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Quantum similarity indices for atomic ionization processes

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Abstract. Quantum similarity is investigated for neutral atoms and singly charged ions by means of their one-particle densities in both position and momentum spaces. As recently observed for neutral atoms, the analysis involving singly charged ions in momentum space provides relevant information concerning structure and periodicity properties. Momentum-space similarity is also revealed to be strongly related to the kind of ionization process the system suffers, to the structural characteristics of the momentum density as well as to the ionization potential.

PACS. 31.10.+z Theory of electronic structure, electronic transitions, and chemical binding – 31.15.-p Calculations and mathematical techniques in atomic and molecular physics

1 Introduction

Quantum Similarity theory [1,2] was originally developed in order to establish quantitative comparisons between molecular systems by means of their fundamental structural magnitudes: electron density functions.

The quantification of similarity between two molecular structures, based on quantum chemistry and on the comparison of their charge densities was firstly proposed by Carbó et al. [1]. Afterwards, the same research group studied the theoretical framework of quantum similarity. Since then, the design of novel procedures, the implementation of new algorithms and measures as well as their practical applications have also been extensively developed [3]. Simultaneously, other research groups adopted quantum similarity, extending the implementation of the theory to various fields and envisaging new applications, giving rise to a great deal of relevant results [4,5]. Since then, molecular similarity has been one of the cornerstones of recent chemical research in molecules [6], complementary to important studies in which information entropies are the main quantities in order to measure the distance between two electron distributions or processes [7–10].

The generality of the method allows it to be used for other quantum objects, such as nuclei or atoms. Nevertheless, very few Quantum Similarity Measures have been employed for studying such systems, dealing only with the position variable $\mathbf{r}$ [11–15]. The basic result concerning atomic systems is that a nearest neighbour similarity is retrieved, masking periodicity, then confirming the earlier work of Carbó et al. [11,12]. Nevertheless, introduction of shape functions [13,14] and the information discriminations concept, with reference to the noble gas atom of the previous row, were found to reveal some features concerning periodicity and shell structure. Very recently, a novel quantum similarity measure has been constructed based on information theory, from which the role of relativistic effects on the electron density is studied [15].

Momentum space concepts, where the momenta of electrons are the basic variables when dealing with the associated density of the system, are common in solid state physics, being much less frequently found in chemistry. In fact, most of the work on quantum similarity has been carried out in the usual position representation $\mathbf{r}$, where problems associated to bonding topology are relevant. However, emphasizing the variation of the long-range position-space electron density strongly requires the use of the conjugate space variable, namely the momentum $\mathbf{p}$ [16].

Both the one particle densities of an N-electron atomic system in position and momentum spaces, $\rho(\mathbf{r})$ and $\Pi(\mathbf{p})$ respectively, are defined in terms of the N-particle wavefunction Ψ and its $3N$ dimensional Fourier transform $\tilde{\Psi}$ as [17]

$$\rho(\mathbf{r}) = \int |\Psi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2 d\mathbf{r}_2 \ldots d\mathbf{r}_N \qquad (1)$$

$$\Pi(\mathbf{p}) = \int |\tilde{\Psi}(\mathbf{p}, \mathbf{p}_2, \ldots, \mathbf{p}_N)|^2 d\mathbf{p}_2 \ldots d\mathbf{p}_N, \qquad (2)$$

normalized to the number of electrons N. The reason for the underlying interest in momentum space concepts to

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questions of chemical similarity is due to the aforementioned Fourier relation between the wavefunction in position and momentum spaces. The spherically averaged momentum space density $\Pi(p)$, compared to its position counterpart $\rho(r)$, tends to be large at high p values. These differences concerning the region from which the corresponding densities are providing the most relevant information can be clearly understood having in mind the respective asymptotic behaviors, an exponentially decreasing one for the position density [18] (conditioned by the value of the atomic ionization potential I) while the momentum density decreases as slowly as p^{-8} for large p [19]. It is worthy to mention that, due to the Fourier transform which connects both conjugate spaces, long-range asymptotic behavior in one space is closely related to short-range properties in the complementary one.

