within 1σ combined (theory + experimental) uncertainties, much better than statistically expected, demonstrating our theory uncertainties are conservative. Together, this demonstrates that the atomic theory is at the same level as most atomic experiment for transition amplitudes, and that theoretical uncertainties can be determined robustly.

We also compare our results to other theoretical evaluations, and discuss the implications for uncertainty analyses of theoretical methods.

In particular, we observed that in many cases there is a large discrepancy between various calculations using coupled-cluster methods, possibly indicative of the sensitivity of such methods to basis choices and the details of the inclusion of triple excitations. Our method, which is based on an exact summation of screening diagrams using a Feynman diagram and Green's function technique, does not suffer from these issues.

Finally, by combining highly accurate calculations of branching ratios with recent experimental data, we extract new high-precision values for several E1 amplitudes of Ca^+, Sr^+, Cs, Fr, and Ra^+.

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