

Jensen–Tsallis divergence and atomic dissimilarity for position and momentum space electron densities

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Quantifying the dissimilarity among two or more many-electron systems by means of their one-particle densities is a hot topic within the physical applications of the information theory. This is a relevant achievement of the so-called “divergence measures,” for which several definitions have been considered, each one with its own advantages and difficulties. Nevertheless, all of them are considered in order to disclose the differences among the involved systems, neutral atoms in the present work, according to their densities in the position and momentum spaces. The pioneering Jensen–Shannon divergence (JSD) constitutes a particular case of the one-parameter Jensen–Tsallis divergence (JTD). The analysis here provided for the JTD of atomic systems generalizes and improves some previous results on the JSD one. Such an improvement mainly arises from the capability of JTD to modify, by means of its characteristic parameter, the relative contribution of relevant specific regions of the atomic densities in both conjugated spaces. © 2010 American Institute of Physics. [doi:10.1063/1.3298911]

I. INTRODUCTION

Information-theoretic divergence measures^{1–3} have been successfully applied in many areas including statistical pattern recognition, machine learning, neuronal networks, signal, image or speech processing, graph theory, computer vision, quantum information theory, or analysis of multielectronic systems. The latter will be the focus of the present paper.

The Kullback-Leibler divergence (Ref. 4) KLD, (also referred as “directed divergence” or “information gain”), one of the Shannon entropy (S) based measures,⁵ is perhaps the most important nonsymmetric divergence measure of information theory and has been extensively studied and applied in a great variety of fields.

Another entropy-based measure is the so-called Jensen–Shannon divergence (JSD).⁶ This divergence measures in fact the statistical dependence between an arbitrary number of probability distributions and there are some important reasons why researchers choose JSD as a measure of divergence, among them: (i) it is a symmetrized and smoothed version of the KLD and hence it shares its mathematical properties and intuitive interpretability, (ii) it has significance in the framework of statistical physics, information theory, and mathematical statistics,⁷ (iii) JSD is related to other information-theoretical functionals (being a special case of the Jensen difference⁸ and the Csiszár divergence⁹) and it is the square of a metric,¹⁰ and (iv) JSD can be generalized in order to measure the distance between more than two distri-

butions, as well as by assigning different weights to each one.⁶ This last point is especially interesting since permits to take into account characteristics such as, for instance, different sizes of the objects we are comparing (e.g., different lengths of the subsequences in DNA analyses¹¹ or different subshells or regions in atomic and molecular dissimilarity analyses¹²).

Due to the aforementioned properties, the JSD can be applied within a wide variety of fields, including signal/image processing, computer vision problems,¹³ and to the analysis of DNA sequences.^{11,14–18} The JSD has also been used for measuring the distance between random graphs,¹⁹ for testing the goodness-of-fit of point estimations,²⁰ in the segmentation of textured images,²¹ and in the statistical characterization of the mobility edge in disordered materials.²²

In addition, the JSD divergence has been employed as measure of distinguishability between mixed quantum states. Distances between quantum states play a central role in quantum information theory. An appropriate measure of distance is the quantum JSD (QJSD) between quantum states. Majtey *et al.*^{10,23,24} studied this distance as a geometrical measure of entanglement and applied it to different families of states.

Exploring quantitatively the level of similarity/dissimilarity between two different systems in terms of meaningful divergence measures appears actually as a very interesting field. Different divergence measures have been recently proposed, including local- and global-character ones (Fisher and Jensen–Shannon divergences, respectively), with the aim of analyzing the similarity and discrepancy among quantum-mechanical or multielectronic models and systems, such as atoms, ions, or relevant parts of them, throughout the

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Periodic Table.²⁵ These systems have been considered as an appropriate benchmark due to their strong hierarchical organization. The studied divergences, not only in the usual position but also in the momentum space, have been shown to provide relevant information on the atomic shell structure and other physical and chemical measurable magnitudes.²⁶

Other relative measures have been recently used with comparative purposes among physical distributions, apart from the aforementioned KLD. For illustration let us mention the “relative Rényi entropy” RRE_q ,²⁷ based in the concept of the “ q -order Rényi entropy” R_q .²⁸ The interpretation of RRE_q in terms of R_q is given in a similar fashion as the KLD in terms of the Shannon entropy S . However, there appear relevant constraints on the allowed values of the characteristic parameter “ q ” (the order), arising from the requirement of non-negativity of the RRE.