Concerning the momentum density $\Pi(\mathbf{p})$, which plays a relevant role in the description of many physical properties of atomic systems [20,21], it is also the essential quantity on defining many different experimentally accessible quantities, which are in fact the main sources of experimental data on the momentum density. Such is the case of the Compton profile $J(\mathbf{q})$ [22] or the reciprocal form factor $B(\mathbf{r})$ [23], given respectively by

$$J(\mathbf{q}) = \frac{1}{2}\int_{p\geq q} \frac{\Pi(\mathbf{p})}{p} d\mathbf{p} \tag{3}$$

$$B(\mathbf{r}) = \int \Pi(\mathbf{p}) \mathrm{e}^{-i\mathbf{p}\cdot\mathbf{r}} d\mathbf{p}. \tag{4}$$

Other structural characteristics of the spherically averaged momentum density $\Pi(p)$ have been also extensively studied, mainly concerning monotonicity properties and displayment of local extrema, for both neutral [24,25] and singly ionized [26] systems. Some of those properties will be also involved in the present work within the framework of quantum similarity.

The Quantum Similarity Measure (QSM) between isolated atoms is defined in a completely similar form as for molecules or other quantum systems [12]:

$$M_{AB} \equiv \int \rho_A(\mathbf{r}_1)\Omega(\mathbf{r}_1,\mathbf{r}_2)\rho_B(\mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_2 \tag{5}$$

where $\rho_A(\mathbf{r}_1)$ and $\rho_B(\mathbf{r}_2)$ are the (spinless) electron density functions of both systems A and B, and $\Omega(\mathbf{r}_1,\mathbf{r}_2)$ is a separation operator. The QSM is complementary to other well-known distances, such as the (symmetrized) Kullback-Leibler entropy [27,28], the Kolmogorov distance [29] or the Jensen-Shannon divergence [30,31].

Most often, Ω is chosen as the Dirac delta function $\delta(\mathbf{r}_1 - \mathbf{r}_2)$ reducing equation (5) to an overlap type integral, and the other most oftenly used operator being $\mathbf{r}_{12}^{-1}$, transforming equation (5) in a Coulomb-type integral. One can generalize these computations by using other positive powers $\mathbf{r}_{12}^{n}$ of the interdistance. Normalization is taken by defining a Quantum Similarity Index (QSI)

$$QSI \equiv \frac{M_{AB}}{\sqrt{M_{AA}M_{BB}}} \tag{6}$$

running between 0 and 1. Evaluation of a similarity index for atoms is straightforward using electron densities of sufficient quality for the isolated atoms. In a completely similar way one can compute similarity indices in momentum space by using the corresponding momentum densities $\Pi_A(\mathbf{p}_1)$ and $\Pi_B(\mathbf{p}_2)$.

M_{AA} (or M_{BB}) is called *quantum self-similarity* or *quantum autosimilarity index* (QAI) and is obtained, independently of the operator, when comparing a system with itself. It is related with the electronic charge density occupation in the space, that is, provides information on the charge concentration of the considered quantum object. When the selected operator is the overlap one, self-similarities can be considered as the square of the norm of the density function in the chosen metric. This is a very important measure of localization, called also *linear entropy* [32], in contrast with the (nonlinear) *Shannon entropy* (both the linear and the Shannon entropies being closely related to Renyi entropies $R_q(\rho)$ of order 2 and 1, respectively, as $M_{AA} = e^{-R_2}$ and $S_\rho = R_1$), or in other contexts, informational energy and inverse participation number [33].

In a recent work [34] in which, to the best of our knowledge, QSI have been, for the first time, calculated and analyzed for neutral atoms throughout the Periodic Table in momentum space, it has been shown the relevant role played by the linear momentum $\mathbf{p}$ as the basic variable of the one-particle momentum density $\Pi(\mathbf{p})$, in order not only to quantify the degree of similarity between two atomic systems but also to provide information on structural characteristics and shell-filling features. In the same work it is also shown, as previously known, that QSI associated to the position-space density $\rho(\mathbf{r})$ only provide information on how close the atoms are located at the periodic table. In order to get additional knowledge on the groups to which the systems belong, shell structure and periodicity, it is necessary to take into account the momentum variable.

