Generalized Jensen Divergence Analysis of Atomic Electron Densities in Conjugated Spaces

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ABSTRACT: Several measures of divergence have been used in the past to quantify the dissimilarity between two or more one-particle atomic densities. The advantages and difficulties of them to capture the differences among different atomic systems in the position and momentum spaces are studied. One of these measures, the Jensen-Shannon divergence, is generalized giving rise to a one-parameter divergence, the Jensen-Rényi divergence, here proposed for a deep study of atomic systems, improving the above previous results. The versatility and power of this divergence is applied to compare different neutral atoms, their composing subshells and each of those atomic densities computed within different models. The parameter of the Jensen-Rényi Divergence allows also to emphasize the study in relevant specific regions of both conjugated spaces. © 2010 Wiley Periodicals, Inc. Int J Quantum Chem 111: 297–306, 2011

Key words: Jensen-Rényi and Jensen-Shannon divergences; atomic one-particle densities; shell-filling patterns; Hartree-Fock and Bare Coulomb Field densities; atomic decomposition in subshells

1. Introduction

The concepts of uncertainty, randomness, or delocalization are basic ingredients in the study, within an information theoretic framework, of relevant structural properties for many different probability distributions appearing as descriptors of several chemical and physical systems and processes. The relevancy of such concepts motivates the search for their appropriate quantification, giving rise to a variety of density functionals, such as the Shannon entropy [1], the Fisher information [2], the disequilibrium or informational energy [3, 4], or the complexity [5], as many others. These information measures have been widely used for describing the information content and behavior of distribution functions in a great variety of fields [6, 7] and, in particular, for the study of many-electron systems [8–13], which are the objects analyzed in this work.

Following the usual procedures carried out within the Information Theory for quantifying the uncertainty or disorder of individual distributions, some extensions have been done to introduce the concepts of distance or divergence between two (or more) distributions, as comparative measures of their dissimilarity [14, 15].

There exists an extensive literature on measures of similarity and dissimilarity between probability densities [16, 17], which have been used in a wide variety of scientific fields including, for instance, sequence analysis [18], pattern recognition [19], diversity [20], classification [21], homology [22], neural networks [23], computational linguistics [24], or quantum theory [25]. The recent explosion in the knowledge based on chemical research has given rise to a surge of interest in chemical similarity. Molecular modelling, quantitative structure activity relationship (QSAR), and quantum information are simple examples of such an interest [26, 27].

Chemical similarity is oftenly described as an inverse of a measure of distance in the appropriate space. In particular, the Quantum Similarity Theory (QST) [28] was originally developed to establish quantitative comparisons between molecular systems by means of their fundamental structural magnitudes, i.e., electron density functions. The obvious motivation was that studying the differences between the electronic charge densities of these species could be related to differences between their respective physical and chemical properties, according to the Density Functional Theory and the Hohenberg-Kohn theorem [29].

In probability, statistics or information theory, different approaches have dealt with the aim of establishing quantitative comparisons among two or more distribution functions, giving rise to a variety of definitions and measures of divergence. All those divergences have their own properties which make them less or more appropriate according to the specific problem we are dealing with [14–17].

The main aim of this work is, far beyond to analyze the capability of the most important information divergence measures as the Quadratic Distance (QD), the Jensen-Shannon Divergence (JSD) and the Fisher Divergence (FD) in the study of dissimilarity between multielectronic systems (Section 2), the comparison to the new proposal here studied. Such a proposal arises from the Rényi entropy, providing a one-parameter generalization of the Jensen-Shannon divergence, namely the Jensen-Rényi divergence (JRD), which allows one to modify the relative weight of the distributions under comparison within specific regions of physical interest, as done for neutral atoms throughout the Periodic Table (Section 3). Additionally, the JRD divergence is applied to the study of dissimilarities between atomic systems which densities are computed within different models (Section 4) and among the whole set of occupied subshells constituing each atom (Section 5). Some concluding remarks are finally given.

The universality of the methods here used allows their application not only for atomic systems but also for many others such as, for instance, molecules and clusters, as well as for the analysis of physical and chemical processes such as ionization and reactions.

