Fisher-like atomic divergences: mathematical grounds and physical applications

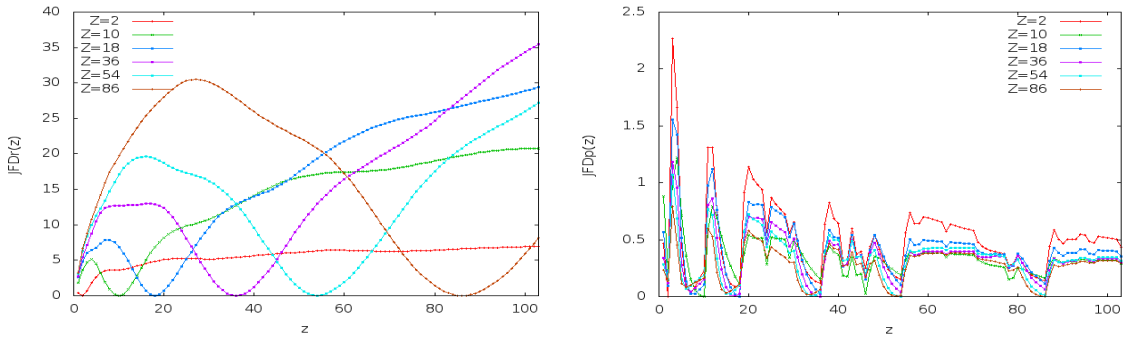
Juan C. Angulo[1,3], Adrián L. Martín[1], Juan Antolín[2,3]

[1]*Departamento de Física Atómica, Molecular y Nuclear, Universidad de Granada, 18071-Granada, Spain*
[2]*Departamento de Física Aplicada, EINA, Universidad de Zaragoza, 50009-Zaragoza, Spain*
[3]*Instituto 'Carlos I' de Física Teórica y Computacional, Universidad de Granada, 18071-Granada, Spain*
angulo@ugr.es

A variety of divergence measures have been applied successfully to the study of many-electron systems [1]. Most usually, measures of global character have been considered, because of their variety and the aims of their use [2]. More scarce and recent are the studies by means of local-character divergence measures [1,3], with a higher sensitivity to differences at smaller scales than those of the global ones.

Two different local divergence measures, the Fisher (FD) and the Jensen-Fisher (JFD) ones, are compared in this work by applying them to atomic one-particle densities in position and momentum spaces. They are defined in terms of the absolute [4] and the relative [5] Fisher information functionals. JFD among each noble gas and all neutral atoms is displayed below in position (left) and momentum (right) spaces.

The analysis here afforded includes not only neutral atoms, but also singly-charge cations. The results are interpreted and justified according to (i) shell-filling patterns, (ii) short- and long-range behaviors of the atomic densities, and (iii) the value of the atomic ionization potential. Strengths and weaknesses of both local measures are emphasized.



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