High-precision study of E1 transition amplitudes for single-valence atoms and ions

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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.

Half our calculated amplitudes are *within the experimental uncertainties*, demonstrating unprecedented theoretical accuracy for many-body atoms. 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 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^+, Cs, Fr, and Ra^+.