2. Dissimilarity Measures: The Jensen-Shannon Divergence

The simplest and most intuitive dissimilarity measure is just the Quadratic Distance (QD) which is defined by the norm of the difference of the distributions:

$$QD(\rho_1, \rho_2) \equiv \left(\int [\rho_1(\vec{r}) - \rho_2(\vec{r})]^2 d\vec{r} \right)^{1/2} \quad (1)$$

A closely related measure of similarity, the so-called Quantum Similarity Index (QSI), can be defined as an overlap integral between the two electronic densities to be compared. This overlap integral can be generalized by introducing other weight operators, different from the Dirac delta one, as for instance the Coulomb operator, leading to additional

molecular quantum similarity measures [28, 30–33]. For the Dirac delta operator, the QSI is given by

$$\text{QSI}(\rho_1, \rho_2) \equiv \frac{\int \rho_1(\vec{r}) \rho_2(\vec{r}) d\vec{r}}{\sqrt{\int [\rho_1(\vec{r})]^2 d\vec{r} \int [\rho_2(\vec{r})]^2 d\vec{r}}} \quad (2)$$

One of the most interesting properties of the QSI is its bounded character, being constrained to the range of values [0, 1].

On the other hand, some other similarity indices based on the concept of an information distance have been proposed and evaluated for different many particle systems, such as atoms or molecules [9, 34, 35].

The Kullback-Leibler divergence or relative entropy [14] is perhaps the most important non symmetric divergence measure in the Information Theory, being defined as

$$\text{KL}(\rho_1, \rho_2) \equiv \int \rho_1(\vec{r}) \ln \frac{\rho_1(\vec{r})}{\rho_2(\vec{r})} d\vec{r} \quad (3)$$

which embodies the well known Shannon entropy [1],

$$S(\rho) \equiv - \int \rho(\vec{r}) \ln \rho(\vec{r}) d\vec{r}, \quad (4)$$

which constitutes a global measure of the spread of the distribution over its whole domain. The KL divergence, as well as its symmetrized version

$$\text{KLS}(\rho_1, \rho_2) \equiv \int \rho_1(\vec{r}) \ln \frac{\rho_1(\vec{r})}{\rho_2(\vec{r})} d\vec{r} + \int \rho_2(\vec{r}) \ln \frac{\rho_2(\vec{r})}{\rho_1(\vec{r})} d\vec{r} \quad (5)$$

have been extensively studied and applied in a great variety of fields such as, for instance, minimum cross entropy estimation [36] or indexing and image retrieval [37].

The so-called "Jensen-Shannon divergence" represents also a symmetrized version of the KL measure and quantifies the deviation (entropy excess) between the Shannon entropy of the mixture of two (or more) distributions and the mixture of the entropies of the distributions. It is given by [38, 39]

$$\text{JSD}(\rho_1, \rho_2) \equiv S\left(\frac{\rho_1 + \rho_2}{2}\right) - \frac{1}{2}[S(\rho_1) + S(\rho_2)], \quad (6)$$

interpreted in this way as the "entropy excess" of the mean density with respect to the mean entropy of the involved distributions.

The JSD preserves the global character of the Shannon entropy, it is a non-negative measure (as a consequence of the convexity of the $S(\rho)$ functional) and equals zero only when $\rho_1 = \rho_2$.

It quantifies, in fact, the statistical dependence among an arbitrary number of probability distributions (as will be shown below), and there are some important reasons because of many researchers choose JSD as a measure of divergence. Among them: (i) it is a smoothed version of the Kullback-Leibler divergence, and hence it shares its mathematical properties and their intuitive interpretability [7, 40], (ii) it provides direct interpretations in the framework of statistical physics, information theory, or mathematical statistics [41], (iii) the JSD is related to other information-theoretical functionals (special case of the Jensen difference [42] and the Csiszár divergence [43]) and it is the square of a metric [44], (iv) the JSD can be generalized to measure the distance between more than two distributions, and (v) it is possible to assign different weights to the distributions, which allows us to take into account different sizes of the objects we are comparing (e.g., different lengths of the subsequences in DNA analyses or different subshells or parts in atomic or molecular similarity analyses [41, 45]). However, its use in the framework of quantum information theory [25, 27] or in the study of multielectronic systems [35, 46, 47] is very recent.

The generalized multiple-density JSD with arbitrary weights can be written as

$$\text{JSD}(\rho_1, \ldots, \rho_n) \equiv S\left(\sum_{k=0}^{n} \omega_k \rho_k\right) - \sum_{k=0}^{n} \omega_k S(\rho_k), \quad (7)$$

the weights $\{\omega_k\}$ verifying $\sum_{k=1}^{n} \omega_k = 1$. The particular case $n = 2$ and $\omega_1 = \omega_2 = 1/2$ provides the initial expression given by Eq. (6), the generalization preserving the mathematical properties verified by the initial JSD.

