Safronova et al. (Phys. Rev. A, Vol. 76, 042504, 2007) published a paper on the study of Francium-like atoms and ions in the range of Z=87-100. Results for the calculation of transition rates show erratic behavior in the high Z range as shown in the figures below.

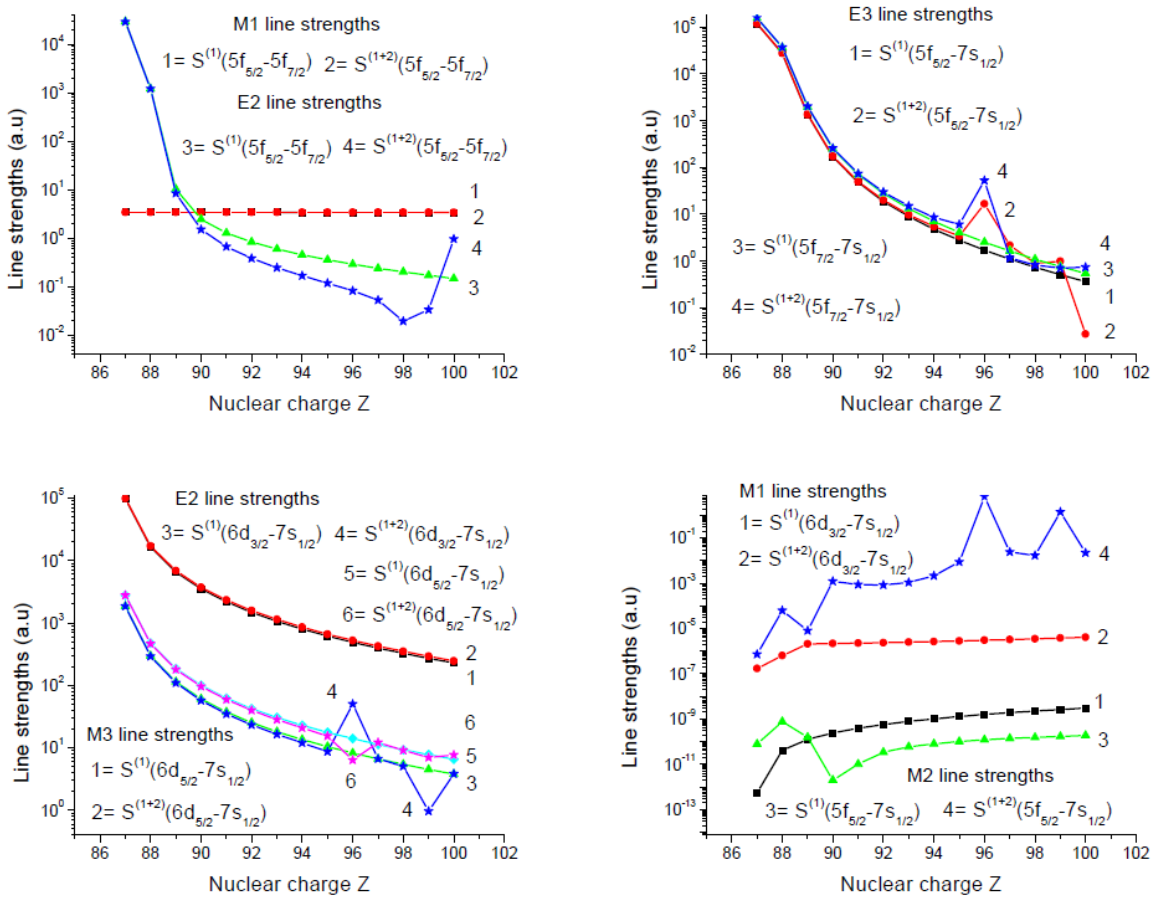

FIG. 6: Multipole line strengths (S in a.u) as functions of Z in Fr-like ions.

A question arises – are these irregularities physical or are they an indication of computational problems?

The DBSR_HF program (O. Zatsarinny and C. Froese Fischer, CPC 202, 287-303 (2016)) uses B-spline expansions for computing the Hartree-Fock wave functions that lead to generalized eigenvalue problems whereas finite difference methods lead differential equations with two-point boundary conditions usually solved by outward and inward integration procedures. For heavy elements, the outward Integration is considerably longer than inward integration and errors accumulate before the matching of occurs.

DBSR_HF has not been used to study heavy elements. In this Project we want to compute wave functions in the range Z=87 – 118 (if possible) for Francium-like atoms and ion. The CPC paper explains the command language for atoms and ions.

For the neutral atom, the ground state is 7s. Orbitals are computed by the command

dbsr_hf Fr.DHF atom=Fr mbreit=1

producing a file Fr.DHF.bsw that contains the B-spline expansions of the orbitals.

The following computes an excited state, with a 6d orbital, using the input from the previous run:

dbsr_hf Fr_6d atom=Fr conf=6d(1) term=LS inp=Fr.DHF.bsw varied=6d,6d- mbreit=1 out_plot=1 plot=aaa

For the ion, DBSR_HF command needs to specify the atom (which determines the nucleus, etc.) and the ion. For the ion, Ra+ (Z=88), the commands would be

dbsr_hf Ra+.DHF atom=Ra ion=Fr mbreit=1

Dbsr_hf Ra+.6d atom=Ra ion=Fr conf=6d(1) term=LS inp=Ra+.DHF.bsw varied=6d,6d- mbreit=1 out_plot=1

Calculations: For Z=87, 88, 90, 92, 94, 96, 98, 100, 103, 106, 109, 112, 115, 118

1. Compute the energies of the ground state (7s) and prepare tables (spread sheet) for which the columns are
   1) Atomic number
   2) Mass number
   3) 7s orbital energy
   4) Coulomb energy (units are not important but maybe eV)
   5) Breit correction
   6) Self-energy
   7) Vacuum Polarization
   8) Sum
   9) Plot Breit/Coulomb and also (Self-energy +Vacuum Polarization)/Coulomb. Are trends smooth?

2. Repeat the above but instead of 6d compute for 5f. Look at some plots of 5f (Z=87,88, higher)
3. Compute some of the line strengths. This requires that we convert the wave functions to GRASP format. We could compute M1 line strength for 5f-5f transitions and 6d-7s and also the E1 6d-5f line strength.