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RESEARCH ARTICLE

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# Phase-space relative Rényi entropy in density functional theory

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## Abstract

The phase-space relative Rényi entropy is introduced using the information theoretical and thermodynamic view of density functional theory. In the special case of constant inverse temperature the phase-space relative Rényi entropy is a sum of the position-space relative Rényi entropy and a term arising from the momentum space. This quantity can be considered as a measure of similarity. It includes more information than the position-space measures, since it also incorporates momentum-space knowledge.

**KEYWORDS**
density functional theory, phase-space relative Rényi entropy

## 1 | INTRODUCTION

Information theoretical concepts have become very effective in quantum chemistry, particularly in density functional theory (DFT) (see e.g., [1–20]). Among others, Rényi entropy [21] or Fisher information [22] have turned to be powerful in several applications. These measures have been mainly employed in position space. Nevertheless, there have been momentum-space [1–5] or even phase-space studies [1–5,23].

Information theoretical concept was applied by Ghosh, Berkowitz and Parr (GBP) [24] in rewriting DFT. In their thermodynamic interpretation the ground-state DFT can be considered a local thermodynamics. They defined a local temperature that later proved to be a useful quantity in chemical reactivity.

Recently, phase-space Shannon, Fisher information, Rényi entropy and complexity [25–28] have been introduced and investigated within a thermodynamic presentation of DFT.

It is interesting that constant temperature can be attained by maximizing the phase-space Shannon information [29,30] or minimizing the phase-space Fisher information [31].

Here, the phase-space relative Rényi information is introduced in the thermodynamic interpretation of DFT and recommended as a measure of quantum similarity. For constant inverse temperature the phase-space relative Rényi entropy is the sum of the position-space relative Rényi entropy and a term coming from the momentum space. The ratio of these terms depends on the order of the phase-space relative Rényi entropy. This novel measure of similarity comprises more information than the position-space measures, because it also involves momentum-space knowledge. This quantity is not restricted to the ground state. Any pair of states can be compared with this measure, only the densities and kinetic energy densities of the states are needed for the analyses.

The paper is organized as follows: the definition and the properties of the phase-space relative Rényi entropy are summarized in Section 2. Section 3 outlines the phase-space information theoretical aspect of DFT. Section 4 presents the phase-space relative Rényi entropy as a novel measure of similarity with simple illustrations. The last section is devoted to discussion.

## 2 | PHASE-SPACE RELATIVE RÉNYI ENTROPY

The Rényi entropy of order $q$ is given by

$$R_f^{(q)} = \frac{1}{1-q} \ln \int [f(\mathbf{r})]^q d\mathbf{r}, \quad \text{for } 0 < q < \infty \text{ and } q \neq 1, \tag{1}$$

where the $D$-dimensional density function $f(\mathbf{r})$ is nonnegative and normalized to 1 ($\int f(\mathbf{r}) d\mathbf{r} = 1$). $r$ denotes $r_1,...,r_D$.

The limit $q \to 1$ yields the Shannon entropy:

$$S_f = -\int f(\mathbf{r}) \ln f(\mathbf{r}) d\mathbf{r}. \tag{2}$$

The relative Rényi entropy of order $q$ defined as

$$R_{f,f_{ref}}^q = \frac{1}{q-1} \ln \int \frac{f^q(\mathbf{r})}{f_{ref}^{q-1}(\mathbf{r})} d\mathbf{r} \tag{3}$$

measures the deviation of $f(\mathbf{r})$ from a reference density $f_{ref}(\mathbf{r})$. The limit $q \to 1$ generates the relative or Kullback–Leibler entropy or cross-entropy [32]

$$I_{KL}(f, f_{ref}) = \int f(\mathbf{r}) \ln \frac{f(\mathbf{r})}{f_{ref}(\mathbf{r})} d\mathbf{r}. \tag{4}$$

In DFT fidelity is defined [27,33] as

$$F(f,g) = \int f^{1/2} g^{1/2} d\mathbf{r}. \tag{5}$$

This quantity also provides a 'difference' between the densities $f(\mathbf{r})$ and $g(\mathbf{r})$.