The Fisher information, I, is another important information quantity [2, 6], being originally introduced as a measure of intrinsic accuracy in statistical estimation theory. It is a measure of the gradient content of a distribution and, therefore, is a local measure which explores deeply the changes in the electronic distribution:

$$I(\rho) \equiv \int \rho(\vec{r}) |\vec{\nabla} \ln \rho(\vec{r})|^2 d\vec{r}, \quad (8)$$

This relevant magnitude is also a measure of the distribution localization, and it has not been used

until very recently to investigate directly electronic densities. Applications in the above field include the studies on single-particle systems governed by a central potential [48], the two-electron entangled artificial atom proposed by Moshinsky [49], the modified Thomas-Fermi atoms [50], and the derivation of analytical relationship between the integrands defining Shannon entropy and Fisher information [51].

In some recent papers, the product of the atomic Fisher information and the Shannon power entropy has been found to show good correlations with the shell structure and pattern of the whole periodic table, giving a measure of the complexity and hierarchy of these systems [52].

Taking into account the divergence character of the symmetrized Kullback-Leibler measure, we define a similar magnitude using now Fisher information. It can be readily verified that the symmetrized relative Fisher information, which will be refered in what follows as "Fisher Divergence" (FD),

$$\text{FD}(\rho_1, \rho_2) \equiv \int \rho_1(\vec{r}) \left| \vec{\nabla} \ln \frac{\rho_1(\vec{r})}{\rho_2(\vec{r})} \right|^2 d\vec{r}$$
$$+ \int \rho_2(\vec{r}) \left| \vec{\nabla} \ln \frac{\rho_2(\vec{r})}{\rho_1(\vec{r})} \right|^2 d\vec{r}, \quad (9)$$

provides relevant information on dissimilarity by performing a comparison between distributions based on the Fisher information. Both the one- and two-density functionals (I and FD, respectively) posses a deep local character in the sense of being more sensitive to strongly localized variations when compared to the behavior of the distribution over its whole domain, as happens with QD and JSD. Nevertheless, all these dissimilarity measures (QD, JSD, and FD) keep as main "distance properties" the non-negativity, the symmetry (invariance under exchange of functions) and saturation (minimal zero value only for identical distributions).

For our present purposes, i.e., the analysis and comparison of neutral atoms throughout the Periodic Table in terms of their one-particle densities in both conjugated position and momentum spaces ($\rho(\vec{r})$ and $\gamma(\vec{p})$, respectively) the definition domain is the whole three-dimensional space. In this sense, it should be pointed out that (i) all expressions given in this work for an specific space (position or momentum) will be also valid in the conjugated one, by only replacing properly the corresponding variables and distributions, and (ii) for atomic systems in the absence of external fields, it is sufficient to deal

with the spherically averaged densities $\rho(r)$ and $\gamma(p)$ defined over the non-negative real line $[0, \infty)$.

Let us first compare these measures among themselves for the quantification of "how similar or dissimilar" the one-particle electronic densities are for neutral atoms in the position (r) and momentum (p) conjugated spaces. The Figure 1, where all noble gases (for illustration) are compared to the rest of atoms in the Periodic Table, allows us to interpret physically the results. Next comments are valid also for all other groups in the Periodic Table. The computations were carried out within a near Hartree-Fock framework [53, 54] for neutral atoms with nuclear charges $Z = 1 - 103$, to obtain the spherically averaged one-particle densities in "r" and "p" spaces, $\rho(r)$, and $\gamma(p)$ respectively.

The comparisons are carried out by means of QD, FD, and JSD in both conjugated spaces, namely position and momentum. Some comments are in order. The most apparent feature is the rich structure displayed by all curves belonging to the three measures when dealing with momentum space, according to the high number of local extrema displayed by all those divergences as compared to the position space ones. The locations and types of extrema (maximum or minimum) are roughly the same for the three measures, at least according to the main peaks, as will be discussed below. The previous comments are not applicable for the position space measures, where a similar structure (not so enhanced as in momentum space) is only displayed by the JSD, as opposite to the unimodal shapes of both QD and FD.

In what concerns the location of the main extrema, it is observed their appearance associated to (i) comparisons between atoms belonging to the same group of the Periodic Table, and (ii) systems suffering the so-called anomalous shell-filling. This comment applies not only for all momentum space measures but also for JSD in the position one. In this sense, the "distance" of a given system to a second one is lower when both them display a higher similarity according to their physical and chemical characteristics, mainly determined by the valence region.