The first aim of the present work is to present a one-parameter generalized divergence, the Jensen–Tsallis divergence (JTD), to explore its advantages as compared to other discrepancy measures and to contrast the results obtained on simple but extremely organized systems like atoms. This divergence can be constructed by simply replacing the Shannon by the q order Tsallis entropy $T^{(q)}$ (Ref. 29) in the JSD divergence definition, as will be described in the next section. The Shannon entropy, a particular case of the Tsallis one as $q \rightarrow 1$, shares the well-known additivity property from which the joint entropy of a pair of independent random variables is just the sum of the individual entropies. In the present work we omit this property as a constraint and, instead, the pseudoadditive Tsallis entropy is considered in order to construct, similarly to JSD, the JTD.

Standard thermodynamics is extensive because of the short-range nature of the interaction between subsystems of a composite system. In other words, when a system is composed of two statistically independent subsystems, then the entropy of the composite system is just the sum of the entropies of the individual systems, and hence the correlations between the subsystems are not accounted. The Tsallis entropy, however, does take into account these correlations due to its pseudoadditivity property. Furthermore, many objects in nature interact through long-range interactions such as gravitational or unscreened Coulomb forces. Therefore the property of additivity is very often violated and consequently the use of a nonextensive entropy is more suitable for real-world applications.

After introducing the aforementioned divergences and the density functionals from which they are defined, a numerical analysis is carried out for all neutral atoms throughout the Periodic Table within a Hartree-Fock framework.^{30,31} In doing so, a comparison among the corresponding one-particle densities in both position and momentum spaces is performed. The results are interpreted according to the following features: (i) the dependence on the parameter q of the JTD divergence for a given pair of atoms, (ii) the behavior of JTD, for fixed q , according to the shell structure of the compared systems, and (iii) the role played by the space (position or momentum) considered for the aforementioned analyses. Finally, some concluding remarks are given.

II. POSITION AND MOMENTUM SPACE DIVERGENCE MEASURES FOR ATOMS

The relevant role played by the one-particle density $\rho(\vec{r})$ in the description of many-electron systems, as shown within a density functional theory framework,³² invites us to think about the extent to which the “similarity” between densities corresponding to two different systems could be interpreted as an indicator of analogy also between their physical and chemical properties, as well as the best way to quantify it. The same applies to the one-particle density $\gamma(\vec{p})$ in the conjugated space, namely, the momentum one because it is also a well-known source of information on the aforementioned properties.³³ In fact, the simultaneous analysis of both the position and the momentum space densities has been proven to provide, in different contexts, a much more complete description.³⁴ In the present work, normalization to unity is chosen for the atomic densities.

The most widely employed double-density functional in order to quantify how similar or different two distributions are, both supposed to be defined over the same domain, is defined in a similar fashion to the usual distance in the L^2 space, namely, the quadratic distance, being in fact the norm of the difference between the considered distributions. Additional measures, proposed as indicators of “information distance” between distributions, includes the quantum similarity index³⁵ and the Fisher divergence,²⁵ which have been also applied to the analysis of many-particle systems, such as, e.g., atoms and molecules.³⁶