Consider distribution functions depending on a parameter $\theta$ and the fidelity with functions $f(\theta)$ and $f(\theta + \delta\theta)$. Then we arrive at the fidelity susceptibility $\chi$ [27,33]

$$\chi = \frac{1}{4} \int \frac{1}{f} \left( \frac{\partial f}{\partial \theta} \right)^2 \tag{6}$$

by expanding $f(\theta + \delta\theta)$ around $f(\theta)$

$$F(\theta, \theta + \delta\theta) = 1 - \frac{1}{2} (\delta\theta)^2 \chi + \ldots \tag{7}$$

We remark that $\chi$ is proportional to the Fisher information

$$I(\theta) = \int \frac{1}{f} \left( \frac{\partial f}{\partial \theta} \right)^2, \tag{8}$$

a key quantity of statistical estimation theory.

Consider now the relative Rényi entropy for the distribution functions $f(\theta)$ and $f(\theta + \delta\theta)$. Expanding $f(\theta + \delta\theta)$ around $f(\theta)$ we are led to [27,34,35]

$$R_{f(\theta), f(\theta+\delta\theta)}^q \approx 2q\chi (\delta\theta)^2. \tag{9}$$

The limit $q \to 1$ provides the Kullback–Leibler entropy:

$$I^{KL}_{f(\theta),f(\theta+\delta\theta)} \approx 2\chi(\delta\theta)^2. \tag{10}$$

Therefore,

$$R^{q}_{f(\theta),f(\theta+\delta\theta)} \approx qI^{KL}_{f(\theta),f(\theta+\delta\theta)}, \tag{11}$$

that is, in this special case the relative Rényi entropy is proportional to the Kullback–Leibler entropy and the ratio is the order $q$.

## 3 | PHASE-SPACE INFORMATION THEORETICAL ASPECT OF DFT

Turn now to the information theoretical and thermodynamic interpretation of DFT invented by Ghosh, Berkowitz and Parr (GBP) [24]. A phase-space distribution function $g(\mathbf{r},\mathbf{p})$ maximizing the information

$$S = -k\int d\mathbf{r}d\mathbf{p}g(\ln g - 1) \tag{12}$$

is searched while keeping the density

$$\int d\mathbf{p}g(\mathbf{r},\mathbf{p}) = \varrho(\mathbf{r}) \tag{13}$$

and kinetic energy density $t(\mathbf{r})$

$$\int d\mathbf{p}\frac{p^2}{2}g(\mathbf{r},\mathbf{p}) = t(\mathbf{r}) \tag{14}$$

fixed. The variation yields a Maxwell–Boltzmann-like distribution function

$$g(\mathbf{r},\mathbf{p}) = e^{-\alpha(\mathbf{r})}e^{-\beta(\mathbf{r})p^2/2}, \tag{15}$$

where $k$ is the Boltzmann constant. The $\mathbf{r}$-dependent Lagrange multipliers $\alpha(\mathbf{r})$ and $\beta(\mathbf{r})$ are given by the conditions (13) and (14). The familiar ideal gas expression

$$t(\mathbf{r}) = \frac{3}{2}\frac{\varrho(\mathbf{r})}{\beta(\mathbf{r})} \tag{16}$$

follows directly from Equations (15) to (14) without any assumption. Owing to Equations (15) and (16) this approach is referred to as a thermodynamic transcription of DFT and $\beta(\mathbf{r})$ is called local inverse temperature.

It should be underlined that the kinetic energy density $t(\mathbf{r})$ is not uniquely defined. Only its integral yielding the kinetic energy $E^{kin} = \int d\mathbf{r}t(\mathbf{r})$ is unique. As a consequence, $\beta(\mathbf{r})$ and $g$ are not unique either. Some forms of $t(\mathbf{r})$ are often applied ([36–38]). Here the form of $t(\mathbf{r})$ that maximizes the phase-space Shannon information [31] (or minimizes the phase-space Fisher information [29]) is selected. This choice is especially appealing as it yields a constant inverse temperature

$$\beta = \frac{3}{2}\frac{N}{E^{kin}}. \tag{17}$$

$N$ is the number of particles.

In the following it is worth using the phase-space distribution function (15) rewritten as

$$f=\frac{1}{N}g=\frac{1}{N}\left[\frac{\beta}{2\pi}\right]^{3/2}\varrho e^{-\beta p^2/2}=\left[\frac{\beta}{2\pi}\right]^{3/2}\sigma e^{-\beta p^2/2}. \tag{18}$$

$f$ normalized to 1. On the other hand, $g$ is normalized to $N$, because $\varrho$ integrates to $N$ as it is usual in DFT. It is advantageous applying shape functions [39] $\sigma(\mathbf{r})=\varrho(\mathbf{r})/N$, which integrate to 1.