Such is not the case of the unimodal measures in positon space, which only provide information on how "far/different" the involved nuclear charges are, the values of the other measures being determined by the atomic shell structure. The minimal value zero is always reached when comparing identical systems, but no additional extrema appear for the position space QD and FD. In fact, these measures quantify the distance between systems as ordered attending exclusively to the nuclear charge, while the
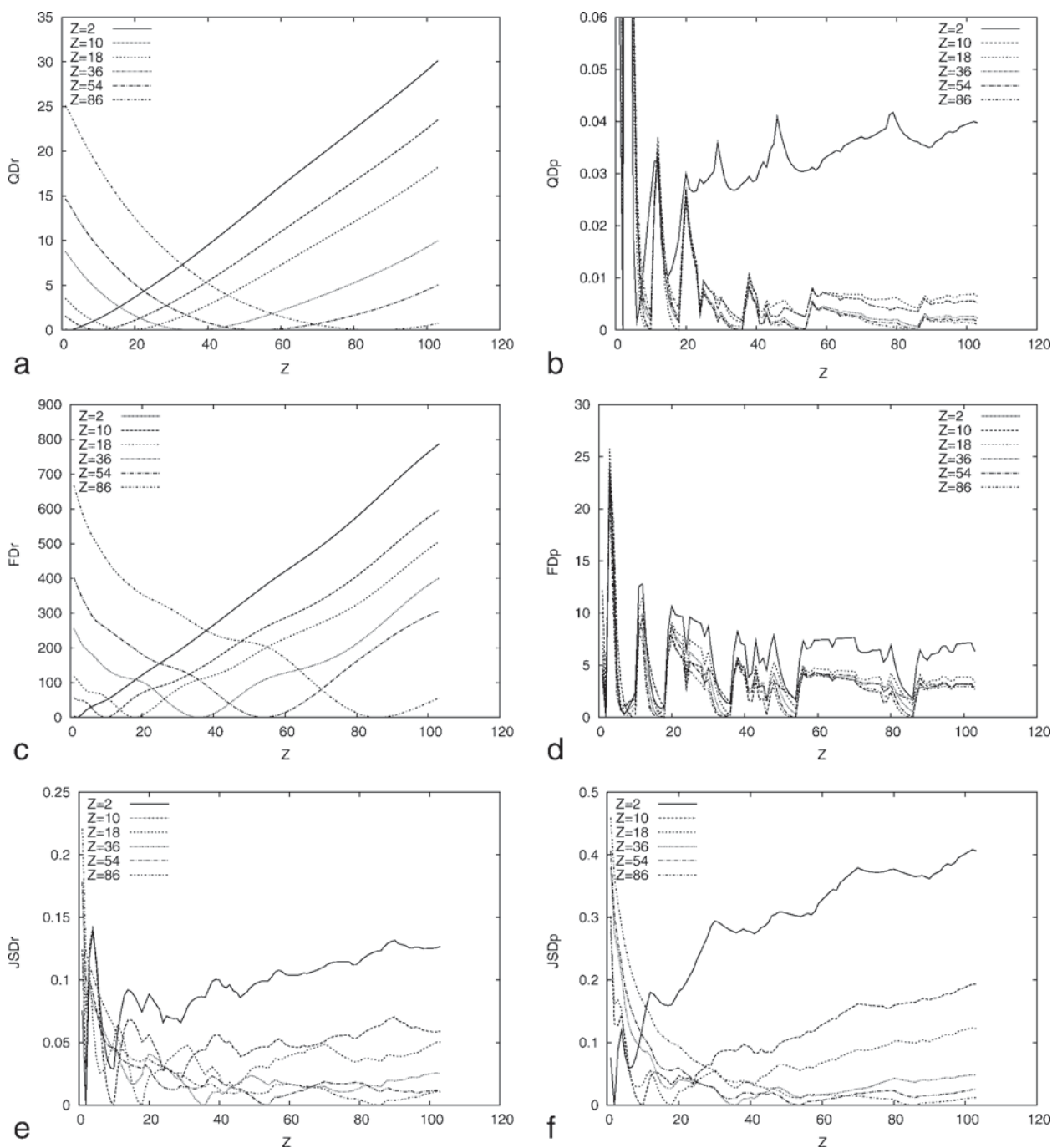
FIGURE 1. Quadratic Distance QD (top), Fisher Divergence FD (middle), and Jensen-Shannon Divergence (bottom) between the one-particle densities of noble gases and those of neutral atoms with nuclear charge $Z = 1 - 103$, in position (left) and momentum (right) spaces. Atomic units are used.

rest of measures quantify their distance according to their location over the highly structured Periodic Table.

