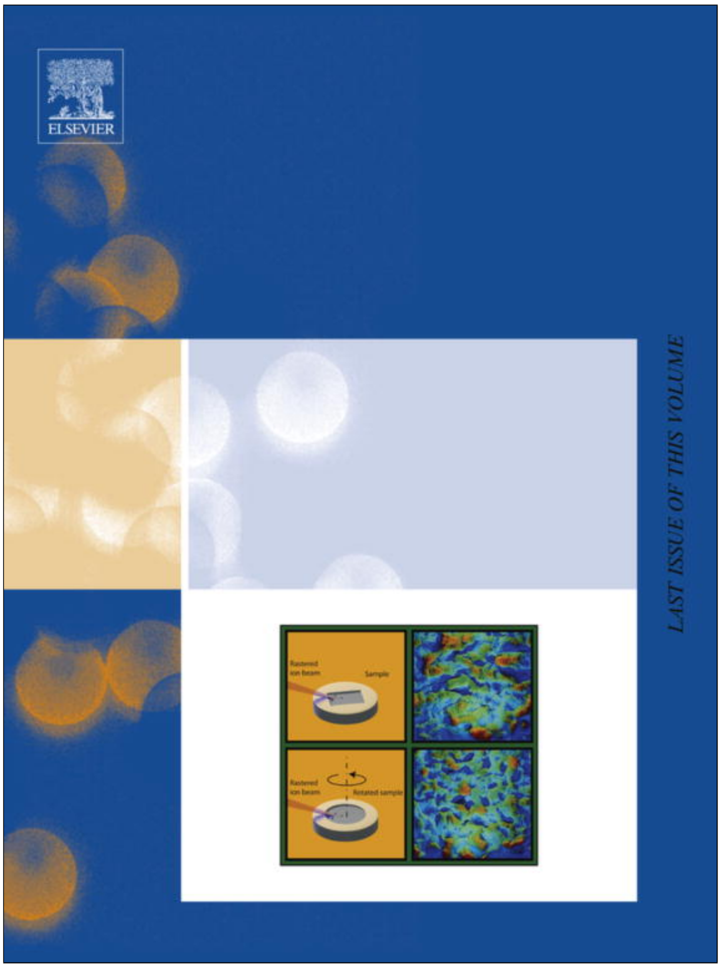
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Generalized Quantum Similarity Index: Applications in atoms

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ABSTRACT

A Generalized Quantum Similarity Index is defined, quantifying the similarity among density functions. The generalization includes, as new features (i) comparison among an arbitrary number of functions, (ii) its ability to modify the relative contribution of different regions within the domain, and (iii) the possibility of assigning different weights to each function according to its relevance on the comparative procedure. The similarity among atomic one-particle densities in both conjugated spaces, and neutral–cation similarity in ionization processes are analyzed. The results are interpreted attending to shell-filling patterns, and also in terms of experimentally accessible quantities of relevance in ionization processes.

1. Introduction

The concepts of similarity and dissimilarity (or divergence) are closely related, both appearing to be of fundamental importance in a wide variety of scientific fields including, for instance, image or texture registration [1–3], sequence analysis [4], pattern recognition [5], biodiversity [6], classification [7], homology [8], neural networks [9], machine learning [10], artificial intelligence [11], computational linguistics [12], fuzzy set theory [13] or quantum information theory [14].

Quantum similarity attempts to give a quantitative measure of the degree of similarity between two quantum objects, having its grounds on the comparison of their one-particle densities with later applications to other quantities, such as e.g. Fukui functions [15]. To quantify the degree of similarity between the compared systems, a general Quantum Similarity Measure [16] can be defined by means of the computation of an integrated measure between the density functions attached to the quantum systems.

The recent explosion in knowledge-based chemical research has created a surge of interest in chemical similarity. Molecular modeling, molecular similarity [16,17] and quantitative structure activity relationship (QSAR) are simple examples of such an interest [18]. More recently the molecular quantum similarity framework has been used to provide a new set of quantum quantitative structure–properties relationship procedures (QQSPR) [19].

