Relativistic effects on information measures for hydrogen-like atoms

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(Dated: February 23, 2009)

Abstract

Position and momentum information measures are evaluated for the ground state of the *relativistic* hydrogen-like atoms. Consequences of the fact that the radial momentum operator is not self-adjoint are explicitly studied, exhibiting fundamental shortcomings of the conventional uncertainty measures in terms of the radial position and momentum variances. The Shannon and Rényi entropies, the Fisher information measure, as well as several related information measures, are considered as viable alternatives. Detailed results on the onset of relativistic effects for low nuclear charges, and on the extreme relativistic limit, are presented. The relativistic position density decays exponentially at large r, but is singular at the origin. Correspondingly, the momentum density decays as an inverse power of p. Both features yield divergent Rényi entropies away from a finite vicinity of the Shannon entropy. While the position space information measures can be evaluated analytically for both the nonrelativistic and the relativistic hydrogen atom, this is not the case for the relativistic momentum space. Some of the results allow interesting insight into the significance of recently evaluated Dirac-Fock vs. Hartree-Fock complexity measures for many-electron neutral atoms.

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PACS:31.10.+z;31.15.-p;31.30.Jv;31.30.-i .

keywords: relativistic H atom; Heisenberg uncertainty relation; Shannon and Rényi entropies; Fisher information measure.

I. INTRODUCTION

The celebrated Heisenberg uncertainty principle [1, 2] of quantum mechanics is specified by means of the position and momentum variances, that are defined in terms of the expectation values of the corresponding (hermitian) operators. Several authors have pointed out that for bimodal distributions this formulation does not provide an adequate measure of the uncertainty of the measurable involved. A variety of information measures have been proposed and investigated in a fairly broad range of contexts. The most familiar of these are due to Shannon [3] and Fisher [4]. They are being increasingly applied in studying the electronic structure and properties of atoms and molecules, and play an important role in the rapidly developing field of quantum information and its anticipated technological offspring.

Due to its fundamental importance in natural sciences, the hydrogen atom has been extensively studied from the *information theoretical* view point. Consequently, the Shannon entropies [5, 6, 7] and Fisher information [8] of the non-relativistic hydrogen-like atom have been studied in considerable detail. We note, with some surprise, a glaring omission, the relativistic hydrogen atom, formulated in terms of the Dirac equation, which is the subject of the present study. Future studies of relativistic effects on the information measures in many-electron atoms will certainly benefit from the presently derived results. Indeed, very recent work on Dirac-Fock vs. Hartree-Fock complexity measures for neutral many-electron atoms [9] allows certain comparisons to be made with results obtained in the present article, that shed additional light on the significance of that study.

The Shannon information entropy S_r of the spatial electron density $\rho(\mathbf{r})$ is defined as

$$S_r = -\int \rho(\mathbf{r})\, \ln \rho(\mathbf{r})\, d\mathbf{r}\ , \tag{1}$$

and the corresponding momentum space entropy S_p is given by

$$S_p = -\int \Pi(\mathbf{p})\, \ln \Pi(\mathbf{p})\, d\mathbf{p}\ , \tag{2}$$

where $\Pi(\mathbf{p})$ denotes the momentum density. The densities $\rho(\mathbf{r})$ and $\Pi(\mathbf{p})$ are each normalized to unity and all quantities are given in atomic units. These two densities are obtained from the corresponding position and momentum space wavefunctions, that are the Fourier transforms of one another. The Shannon entropy sum $S_T = S_r + S_p$ contains the net information and obeys the well known lower bound derived by Bialynicki-Birula and Mycielski [10],

$$S_T = S_r + S_p \geq n\,(1 + \ln \pi)\ , \tag{3}$$

where n is the number of dimensions. The lower bound is attained by a Gaussian distribution. This entropic uncertainty-like relation represents a stronger version of the Heisenberg uncertainty principle of quantum mechanics. The individual entropies S_r and S_p depend on the units used to measure r and p respectively, but their sum S_T does not, i.e., it is invariant under uniform scaling of coordinates.

The Shannon entropies provide a global measure of information about the probability distribution in the respective spaces. A more localized distribution yields a *smaller* value of the corresponding information entropy. For applications of Shannon information entropy in chemical physics we refer the reader to the published literature [5, 11].

In the context of the quantum theory of one-particle systems the Fisher position information measure is defined as

$$I_r = \int \frac{|\nabla \rho(\mathbf{r})|^2}{\rho(\mathbf{r})}\, d\mathbf{r} \tag{4}$$

and the corresponding momentum space measure is given by

$$I_p = \int \frac{|\nabla \Pi(\mathbf{p})|^2}{\Pi(\mathbf{p})}\, d\mathbf{p}. \tag{5}$$

For a general definition of the Fisher information measure and a careful exposition of its significance we refer to the definitive monograph by Rao [12].

The individual Fisher measures are bounded through the Cramer-Rao inequality [12, 13] according to $I_r \geq \dfrac{1}{V_r}$ and $I_p \geq \dfrac{1}{V_p}$, where V's denote the corresponding spatial and momentum variances, respectively. In position space the Fisher information measures the sharpness of the probability density, and for a Gaussian distribution is exactly equal to the inverse of the variance [14]. A sharp (smooth) and strongly localized (well spread-out) probability density gives rise to a *larger* (*smaller*) value of the Fisher information in the position space. With a differential probability density as its content, the Fisher measure is better suited to study the localization characteristics of the probability distribution than the Shannon information entropy [15, 16]. Unlike $S_r + S_p$, for which eq. 3 specifies a lower bound, general bounds are as yet unknown for the Fisher product $I_r I_p$. Since localization (i.e., low uncertainty) means high values of the Fisher information measures, the counterpart of the Heisenberg or Shannon bound should be an upper bound on the product of position and momentum Fisher information measures. For a single particle under the influence of a central potential Dehesa *et al.* [17] have very recently reported a lower bound on the Heisenberg product [18, 19, 20, 21] which can be directly related to the Fisher information. For the application of the Fisher information measure as an underlying guideline for the formulation of fundamental physical principles we refer to the recent book by Frieden [14], and for applications to the electronic structure of atoms, to the pioneering work of Dehesa *et al.* [22, 23, 24, 25].