Probably the most relevant divergence measure introduced within the information theory is the KLD or relative entropy,⁴ as mentioned in the introduction. It is defined as

$$\text{KLD}(\rho_1, \rho_2) \equiv \int \rho_1(\vec{r}) \ln \frac{\rho_1(\vec{r})}{\rho_2(\vec{r})} d\vec{r}, \quad (1)$$

having its roots in the Shannon entropy⁵

$$S(\rho) \equiv - \int \rho(\vec{r}) \ln \rho(\vec{r}) d\vec{r}, \quad (2)$$

a well-known information-theoretic measure of uncertainty which, in particular, quantifies how the distribution spreads over its whole domain, possessing consequently a “global character” as opposite to other information measures, more sensitive to relevant local changes, such as e.g., the Fisher information.^{37,38}

The absence of symmetry of the KLD divergence induces its symmetrized version $\text{KLS}(\rho_1, \rho_2) \equiv \text{KLD}(\rho_1, \rho_2) + \text{KLD}(\rho_2, \rho_1)$, in order to get an appropriate interpretation of this quantity as an information distance. Both divergences KLD and KLS have been widely studied, finding applications in a great variety of fields such as, for instance, minimum cross entropy estimation³⁹ or indexing and image retrieval.⁴⁰

An information measure of divergence strongly related to both the Shannon and the relative entropies is the so-called “JSD.” It is characterized for quantifying the “Shannon entropy excess” of a mixture of distributions with respect to the mixture of their entropies. More specifically, it is given by^{19,41}

$$\text{JSD}(\rho_1, \rho_2) \equiv S\left(\frac{\rho_1 + \rho_2}{2}\right) - \frac{1}{2}[S(\rho_1) + S(\rho_2)], \quad (3)$$

the mathematical definition clarifying the above interpretation as entropy excess of the mean density with respect to the mean entropy of the involved distributions.

Apart from preserving the global character of the Shannon entropy, the JSD possesses the main properties required for a measure to be interpreted as an informational distance, namely, non-negativity [as a consequence of the convexity of the $S(\rho)$ functional], symmetry, and the minimum value 0 being reached only when $\rho_1 = \rho_2$.

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 the present 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 $(0, \infty)$.

The Shannon entropy S constitutes a particular case of the so-called *Tsallis entropy of order q* (Ref. 29)

$$T^{(q)}(\rho) \equiv \frac{1 - \omega^{(q)}(\rho)}{q - 1}, \quad (4)$$

with $\omega^{(q)}(\rho) \equiv \int \rho^q(\vec{r}) d\vec{r}$ being the frequency moment of the order of q of the distribution $\rho(\vec{r})$. Both the Tsallis 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 $q \rightarrow 1$, taking into account the normalization constraint $\omega^{(1)}(\rho) = 1$, provides the Shannon entropy: $T^{(1)}(\rho) = S(\rho)$.

Replacing the Shannon entropy by the Tsallis one in the JSD definition gives rise to a new double-density functional, the JTD of order q ^{42,43}

$$\text{JTD}^{(q)}(\rho_1, \rho_2) \equiv T^{(q)}\left(\frac{\rho_1 + \rho_2}{2}\right) - \frac{1}{2}[T^{(q)}(\rho_1) + T^{(q)}(\rho_2)], \quad (5)$$

in such a way that $\text{JTD}^{(1)} = \text{JSD}$, the new divergence generalizing the previously introduced JSD one and preserving its main properties as mentioned in the introduction. Nonextensive divergences closely related to the JTD divergence above defined have been applied in the fields of symbolic sequence segmentation, ⁴⁴ geological, or medical image registration ⁴² and machine learning techniques. ⁴³

The non-negativity of $\text{JTD}^{(q)}$ is guaranteed for $q > 0$, property 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. A detailed analysis of the behavior of

JTD according to its dependence on the parameter q , the characteristics of the involved systems and the conjugated space where the densities are defined is carried out in the next section.