For the case of molecules or atoms this kind of similarity measures can be defined as the scalar product between the first order density functions weighted with a bielectronic definite positive operator [20]. The simplest choice, the Dirac delta operator, leads to the well-known Quantum Similarity Index (QSI) [21]

$$\mathrm{QSI}(\rho_1,\rho_2) \equiv \frac{\int \rho_1(\vec{r})\rho_2(\vec{r})d\vec{r}}{\sqrt{\int \rho_1^2(\vec{r})d\vec{r} \int \rho_2^2(\vec{r})d\vec{r}}}. \qquad (1)$$

Chemical similarity is often described as an inverse of a measure of distance or divergence in the appropriate space. Recently different divergence measures [22] have been used in the framework of quantum information theory. In particular, the Jensen–Shannon divergence [23] was applied as a measure of entanglement [24,14], and also together with other similarity measures in the study of multielectronic systems [25–28].

Quantifying the dissimilarity among two or more many-electron systems by means of their one-particle densities is also a hot topic within the physical applications of the information theory. Some fundamental measures of information have been used with this aim: Shannon [29], Rényi [30] and Tsallis [31] entropies and Fisher information [32,33], as well as their associated divergences [34–37]. Among those divergence measures susceptible of being employed to study atomic or molecular systems, especially relevant are the 'Kullback–Leibler or relative entropy' [38], the Fisher divergence [34], and the Jensen–Tsallis divergence [35] which constitutes a powerful generalization of the Jensen–Shannon divergence [34].

The aim of this work is to present a new general similarity measure. Its definition, as compared to the pioneering QSI, constitutes a generalization modifying the number of functions to be compared and the weights of each of them in different regions of their domain of definition. The usefulness of the new comparative quantifier is illustrated with applications for one-particle densities in

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position and momentum spaces. These densities are used as a benchmark to study a known but extremely hierarchical and complex [39] set of quantum objects: atoms, but the universality and versatility of this technique allows its application to other more complex or less known molecular or nuclear systems.

The Quantum Similarity Index (QSI) constitutes a particular case of a one-parameter Generalized Quantum Similarity Index $\mathrm{QSI}^{(q)}$. The analysis here provided for the $\mathrm{QSI}^{(q)}$ of atomic systems generalizes and improves some previous results on the QSI one. Such an improvement mainly arises from the capability of $\mathrm{QSI}^{(q)}$ to modify, by means of its characteristic parameter, the relative contribution of relevant specific regions of the atomic densities in both conjugated spaces. The $\mathrm{QSI}^{(q)}$ allows a deep introspection within the structure of the atomic one-particle densities, capturing relevant differences in any of the conjugated spaces. This is not the case of other measures of divergence or similarity employed with multielectronic systems, as for instance, the own QSI.

The Letter is structured as follows: Section 2 is devoted to define the Generalized Quantum Similarity Index, and the analysis of its main theoretical features including its advantages with respect to the original similarity index QSI. In Section 3, applications to the similarity-based study of atomic one-particle densities are carried out, dealing with neutral (Section 3.1) and ionized species (Section 3.2). Concluding remarks and open problems are given in Section 4.

2. Generalized Quantum Similarity Index

Let us consider a couple of functions, $f(\vec{r})$ and $g(\vec{r})$, with identical domain Δ in the D-dimensional space $\mathbb{R}^D$. In what follows, all integrations are understood to be performed over the common domain Δ. The well-known Hölder's inequality [40] establishes the relationship

$$\int fg d\vec{r} \leqslant \left(\int f^p d\vec{r}\right)^{1/p} \left(\int g^q d\vec{r}\right)^{1/q} \tag{2}$$

for any $p, q > 1$ verifying $\frac{1}{p} + \frac{1}{q} = 1$. Equality in the above expression is reached if and only if $f(\vec{r}) = g(\vec{r})$.

The definition of the quantum similarity index $QSI(f,g)$, given by Eq. (1), together with Hölder's inequality for the particular case $p = q = 2$, allows to assert that $QSI(f,g) \in [0,1]$, with $QSI(f,g) = 1$ if and only if $f(\vec{r}) = g(\vec{r})$.

The Hölder's inequality in Eq. (2) constitutes a particular case of the so-called 'generalized Hölder's inequality' [40], given by

$$\left[\int (fg)^m d\vec{r}\right]^{1/m} \leqslant \left(\int f^p d\vec{r}\right)^{1/p} \left(\int g^q d\vec{r}\right)^{1/q}, \tag{3}$$

with $p, q > m > 0$ verifying $\frac{1}{p} + \frac{1}{q} = \frac{1}{m}$. The particular case $m = 1$ provides Hölder's inequality, namely Eq. (2).