A widely used generalization of the Shannon entropy is the Rényi entropy. The Rényi position entropy (that, when a more precise designation is required, we shall address as the a-Rényi position entropy) is defined as [26]

$$H_a^{(r)} = \frac{1}{1-a} \log \left(\int_0^\infty [\rho(r)]^a 4\pi r^2 dr \right) \ . \tag{6}$$

The symmetrized Rényi position entropy is

$$\mathcal{H}_s^{(r)} = (H_a^{(r)} + H_b^{(r)})/2 \tag{7}$$

where

$$a = \frac{1}{1-s}, \quad b = \frac{1}{1+s}, \quad -1 \leq s \leq 1, \quad \text{i.e.,}\ \frac{1}{2} \leq a, b \leq \infty, \quad \frac{1}{a} + \frac{1}{b} = 2.$$

The Rényi momentum entropies are similarly defined in terms of the momentum density $\Pi(p)$. For $a = 1$ one obtains, using l'Hôpital's rule,

$$\lim_{a \to 1} H_a^{(r)} = -\int_0^\infty \rho(r) \log[\rho(r)] 4\pi r^2 dr = S_r \ ,$$

where S_r is the Shannon position entropy [3]. For an n dimensional system, the sum of the a-Rényi position entropy and the b-Rényi momentum entropy, for a and b satisfying $\frac{1}{a} + \frac{1}{b} = 2$, was recently shown by Bialynicki-Birula [26] to satisfy the inequality (uncertainty-like relation)

$$H_a^{(x)} + H_b^{(p)} \geq n \left[\frac{1}{2} \left(\frac{\log(a)}{a-1} + \frac{\log(b)}{b-1} \right) + \log(\pi) \right] \ . \tag{8}$$

The properties of the Shannon entropies and several other information measures under coordinate scaling have been examined in ref. [27]. It was pointed out that upon scaling the coordinates via $\tilde{r} = \zeta r$, normalization of the density requires that

$$\tilde{\rho}(r) = \frac{1}{\zeta^3}\rho\left(\frac{r}{\zeta}\right) .$$

It follows that

$$\begin{aligned}\tilde{H}_a^{(r)} &= \frac{1}{1-a}\log\left(\int_0^\infty [\tilde{\rho}(r)]^a 4\pi r^2 dr\right) \\ &= \frac{1}{1-a}\log\left(\zeta^{3(1-a)}\int_0^\infty [\rho(x)]^a 4\pi x^2 dx\right) = 3\log(\zeta) + H_a^{(r)} .\end{aligned}$$

The scaling of the coordinates introduced above implies scaling of the momenta according to $\tilde{p} = \frac{p}{\zeta}$, so

$$\tilde{H}_{a'}^{(p)} = -3\log(\zeta) + H_{a'}^{(p)} .$$

Hence,

$$\tilde{H}_a^{(r)} + \tilde{H}_{a'}^{(p)} = H_a^{(r)} + H_{a'}^{(p)} .$$

Note that a and a' are entirely independent of one another.

For a system whose hamiltonian is of the form $\mathcal{H} = \hat{T} + \lambda V(r)$, where $\hat{T} = -\frac{1}{2}\nabla^2$, if the potential is homogeneous, i.e., $V(\zeta r) = \zeta^k V(r)$, scaling of the coordinates via $\tilde{r} = \zeta r$ is equivalent to scaling the coupling constant via $\tilde{\lambda} = \zeta^{k+2}\lambda$ [27]. Hence, for such potentials the sum of an a-Rényi position entropy and an a'-Rényi momentum entropy is independent of the coupling constant λ.

Since the position density has dimensions of inverse volume and the momentum density has dimensions of inverse momentum cubed, the Shannon, Fisher and Rényi entropies can be converted into quantities that have dimensions of length or momentum. This property is used to facilitate comparison among the different information measures. We refer to these transformed quantities as "length" and "impetus", respectively. This practice allows a clear distinction between variance-based uncertainty measures and information based measures that have units of position or momentum although they do not involve expectation values of the corresponding quantum-mechanical operators. "Impetus" is a pre-Newtonian synonym of momentum.

A different class of information measures, involving ratios between relativistic and nonrelativistic densities [28, 29], is considered as well. Since these information measures are pure numbers they cannot be transformed into quantities with units of length or momentum. However, they allow the onset of relativistic effects upon increase of the nuclear charge to be followed very transparently.

A third class of information measures is represented by the Tsallis entropy [30],

$$\epsilon_a = \frac{1}{a-1}\left(1 - 4\pi \int_0^\infty (\rho(r))^a r^2 dr\right) ,$$

that has been invoked for non-extensive systems, and which is not homogeneous under coordinate scaling. The Tsallis entropy is closely related to the Rényi entropy via

$$\epsilon_a = \frac{1}{a-1}\left(1 - \exp\left((1-a)H_a^{(r)}\right)\right) .$$

For $a \rightarrow 1$ these two entropies coincide with one another as well as with the Shannon entropy.

Upon attempting to evaluate the various uncertainty and information measures for the relativistic hydrogen atom we encountered three somewhat surprising obstacles. The first has to do with the fact that the radial momentum does not have a proper (self-adjoint) quantum-mechanical counterpart. This fact has been known for a while, and its consequences in the present context are explained below. Another surprise had to do with the fact that the momentum-space solutions of the Dirac equations are still subject to controversy [31, 32]. Finally, we find it intriguing that for the relativistic hydrogen atom the position space information measures could be evaluated analytically, but for the momentum space measures we had to apply numerical integration. The first difficulty suggests that the various uncertainty-like principles that do not involve the variance of position or momentum have even stronger merits for multi-dimensional systems than those extensively pointed out in previous studies on one dimensional systems. We addressed the second difficulty by adhering to the version of the momentum wavefunction that in our judgement was the most natural and straightforward [33] without bothering to explore its equivalence (or lack of it) with other formulations.

This article is structured as follows: In sections 2 and 3 we consider the radial position and momentum variances for the nonrelativistic and the relativistic hydrogen atom, respectively, presenting very explicitly the consequences of the non self-adjointness of the commonly invoked radial momentum operator. The Shannon entropies are investigated in section 4, and the Fisher information measures in section 5. In section 6 we study the Rényi entropies, also considering the average density, that is essentially a special case of these. This allows a brief discussion of complexity measures, with a rather surprising comparison with a recent Dirac-Fock study of neutral many-electron atoms [9]. Scale invariant entropies are discussed in section 8, and some concluding remarks are made in section 9.

II. UNCERTAINTY MEASURES FOR THE NONRELATIVISTIC HYDROGEN-LIKE ATOMS

The most familiar measures of uncertainty are the position and momentum variances, which for a one dimensional system defined over the whole real axis are given by
$(\delta x) = \sqrt{< x^2 > - < x >^2}$ and $(\delta p) = \sqrt{< p^2 > - < p >^2}$, where

$$\begin{aligned} < x^k > &= \int_{-\infty}^{\infty} x^k |\psi(x)|^2 dx = \int_{-\infty}^{\infty} \phi^*(p) \left(i\hbar \frac{d}{dp} \right)^k \phi(p) dp \\ < p^k > &= \int_{-\infty}^{\infty} p^k |\phi|^2 dp = \int_{-\infty}^{\infty} \psi^*(x) \left(-i\hbar \frac{d}{dx} \right)^k \psi(x) dp \, . \end{aligned} \tag{9}$$

Here, $\psi(x)$ and $\phi(p)$ are the position and momentum wavefunctions, which are the Fourier transforms of one another. Eq. 9 emphasizes the correspondence between position and momentum space expectation values of the (hermitian) position and momentum operators, a correspondence that, as we shall explicitly demonstrate below, fails for the (non self-adjoint) radial momentum operator.