III. NUMERICAL ANALYSIS OF THE JTD FOR ATOMS IN CONJUGATED SPACES

As discussed in the previous section, the main feature of the $\text{JTD}^{(q)}$ as compared to other ones and, particularly, to the JSD, is its capability of enhancing/diminishing the relative contribution of different regions within the domain of the distributions under comparison. To the best of our knowledge, the only relative measure with a characteristic parameter applied in the past for multielectronic systems is the RRE, ²⁷ by comparing their densities only with hydrogenic ones. The RRE of order q , built up in terms of the Rényi entropy, ²⁸ embodies the KLD divergence as a particular case. The non-negativity of the relative Rényi measure requires the fulfillment of the very strong constraint $0 < q < 1$ for its characteristic parameter. Such is not the case of $\text{JTD}^{(q)}$, where the only constraints on the value of q arise from the convergence conditions on the involved frequency moments according to the long- and short-range behaviors of the distribution, conditions also required with the Rényi relative entropy even for order q below 1.

Let us consider, as a first step, a fixed neutral system for computing its $\text{JTD}^{(q)}$ divergence with respect to all neutral atoms through the Periodic Table with nuclear charges $Z = 1-103$. This will be done for several values of the parameter q as well as in both conjugated spaces. For illustration, we choose as initial system the Mg atom ($Z=12$) and the values $q=0.6, 1.0, 1.4, 2.0$, as well as $q=0.2$ in position space. Let us remark that the last value is not allowed in momentum space, where the convergence conditions require $q > 3/8 = 0.375$ due to the long-range behavior of the momentum density ⁴⁵ while the exponential decrease for the position density ⁴⁶ guarantees the convergence for any $q > 0$.

The corresponding JTD curves are displayed in Fig. 1, for position and momentum spaces [Figs. 1(a) and 1(b), respectively]. Some comments are in order. In both spaces, it is clearly observed that the structure of the curves strongly depends on the value of q . In fact, if we consider the smoothest curve in a figure (understood according to the number and enhancement of local extrema), varying the q value in a monotone way provokes that the curves increase their level of structure progressively, as measured by the number of extrema and their enhancement. After crossing a critical value, the successive curves lose the unimodal shape, keeping always their minimal value 0 at $Z=12$. In fact, the value $q=1$ which provides the JSD through the equality $\text{JTD}^{(1)} = \text{JSD}$ appears very close to the critical one in both spaces, in spite of the number of extrema displayed by the JSD at this level. However, the aforementioned variation follows opposite trends in each space. While the highly structured curves are displayed for low q values in position space, the situation for momentum space is absolutely different in that higher values of q are required in order to depart from unimodality.