It is also remarkable the very similar ranges of JSD values in both spaces, whereas those of both QD and FD are absolutely different as comparing the position and momentum spaces.

To provide a physical interpretation of the above discussed results, it is worthy to remember the decreasing trend of both densities and their physical

meaning. Higher values of $\rho(r)$ and $\gamma(p)$ correspond to low "r" and "p", respectively. Low "r" is associated to electrons surrounding the nucleus, whereas low "p" (i.e. low speed) electrons are the outermost ones, located in the valence region. The overlap and the gradient integrals (those of QD and FD) are mainly determined by the aforementioned regions: in position space, that governed by the nuclear charge Z, while in momentum space the valence subshell which appears as the essential ingredient for a physically relevant comparison among atomic systems.

In what concerns the structure in position space for JSD, when compared to QD and FD, it should be pointed out the "logarithmic attenuation" of the integrands defining the JSD, which makes possible this measure to quantify, at least slightly, the outermost contribution even in position space.

It appears also as a very intereting aim to deal with a measure, in a similar fashion as those considered in this section, allowing to perform a comparison among distributions but including additionally the availability to define specific regions as main domains to be compared, as well as to enhance or diminish appropriately the level of structure in the sense discussed above. Both aims will be get, as described in the next section, by means of the "Jensen-Rényi Divergence" JRD.

3. Jensen-Rényi Divergence (JRD) Among Neutral Atoms

The Shannon entropy S constitutes a particular case of the so-called Rényi entropy of order q [55],

$$R^{(q)}(\rho) \equiv \frac{1}{1-q} \ln \omega^{(q)}(\rho), \qquad (10)$$

with $\omega^{(q)}(\rho) \equiv \int \rho^q(\vec{r})d\vec{r}$ being the frequency moment of order q of the distribution $\rho(\vec{r})$. Both the Rényi entropy and some frequency moments play a relevant role in the description of quantum many-body systems by means of their one-particle densities. The convergence of the involved integral depends on the short- and long-range behavior of the distribution we are dealing with.

The limiting case $q \to 1$, taking into account the normalization constraint $\omega^{(1)}(\rho) = 1$, provides the Shannon entropy: $R^{(1)}(\rho) = S(\rho)$. Consequently, $R^{(q)}(\rho)$ constitutes a generalization of the Shannon entropy $S(\rho)$.

Replacing the Shannon entropy by the Rényi one in the JSD definition gives rise to a new double-density functional, the Jensen-Rényi Divergence [42]

$$\mathrm{JRD}^{(q)}(\rho_1, \rho_2) \equiv R^{(q)}\left(\frac{\rho_1 + \rho_2}{2}\right) - \frac{1}{2}\left[R^{(q)}(\rho_1) + R^{(q)}(\rho_2)\right]$$

in such a way that $\mathrm{JRD}^{(1)} = \mathrm{JSD}$, the new divergence generalizing the previously introduced JSD one. Scarce applications of the JRD measure have been carried out, only in fields (to the best of our knowledge) such as image registration [56, 57] or document categorization [58].

The non-negativity of $\mathrm{JRD}^{(q)}$ is guaranteed for $0 < q < 1$, constraint which arises from the convex/concave character of the frequency moments $\omega^{(q)}$ according to the value of "q". This parameter acts by smoothing the integrands for lower "q" values and enhancing the contribution of the outermost region of the atomic domain.

The computations of $\mathrm{JRD}^{(q)}$ for the particular values $q = 0.4, 0.8$, when compared to the limiting case $q \to 1$ which corresponds to JSD, provides the results shown in Figure 2 for the divergence between Krypton (nuclear charge $Z = 36$) and all neutral atoms throughout the Periodic Table. These results extend previous studies performed in a similar fashion as done here, but only by means of the JSD measure [35].

It is clearly observed that lowering the value of the parameter "q" below 1 enhances or diminishes different contributions of the density domain according to the considered space (position or momentum) in an opposite way: enhancing the valence region in position space and the nuclear region in the momentum one. This is a consequence of the structural properties of both one-particle atomic densities for which their maximum values are located at the origin (systematically in position space and frequently in the momentum one) or very close to it. As explained before, the valence subshell is far from the origin when compared to the other ones, and the exponential decrease of the density makes the contribution of such a region to the JRD value to be very small, unless enhancing it by powering the density with a small exponent "q". The Figure 2(a) reveals that to get shell-filling patterns by means of $\mathrm{JRD}^{(q)}$ in position space low values of the parameter "q" are required.