Substituting $f$ Equations (18) into (3) we obtain

$$R^q_{f,f_{ref}}=\frac{1}{q-1}\ln\int\left[\left(\frac{\beta(\mathbf{r})}{2\pi}\right)^{3q/2}\left(\frac{\beta_{ref}(\mathbf{r})}{2\pi}\right)^{3(1-q)/2}\sigma^q(\mathbf{r})\sigma^{1-q}_{ref}(\mathbf{r})e^{-[q\beta(\mathbf{r})+(1-q)\beta_{ref}(\mathbf{r})]p^2/2}d\mathbf{r}d\mathbf{p}\right]. \tag{19}$$

Obviously, the integral exists only if

$$q\beta(\mathbf{r})+(1-q)\beta_{ref}(\mathbf{r})>0. \tag{20}$$

It is a constraint for the choice of the kinetic energy density. Or we can select only those values of $q$ for which the inequality holds. Performing the integration in the momentum space, the phase-space relative Rényi entropy takes the form

$$R^q_{f,f_{ref}}=\frac{1}{q-1}\ln\int\left(\frac{\beta^q\beta^{1-q}_{ref}}{q\beta+(1-q)\beta_{ref}}\right)^{3/2}\sigma^q\sigma^{1-q}_{ref}d\mathbf{r}. \tag{21}$$

In the special case of constant inverse temperature Equation (21) yields

$$R^q_{f,f_{ref}}=R^q_{\beta,\beta_{ref}}+R^q_{\sigma,\sigma_{ref}}, \tag{22}$$

where

$$R^q_{\beta,\beta_{ref}}=\frac{3}{2(q-1)}\ln\left[\left(\frac{\beta^q\beta^{1-q}_{ref}}{q\beta+(1-q)\beta_{ref}]}\right)\right] \tag{23}$$

and

$$R^q_{\sigma,\sigma_{ref}}=\frac{1}{q-1}\ln\left[\int\sigma^q\sigma^{1-q}_{ref}d\mathbf{r}\right] \tag{24}$$

is the position-space relative Rényi entropy expressed with the shape functions [39]. That is, the phase-space relative Rényi entropy is the sum of the position-space relative Rényi entropy obtained by the shape functions and the momentum-space term depending only on the inverse temperatures.

As we can see from Equations (12) to (16) the procedure described above is valid both for the true interacting and the non-interacting KS (Kohn–Sham) systems. Certainly, only $\varrho(\mathbf{r})$ is the same and the other quantities (e.g., $f(\mathbf{r},\mathbf{p})$, $t(\mathbf{r})$, $E^{kin}$, $\beta$) are different. It can be advantageous taking interacting kinetic energy because in Coulomb systems at equilibrium nuclear geometry the virial theorem

$$E=-E^{kin} \tag{25}$$

can be employed. $E$ is the total energy. Then, Equation (22) can be expressed with $E$ instead of $\beta$ utilizing Equation (17).

## 4 | PHASE-SPACE RELATIVE RÉNYI ENTROPY AS A NOVEL MEASURE OF SIMILARITY

Quantum similarity measures have turned to be very useful in quantum chemistry (see e.g., [40]). A well-known similarity indicator between the molecular electron densities $\varrho_A(\mathbf{r})$ and $\varrho_B(\mathbf{r})$ is the Carbó index [41]

$$R_{AB} = \frac{\int d\mathbf{r} \varrho_A(\mathbf{r}) \varrho_B(\mathbf{r})}{\sqrt{\int d\mathbf{r} \varrho_A^2(\mathbf{r}) \int d\mathbf{r} \varrho_B^2(\mathbf{r})}}. \tag{26}$$

The generalization of this marker is the generalized quantum similarity index (QSI) [42]

$$QSI^{\gamma} = \frac{\int d\mathbf{r} (\tilde{g}_1 \tilde{g}_2)^{\gamma/2}}{\sqrt{\int d\mathbf{r} \tilde{g}_1^{\gamma} \int d\mathbf{r} \tilde{g}_2^{\gamma}}} \tag{27}$$

that measures the 'distance' between the distribution functions $\tilde{g}_1$ and $\tilde{g}_2$ and $\gamma$ is a real number. Clearly, $\gamma = 2$ yields the Carbó index, while $\gamma = 1$ leads to the fidelity.

Here, a novel marker of similarity, the phase-space relative Rényi entropy is proposed. For constant inverse temperature this quantity (Equation 22) is a sum of two terms. The first arises from the momentum space, while the second is the position-space relative Rényi entropy. We can select two interesting cases. If the two states compared have the same energy (for example degenerate states are taken), the phase-space relative Rényi entropy is reduced to the position-space relative Rényi entropy.