Here we investigate the unexplored momentum space similarity for singly charge ions, firstly (Sect. 2) by showing the very different behaviors of the QSI between two ionized systems when dealing with the position or the momentum variable. Having in mind the importance of the atomic ionization potential I when describing structural characteristics (e.g. asymptotic behavior) of the density, a study of the relationship among the Quantum Similarity Index QSI_p of two *consecutive* neutral systems (i.e. neutral atoms differing by one electron), the Quantum Autosimilarity Index QAI_p and the ionization potential I is carried out in Section 3, where again periodicity properties are displayed due to the involvement of the momentum variable. Other local properties of the momentum density and its corresponding radial function (e.g. location of local extrema) are also shown (Sect. 4) to be strongly related to the values of the above quantities, specially when considering the process involved in the ionization of each neutral atom to obtain their corresponding singly ionized systems, namely cations and anions. The appropriate concluding remarks based on the aforementioned results are finally given (Sect. 5).

2 Position and momentum space similarities for ions

The main aim of this section is to analyze the Quantum Similarity Index (QSI) of two singly-charged ions (cations or anions) in both position and momentum spaces, by considering the associated one-particle densities $\rho(r)$ and $\Pi(p)$, respectively. It is known [34] that the QSI coming from the position-space densities (QSI_r) of two atoms with nuclear charges Z_1 and Z_2 only provides information on the difference $|Z_1 - Z_2|$, attaching the maximum value 1 for identical systems (i.e. $Z_1 = Z_2$) and decreasing monotonically when increasing such a difference or, equivalently, when dealing with more *distant* systems in the periodic table. That is, the quantity QSI_r masks any information concerning periodicity properties, groups to which the systems belong and so on. However, the corresponding quantity QSI_p involving momentum densities take values according to shell-filling and the occupation number of valence orbitals, displaying maxima when the pair of considered atoms belong to the same group.

An identical analysis for singly charged ions is here also carried out by computing the similarities QSI_r and QSI_p. In doing so, the atomic wavefunctions of Koga et al. [35] have been employed, for systems with a number of electrons up to 54. Additional results will be also obtained for neutral atoms up to $Z = 103$ by employing the wavefunctions also given in the same reference.

These wavefunctions are analytically expressed as linear combinations in a Slater type basis, giving rise to a variational approximation to the Hartree-Fock wavefunction for the experimental ground state of the considered system. They are constrained by the electron-nuclear cusp condition (of each orbital) as well as the long-range behavior. The total energy provided by the variational approximation is not more than a few microHartrees above the numerical Hartree-Fock limit values.

Both similarities are represented, respectively, in Figures 1 and 2 for anions as functions of the nuclear charge Z (similar results are also obtained for cations). It is immediate to extract the same conclusions for singly charged ions and neutral atoms, i.e. the necessity of dealing with momentum densities in order to obtain information on periodicity properties when comparing a pair of anions, cations or neutral atoms.

This fact is also observed when comparing a couple of systems with identical nuclear charge Z but differing on the number of electrons, namely the pairs anion-neutral (AN), neutral-cation (NC) and anion-cation (AC). Again the study is performed in both conjugated spaces.

Concerning position space, all computed values of the QSI_r for the aforementioned pairs of atomic systems almost reach the maximum value 1. Such values are always above from 0.99996, 0.99974 and 0.99960 for the pairs AN, NC and AC, respectively. Then, it is shown that charge densities do not essentially vary when adding or removing an electron.

