Electronic factors for isotope shifts

Thomas Carette[*], Jiguang Li[†,*], Cédric Nazé[*], Stephan Fritzsche[‡], Per Jönsson[§] and Michel Godefroid[*] [1]

[*] Chimie Quantique et Photophysique, Université Libre de Bruxelles, B-1050 Brussels, Belgium
[†] Department of Physics, Lund University, S-221 00 Lund, Sweden
[‡] Helmholtz-Institut Jena, D-07743 Jena, Germany
[§] School of Technology, Malmö University, S-205 06 Malmö, Sweden

Synopsis Progresses have been made in the ab initio calculation of the electronic factors contributing to the mass and field isotope shifts of atomic spectral lines. We will illustrate these progresses and underline the current limitations.

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

$$\delta\nu_k^{A,A'} = M_k \, \frac{A' - A}{AA'} + F_k \, \delta\langle r^2\rangle^{A,A'} \, ,$$

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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[1] E-mail: mrgodef@ulb.ac.be