A straightforward interpretation of the observed opposite

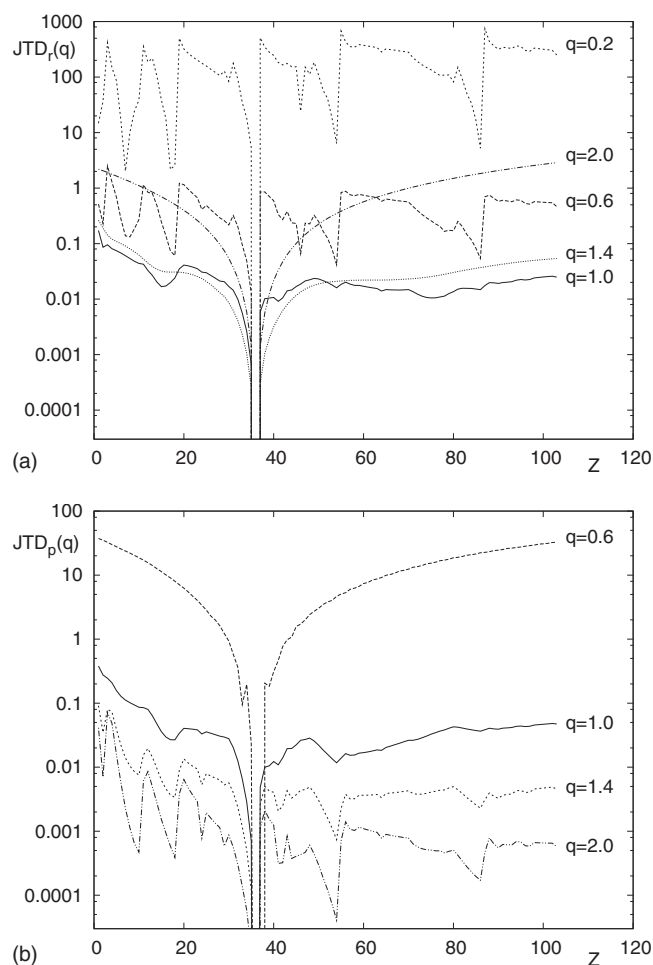


FIG. 1. Jensen–Tsallis Divergence $JTD^{(q)}$ between Mg (nuclear charge $Z=12$) and all neutral atoms with the $Z=1–103$, (a) in position space for $q=0.2, 0.6, 1.0, 1.4, 2.0$ and (b) in momentum space for $q=0.6, 1.0, 1.4, 2.0$. Atomic units are used.

behaviors noted above might be obtained by considering the physical meaning of the position and momentum densities, as well as their respective structural properties. A well-known fact on the position density for ground-state neutral atoms is that the maximum value is systematically reached at the origin. The same is also true in momentum space for a numerous group of systems while for the others the maximum appears shifted from the origin but not significantly.

The differences between the short- and large-range values are enhanced if the power of the density within the integrand of $\omega^{(q)}(\rho)$ increases, making the value of JTD to be strongly determined by the region of the density around the origin. Conversely, decreasing the value of the parameter q smoothes the integrand, raising up the relative contribution of the outermost region.

In the position space, the neighborhood of the origin corresponds to the region of the electron cloud surrounding the nucleus, which is governed by the nuclear charge Z and the Coulombic potential. However, the origin in momentum space is associated to electrons with low values of the linear momentum or, equivalently, with low-speed electrons which are just those located in the outermost or valence region of the atomic system. This fact justifies the observed opposite trends in terms of q : as its value increases, the enhancement

in position space corresponds to the nuclear region, whereas in momentum space corresponds to the valence one.

Taking into account that the shell-filling patterns are determined by the valence region, they are clearly observed in momentum space for large q . Then, the JTD divergence value is mainly based on the different characteristics of the systems under comparison according to their dissimilarity in what shell-filling concerns, while the comparison in position space is mainly determined by the values of their nuclear charges. Opposite trends are observed when decreasing the value of the parameter q . The same reasoning given above for explaining the JTD behavior as q increases also applies for the decreasing case. So that, the role played by the value of the parameter q allows one to obtain a higher level of information on the shell-filling effects by enhancing the relative contribution of different specific regions according to the space we are dealing with. A continuous variation in q makes the contribution to the comparative measure of the outermost spatial region or, equivalently, of the valence subshell containing the low-speed electrons, to vary also in a continuous way.

Concerning the structure of the curves displayed, their local extrema can be classified according to two different characteristics: (i) the lower JTD divergence when comparing an atomic system to another one belonging to the same group and (ii) JTD values when one of the involved atoms belongs to the so-called “anomalous shell-filling” set of atomic systems. As will be shown below, this is a common feature in the study of dissimilarity based on the JTD divergence. The main achievement of the JTD in the present application is its ability to quantify the dissimilarity between atomic systems according to one of the more physically relevant characteristics, namely, the shell-filling process which determines most of the atomic chemical properties, being strongly related also to some experimentally accessible quantities, such as, e.g., the first ionization potential.³²

The present comparative performance is far from the concept of “distances among atoms” according to the values of their nuclear charges, essentially interpreted as size or weight for neutral atoms. This fact is clearly displayed in the Fig. 2, where the JTD of both $Z=36, 38$ atoms along the Periodic Table is displayed. Those systems have been chosen in order to consider a couple of atoms with very similar nuclear charges but strongly different valence subshells as well as many other physical characteristics. In doing so, the JTD are given for $q=0.5$ (below 1), $q=1.5$ (above 1), and the limiting case $q=1$ for which JTD turns out to be JSD. For the JSD divergence, there appear slight differences between the curves for $Z=36$ and $Z=38$, independently of the space considered. It is also worth noting that the range of values for JSD in both spaces is roughly the same.