On the other hand, if the two densities are equal, only the first term remains in $R^q_{f,f_{ref}}$. This happens, for example, if we compare the true interacting and the non-interacting KS systems. Both have the same density, therefore the position-space relative Rényi entropy disappears. The remaining first term in Equation (22) can be given by the interacting and non-interacting kinetic energies. Morrison and Zhao [43] used accurate, correlated wave functions to calculate the densities and obtained the solutions of the KS equations corresponding to these accurate densities for the neutral atoms from He through Ar. $R^q_{\beta,\beta_{ref}}$ have been calculated using their data and plotted on Figure 1 for $q = 2$. As these numbers are very small, they are multiplied by $10^5$ for better visibility. KS values have been taken as reference. As Figure 1 demonstrates the interacting and the KS systems are really very similar. The KS inverse temperature is $\beta_s = \frac{3N}{2E_s^{kin}}$, where $E_s^{kin}$ is the non-interacting KS kinetic energy. For the true interacting system $\beta = \frac{3N}{2E^{kin}}$, where $E^{kin}$ is the interacting kinetic energy. The difference

$$E_c^{kin} = E^{kin} - E_s^{kin} \tag{28}$$

is very small [43]. The Fisher information of Equation (8) with parameter $\beta_s$ is $I = \frac{3}{2\beta_s^2}$ [29]). As the difference of $\beta$ and $\beta_s$ is small, Equation (9) can be used to obtain $R^q_{\beta,\beta_s}$. It is also plotted on Figure 1 and we can see that it is a very good approximation. $R^q_{\beta,\beta_s}$ is plotted as a function of the atomic number $Z$. For neutral atoms $Z = N$. Connecting the points on Figure 1 we can notice that the tangent changes at $Z = 4$ and $Z = 10$. That is, Figure 1 reveals a shell structure. We can obtain similar plots for other values of $q$.

Finally, a simple example is presented to illustrate the relation of $R^q_{\beta,\beta_{ref}}$ and $R^q_{\sigma,\sigma_{ref}}$. Consider H-like ions with atomic number $Z$. The shape function is $\sigma = \frac{Z^3}{\pi} e^{-2Zr}$. The constant inverse temperature is $\beta = 3/Z^2$ [29]). Then Equations (23) and (24) lead to

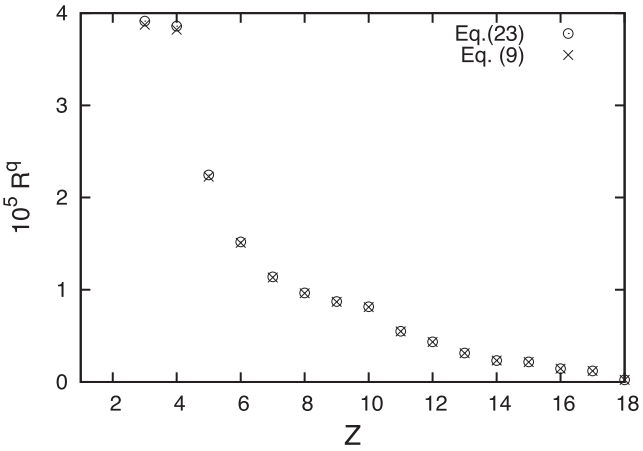


**FIGURE 1** Phase-space relative Rényi entropy of atoms multiplied by $10^5$ for $q = 2$. True interacting values compared to the non-interacting KS ones.

$$R^q_{\beta,\beta_{ref}} = \frac{3}{2(q-1)} \ln\left(\frac{\zeta^{-2q}}{q\zeta^{-2}+(1-q)}\right) \tag{29}$$

and

$$R^q_{\sigma,\sigma_{ref}} = \frac{3}{q-1} \ln\left(\frac{\zeta^{q}}{q\zeta+(1-q)}\right), \tag{30}$$

where

$$\zeta = \frac{Z}{Z_{ref}}. \tag{31}$$

The constraint (20) yields

$$q+(1-q)\zeta^2 > 0. \tag{32}$$

Taking the H-atom as reference ($Z_{ref}=1$), $R^q_{\sigma,\sigma_{ref}}$, $R^q_{\beta,\beta_{ref}}$ and $R^q_{f,f_{ref}}$ are plotted on Figures 2 and 3 for $q=0.0005$ and $q=0.9$. In the first case $R^q_{\sigma,\sigma_{ref}}$ is larger than $R^q_{\beta,\beta_{ref}}$, while in the second case $R^q_{\beta,\beta_{ref}}$ exceeds $R^q_{\sigma,\sigma_{ref}}$. All of them monotonically are increasing functions of $Z$. The weight of the