An iterative use of the above expression allows to generalize the inequality for an arbitrary number $n \geqslant 2$ of functions $\{f_1, f_2, \ldots, f_n\}$:

$$\left[\int (f_1 \ldots f_n)^m d\vec{r}\right]^{1/m} \leqslant \left(\int f_1^{p_1} d\vec{r}\right)^{1/p_1} \ldots \left(\int f_n^{p_n} d\vec{r}\right)^{1/p_n}, \tag{4}$$

with $\frac{1}{p_1} + \cdots + \frac{1}{p_n} = \frac{1}{m}$.

Raising to 'm' and defining $\lambda_i \equiv m/p_i$ the inequality reads as

$$\int (f_1 \ldots f_n)^m d\vec{r} \leqslant \left(\int f_1^{p_1} d\vec{r}\right)^{\lambda_1} \ldots \left(\int f_n^{p_n} d\vec{r}\right)^{\lambda_n}, \tag{5}$$

with $\sum_{i=1}^n \lambda_i = 1$.

We now define new functions $g_i(\vec{r})$ through the identity $f_i = g_i^{q/p_i}$ for an arbitrary $q > 0$, so that

$$\int (g_1^{\lambda_1} \ldots g_n^{\lambda_n})^q d\vec{r} \leqslant \left(\int g_1^q d\vec{r}\right)^{\lambda_1} \ldots \left(\int g_n^q d\vec{r}\right)^{\lambda_n}. \tag{6}$$

The left- and right-hand-side terms in the last inequality give rise to a quotient not greater than 1, as also occurred when defining QSI. This is the essential ingredient that allows to define the 'qth order Generalized Quantum Similarity Index':

$$\mathrm{QSI}^{(q)}(\{g_i, \lambda_i\}_{i=1}^n) \equiv \frac{\int (g_1^{\lambda_1} \ldots g_n^{\lambda_n})^q d\vec{r}}{\left(\int g_1^q d\vec{r}\right)^{\lambda_1} \ldots \left(\int g_n^q d\vec{r}\right)^{\lambda_n}} \quad \text{with} \quad \sum_{i=1}^n \lambda_i = 1, \tag{7}$$

and $0 < \lambda_i < 1$ for all $i = 1, \ldots, n$. It is worthy to remark that (i) $\mathrm{QSI}^{(q)} \in [0,1]$ for any $q > 0$, and (ii) the quantity $\mathrm{QSI}^{(q)}$ does not depend on the normalization of the chosen functions $g_i(\vec{r})$, as also happens with the usual QSI. The last point implies that the similarity index constitutes a measure of how similar the distributions are according to their shapes rather than to their absolute values or sizes, contrary to the aforementioned divergences.

The definition of the above similarity index, as compared to the pioneering QSI measure, constitutes a generalization in three different ways, namely:

- The number 'n' of functions $g_i(\vec{r})$ under comparison, not necessarily $n = 2$ as for the QSI which constitutes a measure of overlap between two densities, while its generalization quantifies the total overlap among an arbitrary number of them.
- The order q, which allows to enhance or diminish the contribution of the 'tails' and, in general, the surroundings of the local extrema of each function, by considering higher or lower values of q.
- The 'weights' λ_i, a set of parameters which control the relative importance of each function in performing the comparison among themselves by means of the generalized similarity index.

For the sake of simplicity in notation, the weights λ_i will be omitted as arguments of $\mathrm{QSI}^{(q)}$ unless necessary. Relevant particular cases of the generalized similarity index $\mathrm{QSI}^{(q)}$ are detailed below:

(a) *Similarity between two densities.*
The usual QSI in Eq. (1) is obtained from the general expression in Eq. (7) by choosing a number of densities $n = 2$, the second order $q = 2$, and equal weights $\lambda_1 = \lambda_2 = 1/2$. That is,

$$\mathrm{QSI}^{(2)}(g_1, g_2) = \mathrm{QSI}(g_1, g_2) \tag{8}$$

For arbitrary order and weights, the generalized similarity index reads as

$$\mathrm{QSI}^{(q)}(g_1, g_2) = \frac{\int (g_1^{\lambda} g_2^{1-\lambda})^q d\vec{r}}{\left(\int g_1^q d\vec{r}\right)^{\lambda} \left(\int g_2^q d\vec{r}\right)^{1-\lambda}} \tag{9}$$

with $0 < \lambda < 1$.