Dealing with position space in Fig. 2(a), the JSD measure allows to observe a slight structure in the curves, which disappears completely for the higher order divergence JTD ($q=1.5$) but which extremely enhances for the low-order $q=0.5$, with both curves displaying in fact absolutely different structures and extrema at similar positions but with opposite maximum/minimum character. So it is concluded the convenience of dealing with low-order JTD in order to get relevant

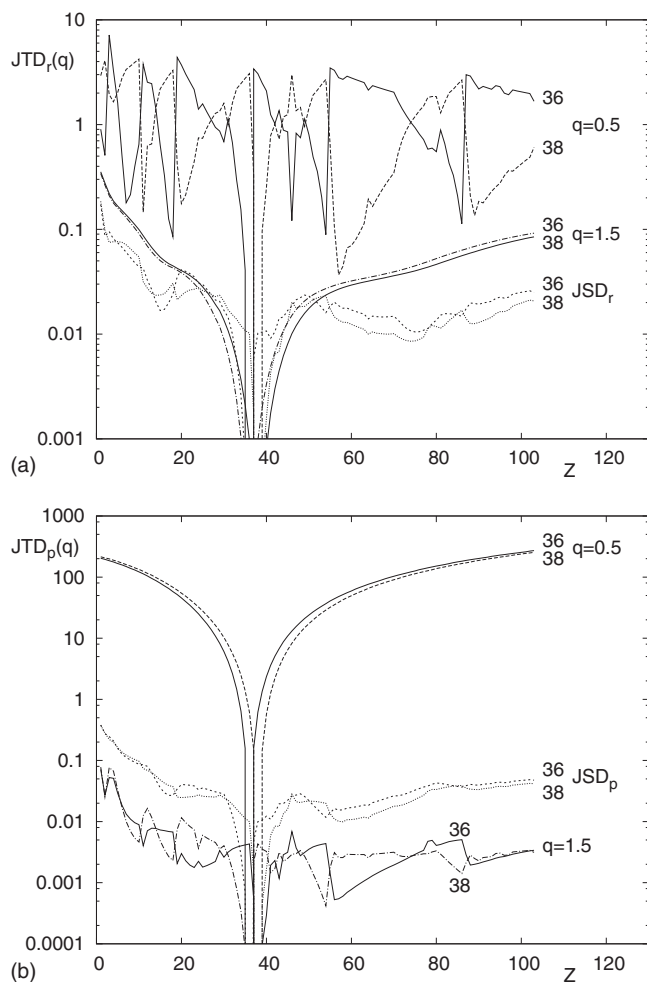


FIG. 2. $JTD_r^{(q)}$ divergences of systems with nuclear charge $Z=36$ (solid) and $Z=38$ (dashed) with respect to all neutral atoms with $Z=1-103$ for $q=0.5, 1.0, 1.5$, in (a) position and (b) momentum spaces. Atomic units are used.

information on the valence characteristics. An opposite trend is displayed in Fig. 2(b) for momentum space, where higher order JTD are the useful ones when analyzing the aforementioned properties. In both spaces, the JTD curves progressively modify their shapes as the parameter q varies in a continuous form, making the number of extrema and their enhancement also to vary in a monotonic way.

