Electronic factors for isotope shifts

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The isotope shift (IS) of the frequency of a given atomic line k between two isotopes A and A' is usually written as

$$\delta \nu_k^{A,A'} = M_k \left[(A'-A)/AA'\right] + F_k \, \delta\langle r^2\rangle^{A,A'}$$

where the two terms represent respectively the mass shift (MS) and field shift (FS) contributions [1]. M_k and F_k are the electronic mass and field shift factors for the considered electronic transition k. Using this relation, the changes in mean-square radii $\delta\langle r^2\rangle^{A,A'}$ of the nuclear charge distribution can be determined from IS measurements provided that the electronic quantities M_k and F_k are known.

As far as MS are concerned, the authors of the present contribution acquired a large experience in the theoretical evaluation of the relevant parameters for highly correlated systems such as neutral atoms and negative ions (see e.g. [2]). The balance between MS and FS contributions to the IS was studied for the resonance doublet lines along the lithium isoelectronic sequence [3]. The “Shabaev” relativistic corrections to the recoil operator [4] affecting the normal mass shift (NMS) and specific mass shift (SMS) factors contributing to M_k have been implemented in the relativistic multiconfiguration Dirac-Hartree-Fock GRASP2K package [5], allowing to test the reliability of the Dirac kinetic energy operator for estimating the NMS [6].

The FS can be estimated in a perturbation approach by expressing the F_k factor as proportional to the change of the electronic total probability density at the origin, calculated for a reference isotope, between the two atomic states involved in the transition, or by a variational method based on two separate electronic calculations for each level, using realistic nuclear densities for both isotopes. The difference between the two calculations reaches 5% for $^{150,142}Nd^{57+}$ [3]. A third approach, more pragmatic, is to assume that both M_k and F_k factors are constants for an isotopic chain. Solving the above equation for the frequency shifts calculated by perturbation for a triplet of isotopes (or more) and using the wave functions of a given stable isotope, allows to estimate the M_k and F_k parameters [1].

All these computational strategies should be compared more systematically. In a joined effort, the authors will focus on some common targets, in answer to the call from the radioactive ion beam physics community who develop highly sensitive in-source laser-photoionization spectroscopy techniques, or perform laser-spectroscopic studies on short-lived radioactive nuclei to explore changes in the nuclear size, spin, and moments for isotopes far away from stability [7].

References

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