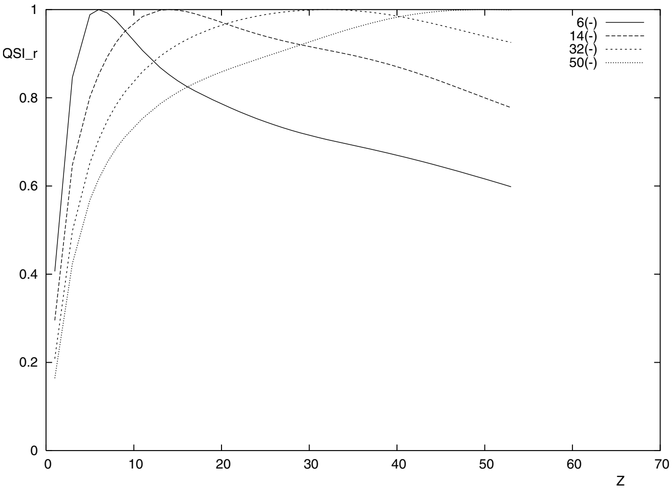

Fig. 1. Quantum similarity index $QSI_r(Z, Z')$ of singly charged anions ($Z' = 6, 14, 32, 50$) in position space.

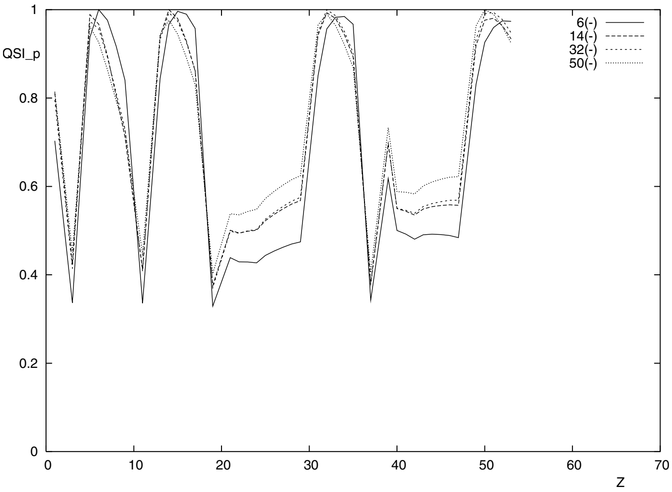

Fig. 2. Quantum similarity index $QSI_p(Z, Z')$ of singly charged anions ($Z' = 6, 14, 32, 50$) in momentum space.

However, results are completely different in momentum space. The ranges of values for QSI_p are strongly dependent on the orbital angular momentum l of the subshells affected by the change on the number of electrons (i.e. if the ionization process concerns 's', 'p' and/or 'd' electrons). Such a dependence is clearly displayed in Table 1, in which the aforementioned ranges of values of QSI_p are given for the three pairs (AN, NC, AC) with identical nuclear charge Z (up to systems with 54 electrons), attending to the quantum number l of the electronic subshells involved in the ionization process. There are a few cases in which, apart from removing an electron, an additional translation of another electron from an 's' to a 'd' subshell also occurs (as denoted in the table).

It is worthy to mention that, when removing an 's' electron in the process NC, there appear two *subranges* (0.367–0.823 and 0.894–0.964) corresponding,

Table 1. Ranges of the Quantum Similarity Index QSI_p between neutral atoms (N), anions (A) and cations (C) and subshells involved in the ionization processes.

Subshell	AN	NC	AC
s	0.716–0.808	0.367–0.964	0.151–0.344
p	0.977–0.991	0.985–0.999	0.924–0.979
d	0.792–0.848	0.977–0.996	
$s(s \rightarrow d)$	0.339	0.487–0.488	
s, d			0.591–0.660
p, d			0.886

respectively, to the cases where the 's' subshell becomes or not empty. The analysis of the data in the table allows to say that higher effects on the momentum densities (i.e. lower values of the associated QSI_p) correspond to ionization processes where 's' electrons are involved and, specially, when an 's' subshell disappears.

Attending to the aforementioned results, in what follows we will only deal with the momentum density $\Pi(p)$ with the aim of describe structural characteristics and physical properties of both neutral and ionized systems.