A. Position and momentum variances for spherically symmetric three-dimensional systems

Qiang and Dong [34], following a time-honored tradition, suggest that the radial momentum operator in the coordinate representation, using atomic units in which $\hbar = 1$, is

$$p_r = -i \left(\frac{\partial}{\partial r} + \frac{1}{r} \right) \, .$$

They justify this expression by noting that

$$p_r^2 = -\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)$$

is (up to a multiplicative constant) the radial part of the Laplacian (i.e., the kinetic energy operator).

Note, however, that the n dimensional generalization

$$p_r = -i\left(\frac{\partial}{\partial r} + \frac{n-1}{2r}\right)$$

satisfies

$$-p_r^2 = \frac{\partial^2}{\partial r^2} + \frac{n-1}{r}\frac{\partial}{\partial r} + \frac{(n-1)(n-3)}{4r^2} ,$$

which, for $n = 2$ and $n > 3$ does not agree with the radial part of the Laplacian,

$$\mathcal{L}_r = \frac{\partial^2}{\partial r^2} + \frac{n-1}{r}\frac{\partial}{\partial r} .$$

Straightforward integration by parts yields

$$< \psi|p_r|\psi >= -iS_n \int_0^\infty \psi(r) \left[\left(\frac{\partial}{\partial r} + \frac{n-1}{2r}\right)\psi(r)\right] r^{n-1} dr = 0 \tag{10}$$

where $S_n = \frac{2\pi^{\frac{n}{2}}}{\Gamma(\frac{n}{2})}$ is the surface area of the n-dimensional unit sphere.

Paz [35] has recently rigorously shown that p_r is not self-adjoint, and has no self-adjoint extension (*cf.*, also, [36, 37, 38], for earlier discussions of this issue). This fact, which is more closely considered below, suggests that using the variance of the radial momentum as an uncertainty measure for (spherically symmetric) three-dimensional systems may be questionable.

B. Position space wavefunction of the nonrelativistic hydrogen atom

The ground state nonrelativistic hydrogenic wavefunction $\psi_{0,0,0}(r) = \left(\frac{Z^3}{\pi}\right)^{\frac{1}{2}} \exp(-Zr)$ yields the density

$$\rho_{NR}(r) = \frac{Z^3}{\pi} \exp(-2Zr) . \tag{11}$$

The expectation values $< r >= \frac{3}{2Z}$ and $< r^2 >= \frac{3}{Z^2}$ yield

$$(\delta r) = \sqrt{< r^2 > - < r >^2} = \frac{\sqrt{3}}{2Z} \approx \frac{0.8660}{Z} \ .$$

Similarly, $< p_r >= 0$ and $< p_r^2 >= Z^2$. The latter value is equal to $< -\nabla^2 >$, because, for a spherically symmetric wavefunction, the angular part of the Laplacian makes a vanishing contribution.

Using these position space expectation values to evaluate $(\delta p_r) = Z$, we obtain the uncertainty product $(\delta r)(\delta p_r) \approx 0.8660$.

C. Momentum space wavefunction of the nonrelativistic hydrogen atom

The momentum space wavefunction for the ground state of the nonrelativistic hydrogen atom [39]

$$\chi_{0,0,0}(p) = \frac{1}{\pi}\left(\frac{2}{Z}\right)^{\frac{3}{2}}\left[\left(\frac{p}{Z}\right)^2 + 1\right]^{-2} , \tag{12}$$

yields the momentum density

$$\Pi_{NR}(p) = \frac{8}{\pi^2 Z^3}\left[\left(\frac{p}{Z}\right)^2 + 1\right]^{-4} , \tag{13}$$

in terms of which we obtain

$$< p >= \int_0^\infty p\Pi_{NR}(p) 4\pi p^2 dp = \frac{8Z}{3\pi} \approx 0.848826Z \ ,$$

and

$$< p^2 >= \int_0^\infty p^2\Pi_{NR}(p) 4\pi p^2 dp = Z^2 \ .$$

The latter value agrees with the position space expectation value of $-\nabla^2$, but the former does not agree with the position space result, eq. 10.

Using these momentum space expectation values we obtain

$$(\delta p) = \frac{Z}{3\pi}\sqrt{9\pi^2 - 64} \approx 0.5287Z \ .$$

Along with the value of δr obtained above we get

$$(\delta r)(\delta p) \approx 0.4578 \ ,$$

which is less than $\frac{1}{2}$. This is probably a manifestation of the questionable status of the radial momentum, pointed out above.

Messiah [40] shows that, in one dimension, $< x^2 >< p_x^2 > \geq \frac{1}{4}$. For a spherically symmetric system $< r^2 >= 3 < x^2 >$ and $< p^2 >= 3 < p_x^2 >$. Hence, $< r^2 >< p^2 > \geq \frac{9}{4}$. The results quoted above imply that for the nonrelativistic hydrogen atom $< r^2 >< p^2 >= 3$, which is larger than the lower bound derived by Messiah.

We conclude this section by emphasizing that the operators r^2 and p^2 can be expressed (in Cartesian coordinates) in terms of manifestly self-adjoint operators. This is not the case for r and p. Further consequences of this distinction are presented in the following section.

III. UNCERTAINTY MEASURES FOR THE RELATIVISTIC HYDROGEN-LIKE ATOMS

A. Relativistic position uncertainty

For the ground state of the Dirac hydrogenic atom the (spin up) wavefunction is of the form

$$\Psi_D = N r^{\gamma-1} \exp(-Zr) \begin{pmatrix} G \\ 0 \\ igY_0 \\ igY_1 \end{pmatrix} \qquad (14)$$

where $G = \sqrt{1+\gamma}$, $g = \sqrt{1-\gamma}$, $Y_0 = \cos(\theta)$ and $Y_1 = \sin(\theta)\exp(i\phi)$. The normalization factor is given by $N = \frac{(2Z)^{\gamma+\frac{1}{2}}}{\sqrt{8\pi\Gamma(2\gamma+1)}}$ where $\gamma = [1-(Z\alpha)^2]^{\frac{1}{2}}$. Here $\alpha \approx \frac{1}{137.03600}$ is the fine-structure constant. In the limit $Z \to 0$ or $c \to \infty$ [remembering that in atomic units $\alpha = 1/c$] it follows that $\gamma \to 1$ and we obtain the nonrelativistic wavefunction $\sqrt{\frac{Z^3}{\pi}}\exp(-Zr)$.

