Precise Atomic Calculations for Low-Energy Searches for Physics Beyond the Standard Model

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Precision atomic metrology gives us an extraordinary probe of physics beyond the Standard Model, enabling searches for new particles, dark matter, variations of fundamental constants, and violations of fundamental symmetries (see, e.g., review [1]). Many of the most sensitive probes extract limits on new physics from differential measurements of heavy atoms with complicated open-shell spectra. This necessitates accurate calculations of these systems for planning and supporting experiments, as well as to interpret the results as limits on new physics.

As an example, recent measurements of the isotope shift of Yb and Yb⁺ have seen strong deviation from theory (the 'King plot nonlinearity' [2]), which could be interpreted as evidence for a new forcecarrying boson that couples electrons and neutrons [3-5]. However, atomic theory is required to quantify (or remove) systematic nuclear effects that might also create the observed deviations, such as quadratic field shifts. Calculations in open-shell atomic systems like Yb⁺ are notoriously difficult to perform with high accuracy.

Novel clocks based on highly charged ions promise significant gains in sensitivity to new physics effects, while simultaneously improving frequency precision [6]. The required accuracy of calculation for these systems increases with ionization stage because of the strong cancellation of binding energies in an optical transition, posing a challenge for atomic structure theory.

I will present some motivations, methods, and results of calculations using the particle-hole CI+MBPT method [7] implemented in the AMBiT code [8]. All-order coupling of selected core

shells allows the method to have accuracy comparable to coupled-cluster methods (Fig. 1) while being applicable across the entire periodic table.

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Fig.1. Grotrian diagram at the 5p – 4f orbital crossing in Pr⁹⁺ [9].
Blue: experiment; Red: CI+MBPT calculations using AMBiT;
Orange: Fock-space coupled-cluster calculations.

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