3 Ionization potential, similarity and autosimilarity

The main physical property involved in describing processes which give rise to an atomic system differing from the starting one by one electron is the atomic ionization potential I. In previous works [9,10] it has been shown to be correlated to different information measures. Such a correlation is also confirmed in this section, where we will deal with neutral atoms of nuclear charge in the range $Z = 1$–103, with the aim of study the correlation between the atomic ionization potential $I(Z)$, the Quantum Similarity Index $QSI_p(Z-1, Z)$ of two consecutive atoms, and the Quantum Autosimilarity Index $QAI_p(Z)$, defined as the Quantum Similarity Measure QSM of the two identical densities $\Pi(p)$, or equivalently

$$QAI_p(Z) = \int \Pi^2(p) d\mathbf{p},$$

which provides information on the momentum concentration of the considered quantum object, being a well-known measure of localization.

Firstly, a comparison of the quantities $QSI_p(Z-1, Z)$ and $I(Z)$ is carried out in Figure 3 for the whole range $Z = 1$–103. It is observed the similar structure of both curves concerning main local extrema, showing a correlation between both quantities which is not displayed when drawing the corresponding *consecutive* position index. In fact, systems displaying common main maxima for both functions posses a completely filled 's', 'p' and 'f' valence subshell ($Z = 2, 4, 10, 12, 18, 36, 54, 70, 86, 102$), while minima are associated to systems with an isolated electron at an 's' or 'p' subshell ($Z = 3, 5, 11, 13, 19, 31, 37, 47, 55, 78, 87$). There are only two exceptions ($Z = 59, 77$) involved in the anomalous shell-filling.

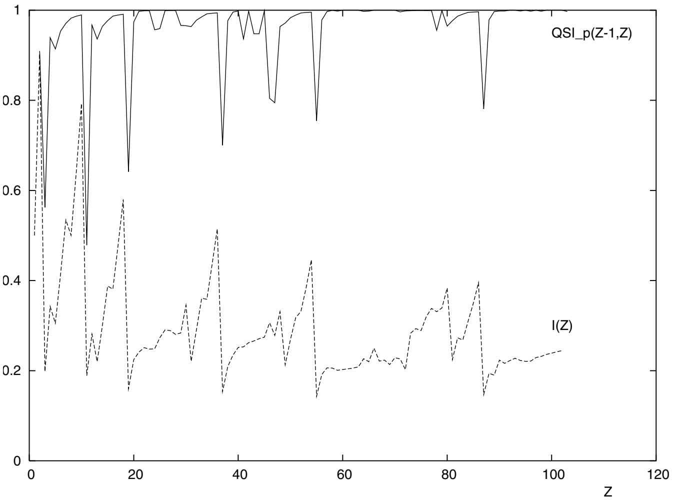

Fig. 3. Quantum similarity index $QSI_p(Z-1, Z)$ of consecutive neutral atoms in momentum space and atomic ionization potential.

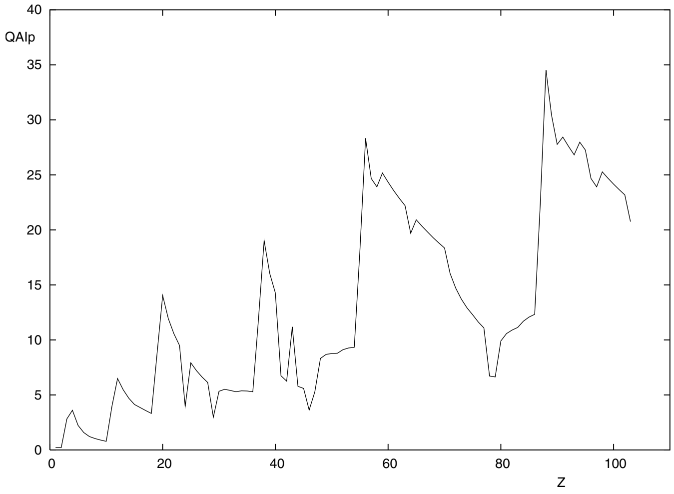

Fig. 4. Quantum autosimilarity index $QAI_p(Z)$ of neutral atoms in momentum space.

Concerning $QAI_p(Z)$, such a quantity is shown for neutral atoms as a function of the nuclear charge $Z = 1$–103 in Figure 4. Again, periodicity patterns are displayed attending to the different monotonically decreasing curves associated to the different groups of the periodic table.