(b) *Uniformly weighted similarity.*
Choosing uniform weights $\lambda_i = 1/n$ in Eq. (7) gives rise to

$$\mathrm{QSI}^{(q)}(g_1, \ldots, g_n) = \frac{\int (g_1 \ldots g_n)^{q/n} d\vec{r}}{\sqrt[n]{\int g_1^q d\vec{r} \ldots \int g_n^q d\vec{r}}}, \tag{10}$$

in particular

$$\mathrm{QSI}^{(q)}(g_1, g_2) = \frac{\int (g_1 g_2)^{q/2} d\vec{r}}{\sqrt{\int g_1^q d\vec{r} \int g_2^q d\vec{r}}}. \tag{11}$$

(c) *Relationship among generalized QSIs of different order.*
From the definition in Eq. (7), we check that

$$\mathrm{QSI}^{(q)}(g_1, \ldots, g_n) = \mathrm{QSI}^{(t)}(g_1^{q/t}, \ldots, g_n^{q/t}) \tag{12}$$

for arbitrary orders q and t. The particular case $t = 2$ provides, in the right-hand-side, the usual QSI, and consequently

$$\mathrm{QSI}^{(q)}(g_1,\ldots,g_n)=\mathrm{QSI}(g_1^{q/2},\ldots,g_n^{q/2}). \tag{13}$$

This means that, in what concerns the dependence on the order q, considering the generalization $\mathrm{QSI}^{(q)}$ is equivalent to evaluate QSI not among the considered functions, but instead among them raised, each one, to the power $q/2$. It is in that way that we better understand the role played by the order q: considering different values of the order implies to carry out a comparative study based on a higher or lower similarity in the short- and long-range domains, in a similar fashion as done in divergence-based previous studies [35,36,41].

3. Numerical analysis with atomic one-particle densities

In this section we analyze the similarity among atomic one-particle densities, in both position and momentum spaces. In doing so, accurate near-Hartree–Fock wavefunctions [42,43] are employed as a benchmark, for both neutral and ionized species with a number of electrons up to 103 and 54, respectively. More accurate numerical frameworks will be considered elsewhere, as pointed out in the last Section. Atomic units (a.u.) will be used throughout.

For the sake of brevity, we will restrict the analysis of the results according to the dependence of the generalized similarity on its order q, dealing with uniformly weighted couples of functions. This description corresponds to the functional

$$\mathrm{QSI}^{(q)}(g_1,g_2)=\frac{\int (g_1g_2)^{q/2}d\vec{r}}{\sqrt{\int g_1^q d\vec{r}\int g_2^q d\vec{r}}} \tag{14}$$

in order to go far beyond the well-known results provided by QSI as obtained for the particular case $q=2$ [25,26]. Further studies including similarity among three or more functions and non-uniform weights will be published elsewhere.

3.1. Pairs of neutral atoms

Let us consider two neutral atoms, A and B, with respective nuclear charges Z_A and Z_B and electron charge densities $\rho_A(\vec{r})$ and $\rho_B(\vec{r})$. In previous studies, the problem of checking the extent to which the *similarity* between the one-particle densities of systems A and B implies a *similarity* among their physico-chemical properties, and conversely, was afforded by quantifying the similarity between ρ_A and ρ_B according to the QSI measure given by Eq. (1). The pioneering and very successful results obtained in comparing molecular densities [21] appeared to be very poor when dealing with atomic densities [25]. The main conclusion was that similarity between atoms A and B is roughly determined by the difference $|Z_A-Z_B|$ among their nuclear charges. So, the quantity QSI (Z,Z') as function of Z for fixed Z' displays an unimodal shape, firstly increasing until reaching the extremal value 1 for $Z=Z'$ and decreasing hereinafter. This kind of information regarding similarity is very far from the physical one, where one should expect the presence of properties such as periodicity or shell-filling patterns, among others. A relevant improvement was provided in Ref. [44], where periodicity patterns are displayed by means of QSI with respect to closed-shell systems.

A complete displayment of periodicity patterns was achieved for arbitrary systems A and B throughout the Periodic Table by considering the atomic momentum densities $\gamma_A(\vec{p})$ and $\gamma_B(\vec{p})$, instead of the position space ones. Within this context, the results obtained were extremely rich, in the sense discussed above: similarity between A and B was strongly determined by the atomic shell-filling patterns, and periodicity was clearly displayed.