The ground state position wavefunction yields the position density

$$\rho_R(r) = \frac{(2Z)^{2\gamma+1}}{4\pi\Gamma(2\gamma+1)} r^{2(\gamma-1)} \exp(-2Zr) \ . \qquad (15)$$

In the extreme relativistic limit $Z \rightarrow \frac{1}{\alpha}$ the position density obtains the form [41]

$$\rho_{ER}(r) = \frac{1}{2\pi\alpha} r^{-2} \exp\left(-\frac{2r}{\alpha}\right) .$$

Using the relativistic wavefunction Ψ_D, eq. (14), we obtain

$$< r >_R = \frac{2\gamma + 1}{2Z}$$

and

$$< r^2 >_R = \frac{(\gamma+1)(2\gamma+1)}{2Z^2} \approx < r^2 >_{NR} - \frac{1}{Z^2}\left(\frac{7}{4}(\alpha Z)^2 + \frac{3}{16}(\alpha Z)^4 + \cdots\right) .$$

hence,

$$(\delta r) = \frac{\sqrt{2\gamma+1}}{2Z} .$$

For future reference we define the ratio $\beta \equiv \sqrt{\frac{< r^2 >_R}{< r^2 >_{NR}}}$, which is plotted in Fig. 1. Evaluating $< p_r >_R = 0$ and

$$< p_r^2 >_R = \frac{Z^2}{2\gamma - 1} \approx < p_r^2 >_{NR} + Z^2\left((\alpha Z)^2 + \frac{5}{4}(\alpha Z)^4 + \cdots\right) \tag{16}$$

it follows that $(\delta p_r) = \frac{Z}{\sqrt{2\gamma - 1}}$. Hence,

$$(\delta r)(\delta p_r) = \frac{1}{2}\sqrt{\frac{2\gamma+1}{2\gamma-1}} .$$

A singularity is observed for $2\gamma - 1 = 0$, that yields $Z = \frac{\sqrt{3}}{2\alpha} \approx 118.68$. We do not know what significance to assign to this nuclear charge.

Since the small components of the Dirac wavefunction for the hydrogen atom depend on the angular coordinates, the expectation value of the Laplacian is not the same as that of $\mathcal{L}_r$, in spite of the fact that the ground state density is spherically symmetric. The angular part of the Laplacian yields

$$< \Psi_D|\frac{1}{r^2}\hat{L}^2|\Psi_D >=$$

$$= \int_0^\infty N^2 r^{2(\gamma-1)} \exp(-2Zr)dr \left\langle \left(G,\ 0,\ -igY_0,\ -ig\overline{Y_1}\right)\left|\hat{L}^2\right| \begin{pmatrix} G \\ 0 \\ igY_0 \\ igY_1 \end{pmatrix} \right\rangle =$$

$$= 4Z^2 \frac{1-\gamma}{2\gamma(2\gamma-1)} \ .$$

Adding the value of $< \Psi_D|p_r^2|\Psi_D >$, eq. 16, we obtain

$$< \Psi_D| -\nabla^2|\Psi_D >= \frac{2-\gamma}{\gamma(2\gamma-1)} Z^2 \ . \tag{17}$$

The singularity at $Z \approx 118.68$ remains

B. Relativistic momentum uncertainty

We use the expression for the relativistic ground state momentum wavefunction due to Sheth [33]. Denoting the radial momentum variable by p and defining

$$x = (\gamma+1)\arctan(\frac{p}{Z}) \ , \tag{18}$$

the momentum density can be written in the form

$$\Pi_R(p) = \frac{\Gamma(\gamma+1)}{2Z^3\pi^{\frac{3}{2}}\Gamma(\gamma+\frac{1}{2})} \frac{F(p)}{(\frac{p}{Z})^2\left((\frac{p}{Z})^2+1\right)^{\gamma+1}}$$

where

$$F(p) = (\gamma+1)\sin^2(x) + \frac{1-\gamma}{\gamma^2}R(p)^2 \tag{19}$$

and $R(p) = (\gamma+1)\cos(x) - \frac{Z}{p}\sin(x)$. Γ is the familiar Γ-function.

In the nonrelativistic limit $\gamma \to 1$ this expression reduces to $\Pi_{NR}(p)$, *cf.* eq. (13).

In the extreme relativistic limit, $Z \to \frac{1}{\alpha}$, the momentum density is obtained by using

L'Hôpital's rule to evaluate $\lim_{\gamma\to 0}\frac{R}{\gamma}=\left.\frac{\partial R}{\partial\gamma}\right|_{\gamma=0}$. It is found to be of the form

$$\Pi_{ER}(p)=\frac{\alpha^3}{2\pi^2}\frac{1}{[\alpha p(1+(\alpha p)^2)]^2}\left[(\alpha p)^2+\left(1-(\alpha p+\frac{1}{\alpha p})\arctan(\alpha p)\right)^2\right]. \qquad (20)$$

The long range decay of the momentum density can be established by noting that for $p\to\infty$

$$\frac{1}{\left(\frac{p}{Z}\right)^2\left(\left(\frac{p}{Z}\right)^2+1\right)^{\gamma+1}}\approx\left(\frac{Z}{p}\right)^{(2\gamma+4)}.$$

Furthermore,

$$x\approx(\gamma+1)\frac{\pi}{2},$$

so that

$$F\approx F_\infty\equiv(\gamma+1)\left(1+\frac{1-2\gamma^2}{\gamma^2}\cos^2\left((\gamma+1)\frac{\pi}{2}\right)\right).$$

To evaluate $<p^2>$ we integrate over p numerically between $p=0$ and $p=p_m$, where p_m is chosen large enough for the density to be close enough to its asymptotic form, and add an integral over the asymptotic momentum density between $p=p_m$ and $p=\infty$. Hence,

$$<p^2>_R=4\pi\int_0^{p_m}\Pi_R(p)p^4dp+\frac{2\Gamma(\gamma+1)}{\sqrt{\pi}\Gamma(\gamma+\frac{1}{2})}Z^{2\gamma+1}F_\infty\frac{p_m^{-(2\gamma-1)}}{2\gamma-1}.$$

The ratio $\mu\equiv\sqrt{\frac{<p^2>_R}{<p^2>_{NR}}}$ is plotted in Fig. 1. The expectation value $<p^2>_R$ was evaluated for the values of Z considered by Qiang and Dong [34]. The results agree with those evaluated analytically by using the position space expectation value of the Laplacian, eq. (17), for $Z=1,\ 11,\ 37$, to ten decimal places, and for $Z=87$ to eight decimal places. The values of $\sqrt{<p_r^2>}$, evaluated in terms of the ground-state wavefunction in the position representation, using Eq. (16) , agree with the values of $(\Delta p_r)_R$ in [34]. It would be nice to show analytically that $<p^2>$ is indeed equal to the right hand side of Eq. (17).

The results presented above clearly expose the difference between the self-adjoint Laplacian and the non-self adjoint radial momentum.