4 Local characteristics of the radial momentum density

Another relevant density function in momentum space is the so-called *radial momentum density* $P(p)$, defined as

$$P(p) \equiv 4\pi p^2 \Pi(p)$$

and which quantifies the probability of finding an electron with a given linear momentum. Such a function displays, for both neutral and ionized systems, a number of local

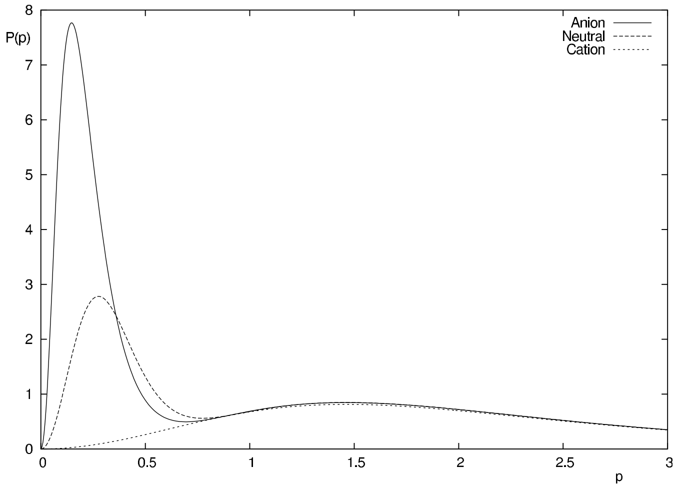

Fig. 5. Radial momentum densities $P(p)$ of Li, Li$^+$ and Li$^-$ (nuclear charge $Z = 3$).

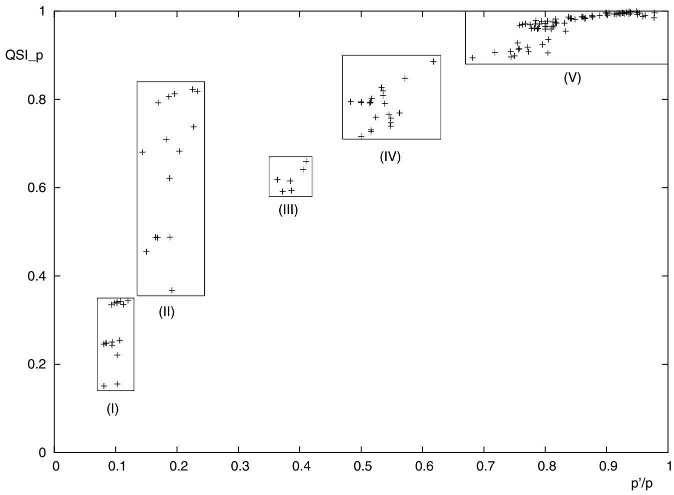

Fig. 6. Quantum similarity index QSI_p among neutral atoms and singly charged ions and ratio p'/p of local maxima of radial momentum densities.

extrema associated to the structure of the momentum density $\Pi(p)$. Nevertheless, it is observed that the most relevant maximum (corresponding to the absolute maximum of the density) is always the first one. The process of ionization (both by adding or removing electrons) produces a translation of the local extrema and, in particular, of the most relevant one. It is also observed a monotonic behavior of the location of extrema when moving across a group or a period, independently of dealing with anions, cations or neutral atoms. In this sense, it is worthy to mention that, when increasing the nuclear charge across a group, both the distance to the origin and the height of the main maximum decrease. An opposite behavior is displayed when moving across a period in what location of the maximum concerns.

As mentioned above, the process of ionization (in which we deal with a pair of systems with identical nuclear charge) translates the main maximum of $P(p)$. This is clearly observed in Figure 5, where the radial momentum densities $P(p)$ of all the neutral atom (Lithium) and its singly charged ions (Li$^+$ and Li$^-$), with nuclear charge $Z = 3$ are drawn, showing the aforementioned changes on the structure of $P(p)$. In order to quantify the magnitude of such a translation when comparing two systems, let us consider the ratio p'/p between the locations of the absolute maxima associated to the systems with a higher and a lower number of electrons, p' and p respectively. It is always observed that $p' < p$ and, consequently, that ratio runs between 0 and 1.