In this section, however, we show that the position-space generalized quantum similarity index $\mathrm{QSI}^{(q)}$ makes possible to get similar information as that provided by $\mathrm{QSI}=\mathrm{QSI}^{(2)}$ in momentum space, by dealing with appropriate values of q other than $q=2$. For illustration, the $\mathrm{QSI}(Z,Z')$ and $\mathrm{QSI}^{(q)}(Z,Z')$ measures in position space (with $q=0.4$) among each of $Z'=18,20$ (Ar and Ca) and all other atoms throughout the Periodic Table ($Z=1-103$) are displayed in Figure 1.

As previously mentioned, both curves for QSI behave in an unimodal way, almost overlapping one with each other because of the closeness of the nuclear charges $Z'=18,20$. Such a similarity between curves disappears progressively as far as q becomes smaller. Changes are dramatic for a value as low as $q=0.4$, not only attending to the different paths followed by each curve, but also because of their higher level of structure, displaying numerous local extrema which location is determined by shell-filling patterns. Let us have in mind that $Z=18$ corresponds to a noble gas (Argon) while $Z=20$ to an alkaline-earth (Calcium), groups of the Periodic Table characterized by extremely different physical properties. In this sense, it is worthy to remark that the main maxima of $\mathrm{QSI}_r^{(04)}(Ar,Z)$ occur for noble gases while those of $\mathrm{QSI}_r^{(04)}(Ca,Z)$ for alkaline-earths. In both cases, additional minor extrema are usually associated to comparisons with systems suffering from an anomalous shell-filling. Similar effects are observed for systems other than $Z'=18,20$.

In order to test the usefulness of the generalized index $\mathrm{QSI}^{(q)}$ as compared to the usual one QSI, let us observe Figure 2 where $\mathrm{QSI}^{(q)}(Kr,Z)$ is displayed ($Z=1$–103) for different values of q, in position (Figure 2a) and momentum (Figure 2b) spaces. The fundamental reason for QSI_r (i.e. $q=2$) to display a so unstructured curve arises from the exponential long-range behavior of the charge density $\rho(\vec{r})$. This fact makes the three integrals included in the definition of QSI to be mainly determined by the values of the densities in the surrounding of the origin, the contribution from outermost regions being almost negligible. Such a quick decrease can be attenuated by raising the density to a low power, as controlled by the parameter q in the definition of $\mathrm{QSI}^{(q)}$. Consequently, decreasing q makes the relative contribution of the outermost regions ('tails') in the evaluation of similarity to increase. Let us keep in mind that the main physical and chemical properties of atomic systems, including the shell-filling pattern, are determined by the value of the density in the valence region, most usually the outermost one. This effect is clearly observed in Figure 2a, with a very apparent increase in the number of local extrema within the curves with $q\leqslant 1$ as compared to the $q=2$ one. Such an increase is progressive, especially in going from $q=2$ to $q=1$, but also for $q<1$.

Let us notice the main features of systems for which $\mathrm{QSI}_r^{(q)}(Kr,Z)$ with $q\leqslant 1$ displays local maxima: (i) other noble gases (e.g. $Z=54,86$ systematically, the rest occasionally), (ii) closed-subshell atoms ($Z=12,30,48,70,80$), (iii) half-filled-subshells ($Z=7,15,43,75$), and (iv) systems with anomalous shell-filling ($Z=24,41,42,44,46,58,64,78,90,93,96,97$).

Concerning momentum space (Figure 2b), highly structured curves were obtained in the recent past by using QSI. A detailed analysis of the number and location of local maxima allows to assert that: (i) a similar structure is obtained for values of the order within the interval $1.5\leqslant q\leqslant 3$, which includes QSI as $q=2$; these maxima correspond to the same systems as in the position case, (ii) in going below such a range, a number of local extrema disappears progressively, as e.g. $Z=2,7,29,78$ (systems characterized in the previous position-space analysis) for the value $q=1$, and (iii) an order as low as $q=0.5$ provides an unimodal curve with the unique maximum at $Z=36$.