IV. SHANNON ENTROPIES FOR THE HYDROGEN ATOM

A. Nonrelativistic position and momentum entropies

The nonrelativistic position entropy $S_r^{NR} = -\int_0^\infty 4\pi r^2 \rho_{NR}(r) \log\Big(\rho_{NR}(r)\Big) dr$ can be easily evaluated for the hydrogenic nonrelativistic ground state position density, yielding

$$S_r^{NR} = 3 + \log(\pi) - 3\log(Z) \approx 4.1447299 - 3\log(Z)\ . \tag{21}$$

Similarly, the nonrelativistic momentum entropy $S_p^{NR} = \int_0^\infty 4\pi p^2 \Pi_{NR}(p) \log\Big(\Pi_{NR}(p)\Big) dp$ can be evaluated for the hydrogenic nonrelativistic ground state momentum density, yielding

$$S_p^{NR} = -\frac{10}{3} + 5\log(2) + 2\log(\pi) + 3\log(Z) \approx 2.4218623 + 3\log(Z)\,. \tag{22}$$

It follows that

$$\begin{aligned} S_r^{NR} + S_p^{NR} &= -\frac{1}{3} + 5\log(2) + 3\log(\pi) \approx 6.5665922 \\ &> 3(1+\log(\pi)) \approx 6.4341897\ . \end{aligned}$$

B. Shannon length and impetus

Since $\exp(S_r)$ has dimensions of volume, we define the Shannon length R_S via

$$\frac{4\pi}{3} R_S^3 = \exp(S_r)\,.$$

We similarly define the Shannon impetus P_S via

$$\frac{4\pi}{3} P_S^3 = \exp(S_p)\,.$$

For the nonrelativistic hydrogen atom we obtain

$$R_S^{NR} = \left(\frac{3}{4}\right)^{\frac{1}{3}} \frac{e}{Z} \approx \frac{2.46972}{Z}$$

and

$$P_S^{NR} = 2(3\pi)^{\frac{1}{3}} \exp(-\frac{10}{9}) Z \approx 1.39071 Z\,,$$

hence,

$$R_S^{NR} P_S^{NR} \approx 3.43466$$

From the entropic uncertainty-like relation

$$S_r + S_p \geq 3(1 + \ln(\pi))$$

it follows that

$$R_S P_S \geq \left(\frac{3}{4\pi}\right)^{\frac{2}{3}} \pi e \approx 3.28639\,.$$

This lower bound is, indeed, lower than the product of the hydrogenic Shannon length and impetus, but fairly close to it.

C. Relativistic position entropy

The position entropy can be evaluated analytically in terms of the relativistic ground state position density, eq. (15), to yield

$$S_r^R = \log\left(\frac{\pi\Gamma(2\gamma+1)}{2Z^3}\right) + (2\gamma+1) - 2(\gamma-1)\Psi(2\gamma+1) \tag{23}$$

where $\Psi(z)$ is the Digamma function, defined as $\Psi(z) = \frac{d\log(\Gamma(z))}{dz}$.

In the nonrelativistic limit $\gamma = 1$ so $\Gamma(2\gamma+1) = \Gamma(3) = 2$ and S_r^R reduces to S_r^{NR}, eq. 21.

The relativistic correction is

$$S_r^R - S_r^{NR} = 2(\gamma-1)(1-\Psi(2\gamma+1)) + \log\left(\frac{\Gamma(2\gamma+1)}{2}\right) \approx -(\alpha Z)^2 + \left(\frac{3}{8} - \frac{\pi^2}{12}\right)(\alpha Z)^4 + \cdots\,. \tag{24}$$

In the extreme relativistic limit

$$S_r = \log\left(\frac{\pi\alpha^3}{2}\right) - 2C + 1 \approx -14.463580 \tag{25}$$

where $C = 0.5772156649..$ is Euler's constant (more commonly denoted γ, a notation we avoid for an obvious reason).

D. Relativistic momentum entropy

The relativistic momentum entropy was evaluated by means of numerical integration. To examine the relativistic corrections to the position and momentum entropies more closely, we consider $\sigma_r \equiv \frac{S_r^R - S_r^{NR}}{(\alpha Z)^2}$ and $\sigma_p \equiv \frac{S_p^R - S_p^{NR}}{(\alpha Z)^2}$. Eq. 24 yields $\sigma_r \approx -1 - 0.4475(\alpha Z)^2 + \cdots$ and a numerical fit yields $\sigma_p \approx 1.80 + 0.65(\alpha Z)^2 + \cdots$, so $\sigma_r + \sigma_p \approx 0.80 + 0.2(\alpha Z)^2 + \cdots$.

E. Relativistic Shannon length and impetus

For the relativistic Shannon length we obtain

$$R_S^R = \frac{1}{2Z}\Big(3\Gamma(2\gamma+1)\Big)^{\frac{1}{3}} \exp\left[1 + \frac{2}{3}(\gamma-1)\Big(1 - \Psi(2\gamma+1)\Big)\right] .$$

Hence,

$$\beta_S \equiv \frac{R_S^R}{R_S^{NR}} = \left(\frac{\Gamma(2\gamma+1)}{2}\right)^{\frac{1}{3}} \exp\left[\frac{2}{3}(\gamma-1)\Big(1 - \Psi(2\gamma+1)\Big)\right] \approx 1 - \frac{1}{3}(\alpha Z)^2 + \cdots .$$

The ratio of the relativistic and nonrelativistic Shannon impeti can be obtained in terms of the numerically determined σ_p, as follows,

$$\mu_S \equiv \frac{P_S^R}{P_S^{NR}} = \exp\left[\frac{(\alpha Z)^2}{3}\sigma_p\right] \approx 1 + 0.60(\alpha Z)^2 + \cdots .$$

Hence,

$$\beta_S \mu_S \approx 1 + 0.27(\alpha Z)^2 + \cdots . \tag{26}$$

In Fig. 1 we present the ratios of the relativistic to nonrelativistic Shannon lengths and impeti, along with the corresponding ratios of the root mean square radius and momentum, and that of the Fisher lengths and impeti (to be discussed below). We note that for large Z the relativistic effect on the momentum uncertainty measures is larger than on their position counterparts. This is most pronounced for the root mean square position and momentum, whereas the relativistic effects on the Fisher measures are almost symmetrical. This is most likely due to the fact that the Fisher measures are sensitive to the local oscillations of the distribution rather than to its long range behavior, where the relativistic momentum distribution varies the most.

V. FISHER INFORMATION MEASURES FOR THE HYDROGEN ATOM

The Fisher position information measure, $I_r = \int_0^\infty 4\pi r^2 \frac{1}{\rho(r)} \left(\frac{d\rho}{dr}\right)^2 dr$ can be easily evaluated for the ground state of the relativistic hydrogen-like atom, yielding

$$I_r^R = \frac{4Z^2}{2\gamma - 1} = 4 < p_r^2 > \approx I_r^{NR} \left(1 + (\alpha Z)^2 + \frac{5}{4}(\alpha Z)^4 + \frac{13}{8}(\alpha Z)^6 + \cdots \right) ,$$

where $I_r^{NR} = 4Z^2$. Since I_r^R has a singularity when $2\gamma - 1 = 0$, *i. e.*, at $Z \approx 118.68$, we do not examine the extreme relativistic limit.