This measure of the *structural alteration* of the density should be expected to be related to other quantities, studied in the previous sections, and which appeared to be strongly related to the ionization process.

This is the purpose of Figure 6, where the similarity QSI_p for all neutral and ionized systems considered in the present work (AN, NC, AC) is drawn as a function of the ratio p'/p. In the figure appear clearly distinguishable five regions, each corresponding to different ionization processes, as described below:

(I) An anion with an 's' subshell completely filled is compared to the system (neutral atom or cation) with the same subshell absolutely empty. Here the range for p'/p is 0.081–0.120.
(II) Corresponds to the process in which a neutral atom loses an 's' subshell. The ratio p'/p belongs to the interval 0.165–0.233.
(III) This region is associated to the comparison between an anion and the associated cation which differ in an 's' and a 'd' electron, being the ratio p'/p within the values 0.364–0.410.
(IV) When a neutral atom gains an 's' or a 'd' electron, the limit values for p'/p are 0.483–0.571.
(V) Resting comparisons (i.e. those only involving 'p' or 'd' electrons, as well as those where a filled 's' subshell only loses one electron) always provide values of p'/p above from 0.617.

Consequently, it is clearly evident the correlation between the similarity QSI_p and the structural variation p'/p, subject to the ionization process connecting both compared systems.

Following a similar reasoning, it appears interesting to study the value of the ionization potential I (the main physical property on describing ionization processes) in terms of the above employed ratio p'/p. This comparison is given in Figure 7 for the process on going from a neutral atom to the corresponding singly charged cation, where again three different regions are distinguished associated to different ranges of p'/p. A similar interpretation to the one given above can be given again:

(I) Region around $p'/p = 0.2$ corresponds to processes in which an 's' subshell becomes completely empty.
(II) Points appearing close to $p'/p = 0.8$ are associated to processes in which a completely filled 's' subshell loses only one electron or those in which a 'd' subshell becomes completely empty.

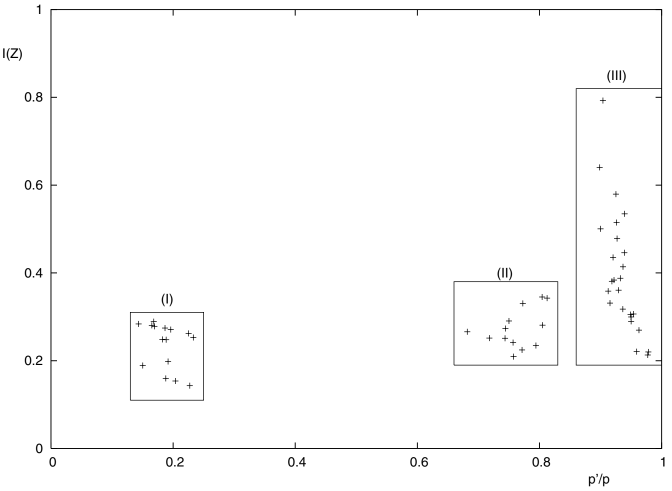

Fig. 7. Atomic ionization potential $I(Z)$ and ratio p'/p of local maxima of radial momentum densities for pairs neutral-cation.

(III) Removing 'p' electrons (as well as the exceptional case $Z = 46$, the only one in which a completely filled 'd' subshell loses one electron) provided the cloud of values of p'/p around 0.9.

5 Concluding remarks

The comparison of ionized and/or neutral atomic systems by means of Quantum Similarity Indices provides relevant information on periodicity properties and shell structure when dealing with one-particle densities in momentum space. However, the corresponding values in position space are only concerned by their closeness at the periodic table.

Such an index in momentum space, as well as the quantum autosimilarity index, are strongly conditioned by structural (e.g. location of local extrema of the densities) and experimentally accessible (e.g. ionization potential) quantities. Additionally, other characteristics (e.g. quantum numbers) of the electrons involved in the ionization processes essentially determine the range of values to which the associated quantum similarity index belongs.

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