The opposite trend is observed in the Figure 2(b), similarly justified as previously. The momentum density around the origin quantifies the relative number of electrons with low linear momentum "p," which are just those located in the outermost region.
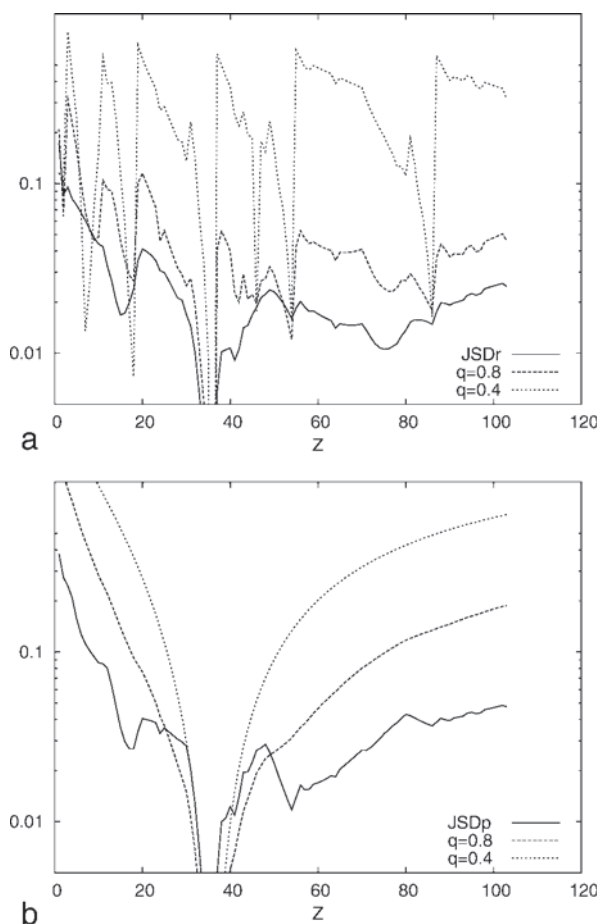
FIGURE 2. Jensen-Rényi Divergence JRD$^{(q)}$ for $q = 0.4, 0.8$ and Jensen-Shannon Divergence $JSD = JRD^{(1)}$ between the one-particle densities of Krypton (nuclear charge $Z = 36$) and those of neutral atoms with $Z = 1$–103, in (a) position and (b) momentum spaces. Atomic units are used.

Consequently, the contribution of that region is now diminished when lowering "p."

Concerning the momentum space, the value $q = 1$ appears as "almost critical", in the sense that going down only up to $q = 0.8$ makes the previous structure to disappear almost completely.

So, the role played by the value of the parameter "q" allows one to obtain a higher level of information on the shell-filling effects according to the space which the density considered belongs to.

The discussion concerning the specific structure of the curves displayed in this figure can be carried out in a similar fashion to that of Figure 1. That is, the location of the main minima corresponds to systems belonging to the same atomic group of Krypton (i.e., noble gases), while other minor ones

are mostly associated to systems suffering the "anomalous shell-filling." This comment is valid for the JRD in both conjugated spaces, for those "q" values for which such a structure is displayed.

4. Jensen Divergences Among Atomic Models

The applications of JSD and JRD go far beyond the comparison of different neutral atoms as previously done. In fact, the divergences can be used by considering two arbitrary distribution functions. Within the framework we are dealing with, a very interesting application is the quantification of the differences between the one-particle densities of a given system but computed within different models. As a very specific ilustration, the Figure 3 shows the corresponding divergences, in each conjugated space, for the Hartree-Fock (HF) and the "Bare Coulomb Field" (BCF) models, in the last one the interelectronic repulsion being neglected. So, the corresponding divergences constitute, in fact, a measure of the changes experienced by the densities when neglecting the repulsive forces and, consequently, of their relevance for the atomic densities, as shown in Ref. 47 for the JSD case.

It is first observed, by comparing Figures 3(a) and (b), that the curves are ordered following opposite trends in the two spaces. Divergences (i.e., differences between the HF and BCF densities) become higher as decreasing (increasing) "q" in position (momentum) space. The interelectronic repulsion mainly affects, consequently, the outermost region as compared to the nuclear one, as can be interpreted according to the results obtained in each space.