In all cases, the appearance of local extrema in the curves is determined, as remarked in the discussion of Fig. 2, by the groups of the Periodic Table which the atoms belong to. The divergence of a system with respect to an atom of the same group is smaller than that of its neighbors displayed in the figures as apparent minima. In the present case, the valence orbital of $Z=36$ is p^6 while for $Z=38$ it is s^2 . Those minima correspond, respectively, to atoms with identical valence orbital. Additional extrema, mainly minima, are associated with systems that suffer from the anomalous shell-filling effects.

The Fig. 3 provides a corroboration of the previous observations. The curves correspond to the JTD values in position space of each atom belonging to the noble gases group, as compared to all the atomic systems throughout the Periodic Table. According to those comments, it should be ex-

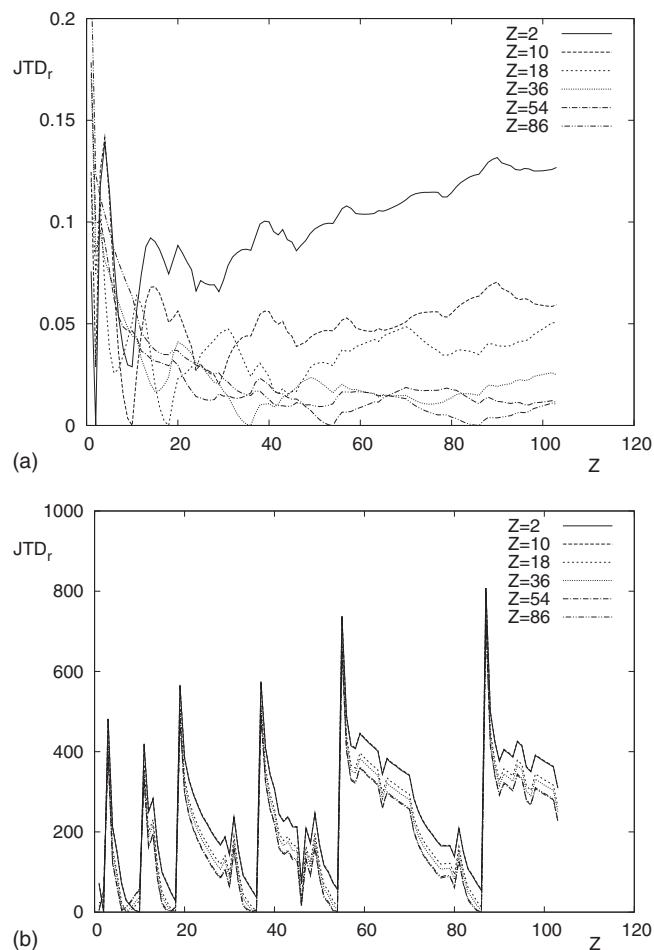


FIG. 3. JTD in position space $JTD_r^{(q)}$ for the noble gases ($Z=2, 10, 18, 36, 54, 86$) with respect to all neutral atoms with $Z=1-103$, for (a) $q=1.0$ and (b) $q=0.2$. Atomic units are used.

pected a similar behavior for all the atoms belonging to the same group. A comparison between the cases $q=1$ and $q=0.2$ [Figs. 3(a) and 3(b), respectively] makes one again to notice that, in spite of the similarity (at least roughly) among the shapes of the curves, they are almost identical for the low q order JTD as compared to the JSD. Similar observations can be noted from Fig. 4 with regard to momentum space, where now the comparison between Fig. 4(a), corresponding to JSD, to the higher q order in Fig. 4(b) makes the curves closer, with the only exception of the $Z=2$ (helium) one. The reason explaining this exception is the different structure of the Helium, with an “ s ” valence subshell, as compared to the “ p ” one for the others in the same group.

The analysis of the JTD divergence between atomic systems carried out above, regarding to the relevancy of the considered divergence order q , the shell structure of the systems under comparison as well as the information provided by the position and momentum densities allow us to consider this comparative measure as a powerful tool in order to appropriately quantify the dissimilarity of atomic systems on the basis of their respective one-particle densities.