Figure 3 shows $\mathrm{QSI}_r^{(0.4)}$, a position space index displaying extremely structured curves for all noble gases. The location of local extrema in each curve is determined according to similar patterns to those just discussed. All curves appear (roughly) ordered according to the nuclear charges of the systems involved. This behavior was

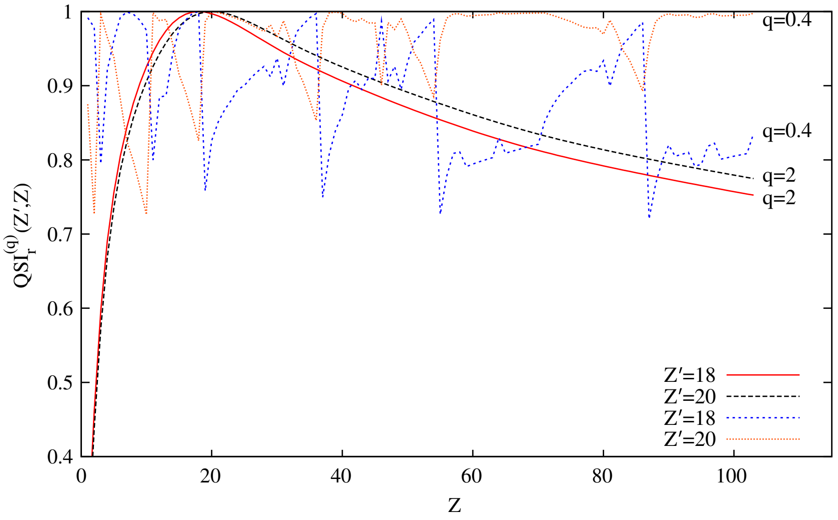

Figure 1. Generalized Quantum Similarity Index $QSI_r^{(q)}(Z',Z)$ (for $q = 0.4$ and 2.0) in position space among each of Argon ($Z' = 18$) and Calcium ($Z' = 20$) with respect to all neutral atoms with nuclear charge $Z = 1$–103. Atomic units are used.

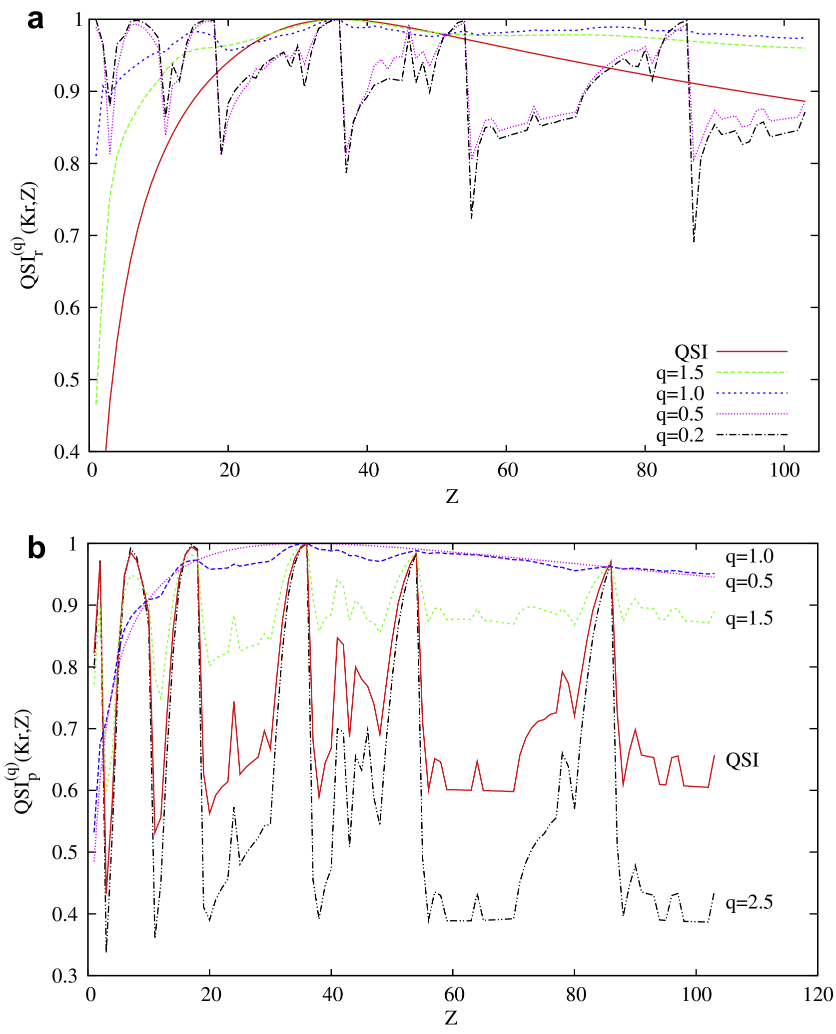

Figure 2. Generalized Quantum Similarity Index $QSI^{(q)}(Kr, Z)$ between Krypton ($Z' = 36$) and all neutral atoms with nuclear charge $Z = 1$–103 for different orders q, in (a) position and (b) momentum spaces. Atomic units are used.