This fact means that, as far as the interelectronic repulsion increases, the electrons start to space out among themselves but more easily in the outermost region because of their spreading there as compared to the vicinity of the nucleus.

Concerning the structural characteristics of the curves, it is also observed that also the extrema in each space follow different trends: local maxima appear in position space in the $q = 0.2$ curve for systems where a new subshell has been added, more apparently when the subshell is of "s" type. This means that the single-electron valence orbitals are more sensitive to the effect of the repulsive forces than those with a higher occupation number. On the other hand, location of maxima in the momentum JSD curve are associated to closed-shell systems.
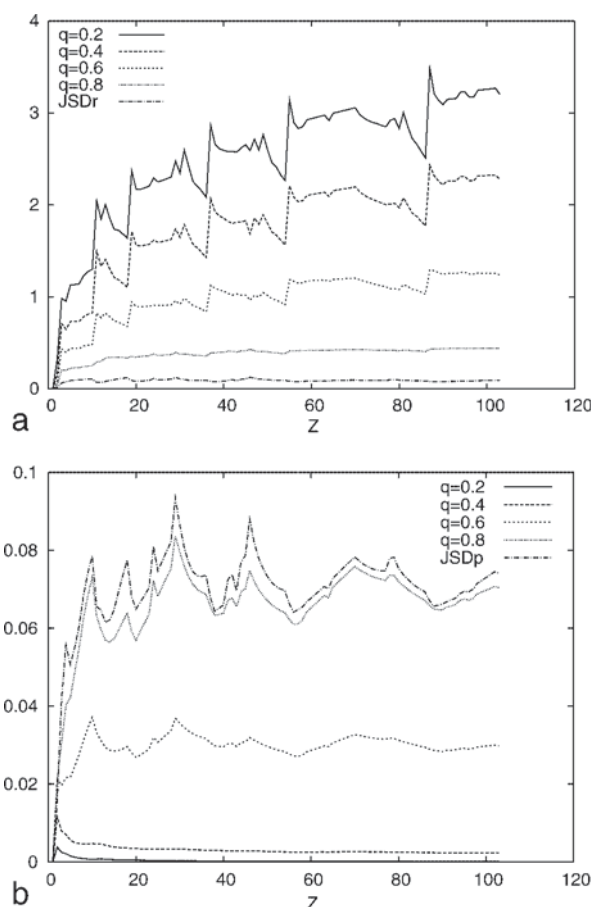
FIGURE 3. Jensen-Rényi Divergence JRD$^{(q)}$ for $q = 0.2, 0.4, 0.6, 0.8$ and Jensen-Shannon Divergence JSD = JRD$^{(1)}$ between the one-particle densities computed within Hartree-Fock (HF) and Bare Coulomb Field models, for neutral atoms with nuclear charge $Z = 1–103$, in (a) position and (b) momentum spaces. Atomic units are used.

Other "q" values make the extrema to progressively soften, even disappearing in some cases.

The universality of the method here used allows its application to the analysis of the effects arising by considering numerical computations or models other than the BCF one. This will be done elsewhere by considering correlated wavefunctions or relativistic effects, among others.

5. Jensen Divergences Among Atomic Subshells

The JSD and JRD definitions can be extended (i) by considering an arbitrary number "M" of distributions, and (ii) by weighting each density according to the desired criteria. This generalization gives rise to

$$\text{JRD}^{(q)}\left(\{\omega_i, \rho_i\}_{i=1}^{M}\right) \equiv R^{(q)}\left(\sum_{i=1}^{M} \omega_i \rho_i\right) - \sum_{i=1}^{M} \omega_i R^{(q)}(\rho_i)$$

(11)

with $\sum_{i=1}^{M} \omega_i = 1$, and similarly for JSD in terms of $S(\rho_i)$. The same properties previously mentioned remain.

The above generalization allows one to quantify the divergence among a collection of distributions, which can be considered as a "mean distance" among them. A particular application of this measure can be performed on the subshells (n, l) composing a given N-electron atom, each one containing N_{nl} electrons and normalized to unity. The total density is expressed then as

$$N \cdot \rho = \sum_{nl} N_{nl} \cdot \rho_{nl}$$

(12)

or equivalently

$$\rho = \sum_{nl} \omega_{nl} \rho_{nl},$$

(13)

the weights being chosen as $\omega_{nl} = N_{nl}/N$ (relative electronic charge of the subshell). This divergence represents the "excess of entropy" (Shannon or Renyi) of the global atom with respect to the mean entropy of its constituents (the subshells). A similar analysis as done in previous works for JSD [45] are now extended to JRD.