It is worthy to remark that, in spite of the availability of other comparative measures, the JTD allows to perform a deeper and more detailed study as compared to the other ones.²⁵ Attending to that comparison, the behavior of the

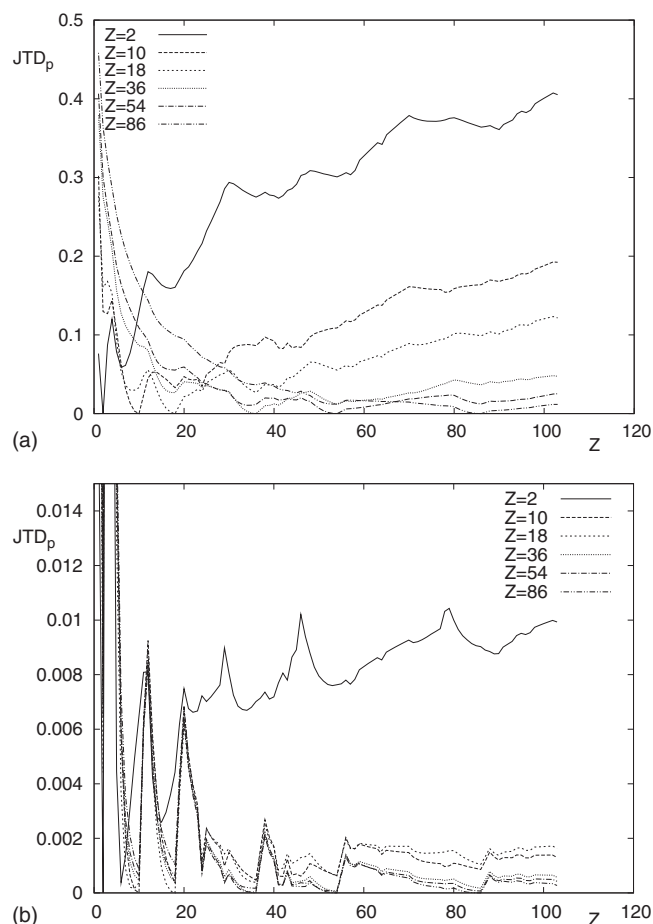


FIG. 4. JTD in momentum space $JTD_p^{(q)}$ for the noble gases ($Z=2, 10, 18, 36, 54, 86$) with respect to all neutral atoms with $Z=1-103$, for (a) $q=1.0$ and (b) $q=2.5$. Atomic units are used.

JTD in the conjugated spaces deserves a relevant comment, concerning its capability to provide relevant information in both spaces, contrary to the case of many other measures, such as for instance the quadratic distance, the quantum similarity index, and the Fisher divergence, which are not able to provide the aforementioned informational description when dealing with the position space, requiring to perform this type of analysis by means of the momentum space density.

IV. CONCLUSIONS

In this work we have proposed a divergence measure, based in concepts taken from the information theory, to study the dissimilarity among several multielectronic distributions. It has been shown how the JTD allows a deep introspection within the structure of the atomic one-particle densities. The JTD captures relevant differences in any of the conjugated spaces. This is not the case of other measures of divergence employed with multielectronic systems. The neutral atoms have constituted a benchmark for the present analysis, displaying their complex and hierarchical organization along the Periodic Table. The employment of the JTD as a divergence measure can be applied not only to compare a couple of probability distributions, but also to an arbitrary number

of them, even assigning different weights to each distribution considered as a whole, apart from the weighting effect of the characteristic parameter of JTD.

Further applications of this generalized divergence are actually being carried out for atoms and molecules, such as the comparisons among (i) distributions computed within different models for a given system, (ii) parts or components of the global system, (iii) atomic species involved in ionization processes, and (iv) initial and final products in chemical reactions. On the other hand, the generality of the techniques here employed allows the extension of this study to many relevant physical and chemical systems and/or processes. The results of those studies are being currently investigated in our laboratories and will be provided elsewhere.

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