emphasized in previous works dealing with the momentum space similarity QSI, instead of the position one as in the present figure. Specially remarkable are (i) the closeness to unity of the main maxima of $QSI_r^{(0.4)}$ when comparing a couple of noble gases, and (ii) the

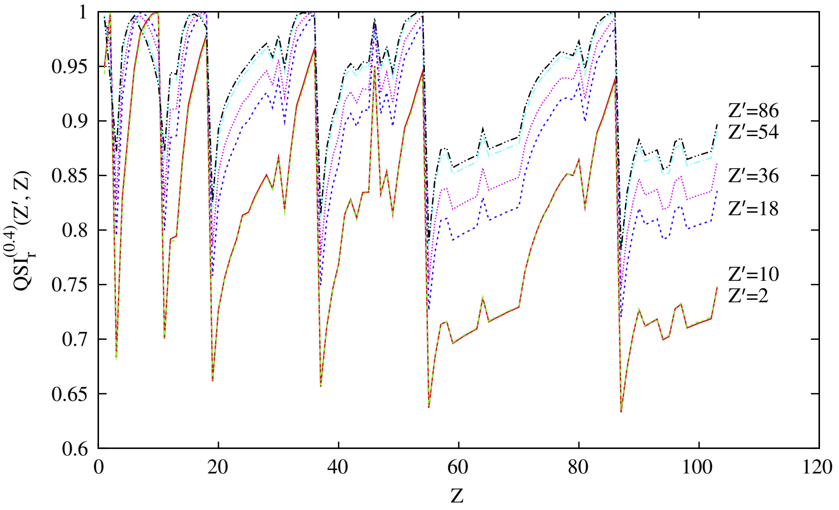

Figure 3. Generalized Quantum Similarity Index $\mathrm{QSI}_r^{(q)}(Z',Z)$ (for $q = 0.4$) in position space of each noble gas with respect to all neutral atoms with nuclear charge $Z = 1$–103. Atomic units are used.

very apparent minima when a noble gas is compared with an alkaline system.

3.2. Ionization processes

The results obtained by means of the similarity indexes and their physical interpretation motivated us to ask ourselves about the following questions: to which extent the ionization of a neutral atom modifies its one-particle densities, in both conjugated spaces? Is the similarity measure an appropriate tool to quantify the modifications in the densities? Is there a connection between neutral–ion similarity and relevant physical properties in describing ionization processes?

All those questions are afforded here, employing the generalized measure $\mathrm{QSI}^{(q)}(NC)$ for different values of the order q. In doing so, a number of neutral atoms and their singly-charged cations are considered in order to compare the respective one-particle densities of the neutral system (N) and its cation (C). The results are interpreted according to shell-filling patterns (in particular the subshell from which the electron is ejected) as well as in terms of the first atomic ionization potential. Such a study is performed in both conjugated spaces. Previous works [26] employing the quantum similarity index QSI (NC) provided more limited results.

We first analyze Figure 4, corresponding to the position space index $\mathrm{QSI}_r^{(q)}(NC)$ for different values of q, together with the atomic ionization potential (AIP) of the neutral system. The most remarkable feature is the increase of structure, according to the number and enhancement of local extrema, as the parameter q becomes smaller. In some cases, most local minima of $\mathrm{QSI}_r^{(q)}(NC)$ correspond to systems displaying local minima in the AIP curve. Such a resemblance does not occur for the position space QSI.

Restricting ourselves to $0.4 \leqslant q \leqslant 1$, the following comments are in order:

1. The systematic appearance of minima in q-similarity for systems $Z = 3, 8, 11, 19, (23, 24), 31, 37, 42, 45, 47, 49$ is associated to ionization processes provoking the disappearance of a subshell (a ‘s’ one, except for $Z = 31$), or a ‘p’ subshell which becomes half-filled ($Z = 8$).
2. The closeness of the above list with that of AIP minima: $Z = 3, 5, 8, 11, 13, 16, 19, 23, 28, 31, 34, 37, 47, 49$. Values included in this list but not in the previous one are $Z = 5, 13, 16, 28, 34$, corresponding again to the disappearance of subshells ($Z = 5, 13, 28$) or half-filled ‘p’ ones in the cation ($Z = 16, 34$).