The JSD and JRD divergences of the aforementioned "collection of subshells" have been computed for all neutral atoms with nuclear charge $Z = 1–103$, and their values are displayed in Figure 4. Some comments are in order:

i. A general decreasing trend of the JRD divergence as "q" increases is observed in both conjugated spaces, almost systematic in momentum space with the corresponding curves ordered appart from few exceptions corresponding to light atoms. So, the Renyi entropy of the global system decreases, when compared to its lower bound given by the mean entropy of the subshells, when increasing "q."
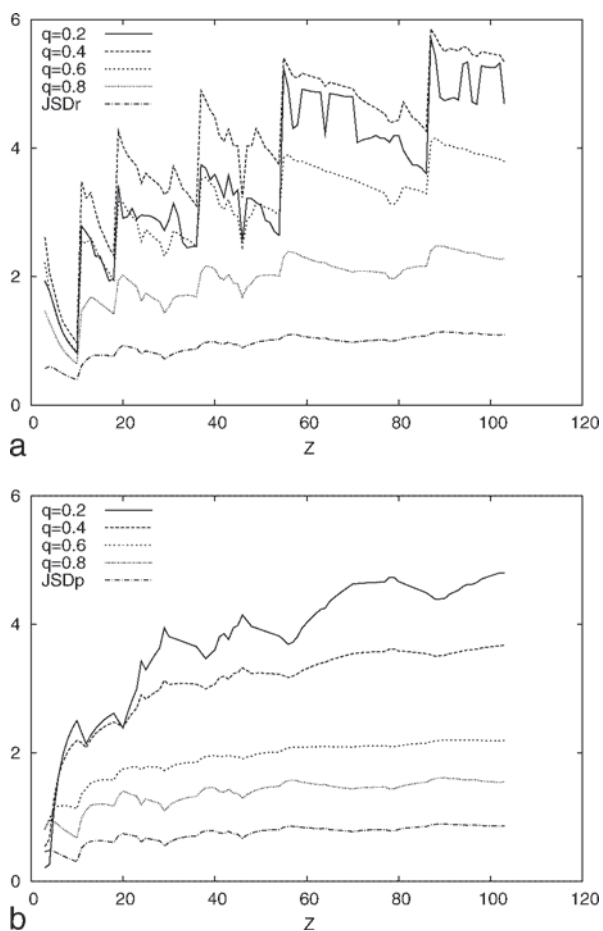
FIGURE 4. Jensen-Rényi Divergence $JRD^{(q)}$ for $q = 0.2, 0.4, 0.6, 0.8$ and Jensen-Shannon Divergence $JSD = JRD^{(1)}$ among the occupied subshells for all neutral atoms with nuclear charge $Z = 1$–103, in (a) position and (b) momentum spaces. Atomic units are used.

ii. According to the interpretation of low and large "q" values', the divergence among subshells is higher when enhancing the contribution of the densities around the origin, independently of the space considered. This fact suggests that the relevant feature for quantifying the global divergence is the region of higher density values instead of the shell-filling pattern.

iii. Location of extrema within each curve does not follow a so systematic pattern as in the applications previously performed. This is in accordance with the previous comment on the reasons for finding a higher or lower divergence.

6. Concluding Remarks

The most important statistical measures of divergence (QD, FD, JSD) are used and compared to study one-electron atomic densities. Concerning QD and FD, the analysis in the momentum space shows how the momentum density carries fundamental information about periodicity and structure of the atomic systems and reveals the pattern of periodic table of elements. This is in contrast with the position space analysis, where instead of those patterns a unimodal behavior is displayed.

This trend is partially avoided by the Jensen-Shannon divergence (JSD), showing at least a little structure in both conjugate spaces. To improve the above results, we have used a well known generalization of the Shannon entropy, namely the Rényi entropy, to build up a one-parameter divergence measure, The Jensen-Rényi divergence (JRD) appears capable of assigning different weights to specific regions of the electronic distribution domains to control the most important contributions of the electronic cloud to the atomic densities in position and momentum spaces. This generalized divergence provide information on the atomic shell structure and shell-filling patterns in both conjugated spaces and has been used to compare quantitatively the dissimilarities of atomic shells, systems and models.

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