The Fisher momentum information measure $I_p = \int_0^\infty 4\pi p^2 \frac{1}{\Pi(p)} \left(\frac{d\Pi}{dp}\right)^2 dp$ for the nonrelativistic momentum distribution can be evaluated analytically, yielding $I_p^{NR} = \frac{12}{Z^2}$. For the relativistic momentum density the Fisher information was evaluated numerically.

A. Fisher length and impetus

The Fisher position information measure I_r has dimensions of inverse area. We define the Fisher length as $R_F = I_r^{-\frac{1}{2}}$. Similarly, we define the Fisher impetus $P_F = I_p^{-\frac{1}{2}}$. For the nonrelativistic hydrogen atom we obtain $R_F^{NR} = \frac{1}{2Z}$ and $P_F^{NR} = \frac{Z}{\sqrt{12}}$. The ratio between the relativistic and the nonrelativistic Fisher lengths is

$$\beta_F \equiv \frac{R_F^R}{R_F^{NR}} = (2\gamma - 1)^{\frac{1}{2}} \approx 1 - \frac{1}{2}(\alpha Z)^2 - \frac{1}{4}(\alpha Z)^4 + \cdots ,$$

The corresponding ratio of Fisher impeti is evaluated by fitting the numerically evaluated ratios to obtain

$$\mu_F \equiv \frac{P_F^R}{P_F^{NR}} \approx 1 + 0.4166(\alpha Z)^2 + 0.23(\alpha Z)^4 + \cdots ,$$

hence,

$$\beta_F \mu_F \approx 1 - 0.0834(\alpha Z)^2 + \cdots . \tag{27}$$

We note that the leading relativistic term is negative, unlike the corresponding term for the product of Shannon length and impetus, eq. 26.

The ratios of the relativistic to nonrelativistic Fisher lengths and impeti are presented in Fig. 1.

VI. RÉNYI ENTROPIES FOR THE HYDROGEN ATOM

A. Rényi position entropies

The Rényi position entropy is defined in eq. 6. The hydrogenic nonrelativistic ground state position density yields

$$H_a^{(r,NR)} = \log\left(\frac{\pi}{Z^3}\right) + 3\frac{\log(a)}{a-1} \ . \tag{28}$$

For $a \to 1$ this expression reduces to $H_1^{(r,NR)} = \log\left(\frac{\pi}{Z^3}\right) + 3$, which is the well-known hydrogenic Shannon position entropy. Substituting in eq. 7 we obtain

$$\mathcal{H}_s^{(r,NR)} = \log\left(\frac{\pi}{Z^3}\right) + \frac{3}{2s}\log\left(\frac{(1+s)^{1+s}}{(1-s)^{1-s}}\right) \ .$$

The hydrogenic relativistic ground state position density yields

$$\begin{aligned} H_a^{(r,R)} &= \log\left(\frac{\pi\Gamma(2\gamma+1)}{2Z^3}\right) + 2(\gamma-1)\log(a) \\ &+ \frac{1}{1-a}\left[\log\left(\frac{\Gamma\Big(2(\gamma-1)a+3\Big)}{\Gamma(2\gamma+1)}\right) - (2\gamma+1)\log(a)\right] \ . \end{aligned} \tag{29}$$

This expression is finite when the argument of the Γ-function satisfies $2(\gamma-1)a+3>0$. This condition can easily be traced back to the singularity of the relativistic density at the origin, cf. eq. 15. Since $0 \le \gamma \le 1$, this condition holds for all Z when $a \le \frac{3}{2}$. For $a > \frac{3}{2}$ divergence will take place when $Z \ge \frac{\sqrt{3(4a-3)}}{2a\alpha}$. For $\gamma = 1$ eq. 29 reduces to eq. 28. In the limit $a \to 1$ we obtain the relativistic Shannon entropy, eq. 23. For $\gamma \to 0$ this expression yields S_r^{ER}.

The relativistic correction $\Delta H_a^{(r)} = H_a^{(r,R)} - H_a^{(r,NR)}$ can be expanded in the form

$$\begin{aligned} \Delta H_a^{(r)} &= \log\left(\frac{\Gamma(2\gamma+1)}{2}\right) + 2(\gamma-1)\frac{a\log(a)}{a-1} - \frac{1}{a-1}\log\left(\frac{\Gamma(3+2a(\gamma-1))}{\Gamma(2\gamma+1)}\right) \\ &= -\frac{a\log(a)}{a-1}\left((\alpha Z)^2 + (\alpha Z)^4/4 + \cdots\right) + a\left(\frac{5}{8} - \frac{\pi^2}{12}\right)(\alpha Z)^4 + \cdots \end{aligned}$$

Using this expansion we obtain

$$\Delta\mathcal{H}_s^{(r)} = -\frac{1}{2s}\log\left(\frac{1+s}{1-s}\right)\left((\alpha Z)^2 + (\alpha Z)^4/4 + \cdots\right) + \frac{1}{1-s^2}\left(\frac{5}{8} - \frac{\pi^2}{12}\right)(\alpha Z)^4 + \cdots$$

In the extreme relativistic limit

$$H_a^{(r,ER)} = \log\left(\frac{\pi\alpha^3}{2}\right) + \frac{1}{1-a}\log\left(\frac{\Gamma(3-2a)}{a^{3-2a}}\right) . \tag{30}$$

Eq. 30 can also be obtained from eq. 29, by taking the limit $\gamma \to 0$. For $a \to 1$ this expression yields eq. 25.

The results presented above imply the commutativity of the diagram

$$\begin{array}{ccccc} \rho_{NR}(r) & \Longrightarrow & H_a^{(r,NR)} & \longrightarrow & S_r^{NR} \\ \uparrow & & \uparrow & & \uparrow \\ \rho_R(r) & \Longrightarrow & H_a^{(r,R)} & \longrightarrow & S_r^{R} \\ \downarrow & & \downarrow & & \downarrow \\ \rho_{ER}(r) & \Longrightarrow & H_a^{(r,ER)} & \longrightarrow & S_r^{ER} \end{array}$$

where

$$\begin{array}{cl} \uparrow & \text{stands for } \lim_{\gamma\to 1} \\ \downarrow & \text{stands for } \lim_{\gamma\to 0} \\ \longrightarrow & \text{stands for } \lim_{a\to 1} \end{array}$$

and

$$X(r) \Longrightarrow Y \ \text{ stands for } Y = \frac{1}{1-a}\int_0^\infty 4\pi r^2 [X(r)]^a dr\,,$$

i.e., the fact that whenever more than one path (respecting the directions of the various arrows) is available between any two nodes, the results along the different paths are identical.