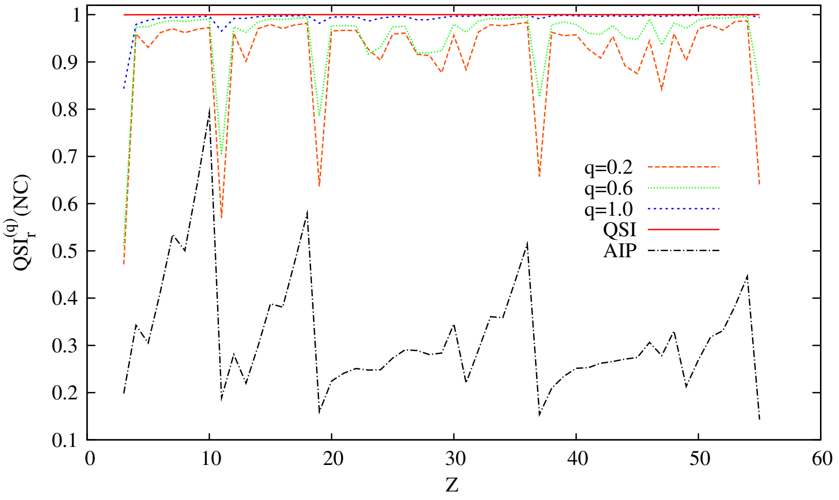

Figure 4. Generalized Quantum Similarity Index $\mathrm{QSI}_r^{(q)}(NC)$ in position space for neutral–cation pairs (nuclear charge $Z = 3$–55) with different orders q. Atomic units are used.

3. Nevertheless, most of the just mentioned ‘additional systems’ are detected by low enough values of q (0.8 for $Z = 13, 16, 34$ and 0.4 for $Z = 5$). Such a detection occurs also for $Z = 52$ (half-filled ‘p’ subshell in cation) with $q = 0.8$, in spite of not displaying a minimum of AIP.
4. Most usually, the main peaks in the curves are associated to ionization ejecting a s-subshell electron, as compared to the ‘p’ or ‘d’ ones. This means that the s-like ionization produces stronger changes in the electron charge density, appreciably more relevant than those produced by removing electrons from other types of subshells.

Conclusions from the analysis in momentum space are roughly the same as those arising from the position space study. A few additional comments are in order: (i) a strong resemblance among lists of minima in generalized similarity for different q’s is observed, even for an interval as wide as $0.5 \leqslant qs \leqslant 3.0$, and (ii) those lists share many systems enclosed in the lists of minima of both position-space generalized similarity for low q and the atomic ionization potential. The interpretation of the physical properties characterizing the systems displaying a minimum in momentum space can be done in a similar fashion as in the position one.

4. Conclusions and open problems

The capability of a generalization of the pioneering quantum similarity index to gain physical insight within the structural properties of many-electron systems has been shown. In doing so, we have taken advantage of its characteristic parameter in order to enhance or diminish the short- and long-range contributions in a similarity-based analysis. The generalized index allows to deal with a set of an arbitrary number of density functions, assigning different weights to each one in accordance with their role within the comparative purpose considered.

For atomic systems, a study based on one-particle densities in position space provides clearly an interpretation by means of shell structure. The generalization introduced in this work allows to deal with densities of any of the conjugated spaces by choosing appropriately the value of its characteristic parameter.

A detailed numerical analysis has been presented, from which it is clearly established the relationship between valence subshell properties of the systems under comparison and the generalized similarity values, as well as the detection of the presence of systems suffering from anomalous shell-filling.

The usefulness of the tool here defined has been shown in the study of ionized systems, by considering the analysis of atomic pairs neutral–cation. It appears a strong resemblance among the extrema of similarity and those of the atomic ionization potential, mostly determined by occupancy numbers of the outermost subshell in neutral and cationic systems. In fact, it is observed that the angular momentum quantum number ‘l’ of the electron ejected plays a relevant role in terms of similarity.

Further applications of the generalized index, arising from its rigorous mathematical properties here described, are planned to be carried out in a near future, including studies (i) on the ability in comparing different quantum models (e.g. configuration interactions, relativistic effects), (ii) comparing more that two functions, e.g. sequence anion–neutral–cation, groups/periods of the Periodic Table, isoelectronic series, ‘parts’ of a given composite system, (iii) assigning appropriate weights to each system according to relevant physical/chemical properties, such as mass, number of electrons, volume. Additional studies of quantum systems (e.g. molecules) and processes (reaction, excitation) will be provided elsewhere.

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