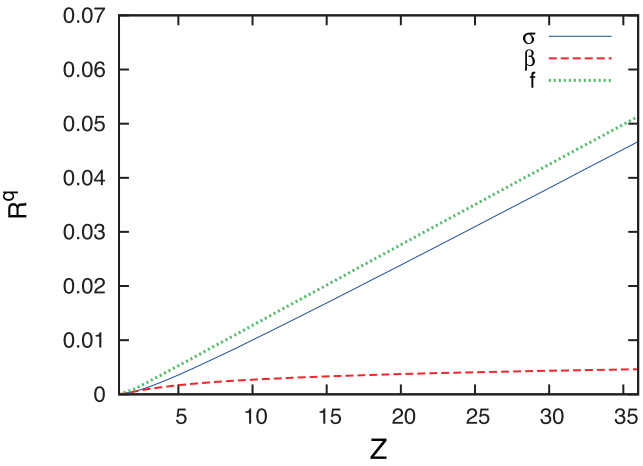


**FIGURE 2** Phase-space relative Rényi entropy of H-like ions for $q=0.0005$ with H-atom as reference (color online).

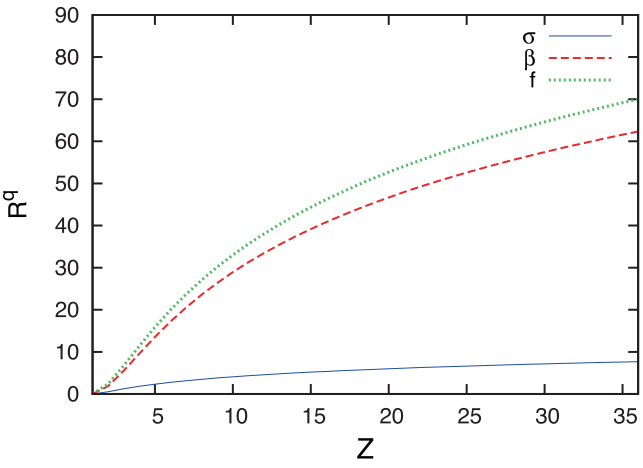


**FIGURE 3** Phase-space relative Rényi entropy of H-like ions for $q=0.9$ with H-atom as reference (color online).

position-space (or momentum-space) term in the phase-space relative Rényi entropy depends on $q$. At $q = 0.45$ (not shown in the figures) the two terms have the same magnitude.

## 5 | DISCUSSION

We can notice that the scheme followed above (Equations 12–16) is not restricted to the ground state. Any state can be taken, $R^q_{\varrho,\varrho_{ref}}$ can compare any pair of states. Only the density and kinetic energy density are needed for the analyses.

The phase-space distribution functions are usually assumed to be nonnegative and supposed to generate the correct marginal distribution functions (see [44–48]). However, the Ghosh–Berkowitz–Parr distribution function studied here has only a correct position-space marginal. On the other hand, it does not produce the correct momentum-space marginal due to the kinetic energy density constraint (Equation 14; instead of a momentum-space density constraint).

It is well-known that in Coulomb systems the density decays as

$$\lim_{r\to\infty} \frac{\partial \ln \overline{\varrho}(r)}{\partial r} = -\sqrt{8(E_0^{N-1} - E)}, \tag{33}$$

where $E_0^{N-1} - E$ is the vertical ionization potential of the $N$-electron system. $E$ is the energy of the given state and $E_0^{N-1}$ is the ground-state energy of the $N-1$ electron system [49–51]. So, if the density is known, $E$ is also given together with $\beta$ owing to the virial theorem. Consequently, $f$ is available by Equation (18). In other words, the density comprises phase-space information. Therefore, selection of constant temperature is particularly advantageous.

The phase-space distribution functions $f$ and $f^{ref}$ can belong to different systems. Therefore, the phase-space relative Rényi entropy can reveal resemblance of different systems.

In conclusion, the phase-space Rényi relative entropy has been introduced utilizing the thermodynamic transcription of DFT. For constant inverse temperature this quantity is a sum of the position-space relative Rényi entropy and a term arising from the momentum space. The ratio of these terms depends on the order $q$. The phase-space relative Rényi entropy can be considered as a measure of similarity. It contains more information than the position-space measures, since it comprises momentum-space information as well.

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### DATA AVAILABILITY STATEMENT

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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