B. Rényi length

Noting that $\exp(H_a^{(r)})$ has dimensions of volume we define the Rényi length R_a via the relation

$$\frac{4\pi}{3}R_a^3 = \exp(H_a^{(r)})\,.$$

It follows that

$$R_a^{NR} = \left(\frac{3}{4}\right)^{\frac{1}{3}} \frac{1}{Z} a^{\frac{1}{a-1}}\,.$$

and

$$\lim_{a\to 1} R_\alpha^{NR} = \left(\frac{3}{4}\right)^{\frac{1}{3}} \frac{e}{Z} = R_S^{NR}\,.$$

Similarly,

$$R_a^R = \left(\frac{3\Gamma(2\gamma+1)}{8}\right)^{\frac{1}{3}} \frac{1}{Z} a^{-\frac{2a(\gamma-1)+3}{3(1-a)}} \left(\frac{\Gamma(2a(\gamma-1)+3)}{\Gamma(2\gamma+1)}\right)^{\frac{1}{3(1-a)}}\,,$$

yielding R_a^{NR} in the limit $\gamma \to 1$.

C. Rényi momentum entropies

The hydrogenic nonrelativistic ground state Rényi momentum entropy is

$$H_b^{(p,NR)} = \log\left(\frac{\pi^2 Z^3}{8}\right) + \frac{1}{1-b}\log\left(I(b)\right)\,, \tag{31}$$

where,

$$I(b) = \frac{32}{\pi}\int_0^\infty (y^2+1)^{-4b} y^2 dy = \frac{8}{\sqrt{\pi}} \frac{\Gamma\left(4b-\frac{3}{2}\right)}{\Gamma(4b)}\,. \tag{32}$$

The dependence of $H_a^{(r,NR)}$, eq. 28, and $H_b^{(p,NR)}$, eq. 31, on the nuclear charge Z is such that the sum, for any choice of a and b, is independent of Z, as demonstrated above for arbitrary homogeneous potentials.

Noting that $I(1) = 1$ we obtain, for $b \to 1$, the nonrelativistic Shannon momentum entropy, eq. 22.

The nonrelativistic momentum density behaves, at large p, as $\Pi_{NR}(p) \sim \frac{1}{p^8}$, so that the integral in $H_b^{(p,NR)}$ diverges unless $8b-2>1$, or $b>\frac{3}{8}$. Indeed, for $b=\frac{3}{8}$ the numerator of eq. 32 vanishes. Note, however, that this value of b is below the lower bound $b > \frac{1}{2}$ allowing the definition of the symmetrized Rényi entropy, eq. 7.

The extreme relativistic momentum density, eq. 20, behaves, for $p \to \infty$, like

$$\Pi_{ER}(p) \sim \frac{1}{p^4} ,$$

so that the integral in the expression for $H_b^{(p,ER)}$ behaves like $\frac{1}{p^{4b-2}}$. Hence, the integral diverges unless $4b - 2 > 1$ or $b > \frac{3}{4}$.

The behavior of the relativistic momentum density is more subtle. For $p \to \infty$ the variable x, defined in eq. 18, satisfies $x \to (\gamma + 1)\frac{\pi}{2}$. As long as $\gamma < 1$ one finds that $F(p)$, defined by eq. 19, becomes a (γ dependent) constant, so that for large p the relativistic momentum density decays as $\Pi_R(p) \sim \frac{1}{p^{2\gamma+4}}$. It follows that the integrand in the expression for $H_b^{(p,R)}$ converges provided that $(2\gamma + 4)b - 2 > 1$ or $b > \frac{3}{2\gamma+4}$. For $\gamma = 0$ this expression yields $b > \frac{3}{4}$, in agreement with the result obtained above for the extreme relativistic momentum density, but for $\gamma = 1$ this expression yields $b > \frac{1}{2}$, which is larger than the bound $b > \frac{3}{8}$ obtained above for the nonrelativistic momentum density. This is a consequence of the fact that by taking the limit $\gamma \to 1$ before the limit $p \to \infty$ one obtains $F = 8\frac{p^2}{(1+p^2)^2}$, that for large p yields $F \approx \frac{8}{p^2}$ rather than the constant obtained when the limits over γ and p are taken in the opposite order. Since $0 \le \gamma \le 1$, it follows that for $b > \frac{3}{4}$ the Rényi entropy converges for all Z, for $b < \frac{1}{2}$ it diverges for all Z, and for $\frac{1}{2} < b < \frac{3}{4}$ it converges for $Z < \frac{3}{2\alpha}\sqrt{(2 - \frac{1}{b})(\frac{1}{b} - \frac{2}{3}}$. Substituting $b = \frac{1}{2-\frac{1}{a}}$ we obtain $Z < \frac{\sqrt{3(4a-3)}}{2a\alpha}$. Comparing with the results obtained above for $H_a^{(r,R)}$ we conclude that $H_a^{(r,R)}$ and $H_b^{(p,R)}$ converge over the same range of Z when a and b are related via $\frac{1}{a} + \frac{1}{b} = 2$.

The relativistic Rényi momentum entropies can only be obtained numerically. The main point to note is that the various sums of Rényi position and momentum entropies exhibit a dependence on Z, unlike the nonrelativistic case. In Fig. 3 we show the sum of the Rényi position and momentum entropies, $H_a^{(r)} + H_b^{(p)}$, where $a = \frac{1}{1-s}$ and $b = \frac{1}{1+s}$, vs. s. The lowest curve corresponds to the lower bound presented in eq. 8, and the curve just above it is the nonrelativistic entropy sum. The relativistic entropy sums are all higher than the nonrelativistic one, exhibiting a rapid increase for higher s values. This behavior anticipates the approaching singularity of the relativistic Rényi momentum entropy for an appropriate value of $s > \frac{1}{3}$, that decreases with increasing Z, as clearly displayed in Fig. 3. Thus, for

$Z = 100$ the Rényi momentum entropy becomes singular for $s = \frac{2\gamma+1}{3} \approx 0.789$.

D. Rényi impetus

The relation

$$\frac{4\pi}{3} P_b^3 = \exp(H_b^{(p)})$$

defines the Rényi impetus P_a. It follows that

$$P_b^{NR} = \left(\frac{3\pi}{4}\right)^{\frac{1}{3}} \frac{Z}{2} \left(\frac{8}{\sqrt{\pi}} \frac{\Gamma(4b - \frac{3}{2})}{\Gamma(4b)}\right)^{\frac{1}{3(1-b)}} .$$

In the limit $b \to 1$ this expression yields the nonrelativistic Shannon impetus.

The relativistic Rényi impeti can be obtained from the numerically evaluated Rényi momentum entropies.

From the uncertainty-like relation for the Rényi entropies, eq. 8, it follows that the length-impetus product satisfies

$$R_a P_b \geq \left(\frac{9\pi}{16}\right)^{\frac{1}{3}} a^{\frac{1}{2(a-1)}} b^{\frac{1}{2(b-1)}} . \tag{33}$$

where $\frac{1}{a} + \frac{1}{b} = 2$.

The ratios of the relativistic to nonrelativistic Rényi lengths (β_R) and impeti (μ_R) are presented in Fig. 2 for conjugate pairs $(a, b) = \left\{(\frac{5}{8}, \frac{5}{2}), (\frac{3}{4}, \frac{3}{2}), (\frac{7}{8}, \frac{7}{6}), (\frac{7}{6}, \frac{7}{8}), (\frac{3}{2}, \frac{3}{4}), (\frac{5}{2}, \frac{5}{8})\right\}$. Like the Shannon measures presented in Fig. 1, the Rényi impeti show a more pronounced relativistic effect than the corresponding lengths. The relativistic effect on the Rényi impeti increases with increasing b; the relativistic effect on the corresponding lengths (that correspond to decreasing a, satisfying $\frac{1}{a} + \frac{1}{b} = 2$) also increases, but more moderately.

E. Average position and momentum densities

The average position density is defined as

$$< \rho >= \int_0^\infty 4\pi r^2 \Big(\rho(r)\Big)^2 dr \, .$$

While closely related to the 2-Rényi entropy, i.e., $<\rho>=\exp\left(-H_2^{(r)}\right)$, the average position density merits special attention since it has recently been invoked as a factor in a proposed measure of complexity [42, 43]. The average density is also known as the Onicescu information measure [44], and is closely related to the linear entropy $\epsilon_r = 1 - <\rho>$, which is the $q = 2$ case of the Tsallis entropy [30].

For the hydrogen atom

$$<\rho_{NR}>=\frac{Z^3}{8\pi}\,,$$

and

$$<\rho_R>=\frac{Z^3\Gamma(4\gamma-1)}{\pi 2^{4\gamma-2}(\Gamma(2\gamma+1))^2}\,.$$

The relativistic expression becomes singular when $4\gamma - 1 = 0$, *i.e.* $Z = \frac{\sqrt{15}}{4\alpha} \approx 132.68$. The onset of relativistic effects is given by $\frac{<\rho_R>-<\rho_{NR}>}{Z^3} \approx 0.055159(\alpha Z)^2 + 0.067737(\alpha Z)^4 + 0.079452(\alpha Z)^6 + \cdots$.

The momentum density expectation value $<\Pi>=\int_0^\infty 4\pi p^2\Big(\Pi(p)\Big)^2 dp$ for the nonrelativistic density was evaluated analytically, yielding $<\Pi_{NR}>=\frac{33}{16\pi^2 Z^3} \approx \frac{0.208975}{Z^3}$. The relativistic counterpart, $<\Pi_R>$, can only be evaluated numerically.

The leading terms in the Taylor series expansion of $Z^3(<\Pi_R> - <\Pi_{NR}>)$ were obtained by differentiating the integrand, $Z^3 4\pi p^2\Big((\Pi_R(p))^2 - (\Pi_{NR}(p))^2\Big)$, with respect to αZ, an appropriate number of times, evaluating it at $Z = 0$, and integrating over p. In this way we obtain

$$Z^3(<\Pi_R> - <\Pi_{NR}>) \approx -0.254464(\alpha Z)^2 + 0.054446(\alpha Z)^4 + 0.001883(\alpha Z)^6 + \cdots\ .$$

or

$$\frac{<\Pi_R>}{<\Pi_{NR}>} \approx 1 - 1.21768(\alpha Z)^2 + 0.26054(\alpha Z)^4 + 0.00901(\alpha Z)^6 + \cdots\ .$$

F. Average length and impetus

Noting that $<\rho>$ has dimensions of inverse volume we define the average length R_A via

$$\frac{4\pi}{3}R_A^3 =<\rho>^{-1}\ .$$

Similarly, the average impetus P_A is defined via

$$\frac{4\pi}{3} P_A^3 =< \Pi >^{-1} \ .$$

As a consequence of the connection between the average entropy and the 2-Rényi entropy $H_2^{(r)}$ the lengths and impeti related to these two information measures coincide. For the nonrelativistic hydrogen atom we obtain

$$R_A^{NR} = \frac{6^{\frac{1}{3}}}{Z} \approx \frac{1.81712}{Z}$$

and

$$P_A^{NR} = Z \left(\frac{4\pi}{11} \right)^{\frac{1}{3}} \approx 1.04538 Z \, .$$

Furthermore

$$\frac{R_A^R}{R_A^{NR}} \approx 1 - 0.46210(\alpha Z)^2 - 0.14040(\alpha Z)^4 - 0.07719(\alpha Z)^6 + \cdots ,$$

and

$$\frac{P_A^R}{P_A^{NR}} \approx 1 + 0.40589(\alpha Z)^2 + 0.24265(\alpha Z)^4 + 0.16806(\alpha Z)^6 + \cdots ,$$

hence,

$$\frac{(R_A P_A)^R}{(R_A P_A)^{NR}} \approx 1 - 0.0562(\alpha Z)^2 + \cdots .$$

This expression is rather similar to the corresponding ratio for the Fisher length and impetus, eq. 27.

G. Complexity measures

The results presented above concerning the relativistic effects on the various information measures for the H-like atoms allow the evaluation of the *statistical* measure of complexity C, defined by López-Ruiz, Mancini, Calbet (LMC) [42, 43]. The LMC measure C is given by

$$C = H \cdot D \ , \tag{34}$$

where H denotes a measure of information and D represents the so called disequilibrium or the distance from equilibrium (most probable state). The form of C is designed such that it vanishes for the two extreme probability distributions corresponding to perfect order ($H = 0$) and maximum disorder ($D = 0$), respectively. It is only very recently [45, 46, 47, 48], that the studies on the electronic structural complexity of *neutral* atoms using the non-relativistic Hartree-Fock (HF) wave functions [49] for atoms with atomic number Z=1-54, have been reported using a variety of information measures. A similar evaluation of a complexity measure for neutral atoms with Z=1-103 was recently carried out in terms of the Dirac-Fock wavefunction, choosing the exponential of the Shannon position entropy as the measure of information, $H = \exp(S_r)$, and the average position density as the measure of disequilibrium, $D =< \rho >$ [9]. While the measure of information exhibits a strong shell effect but insignificant relativistic effect, the measure of disequilibrium was found to be a monotonically increasing function of Z exhibiting a strong relativistic effect. It is remarkable that the ratio of the relativistic to the nonrelativistic measures of disequilibrium (average position densities) obtained for neutral many-electron atoms is in almost quantitative agreement with the corresponding ratio obtained in terms of the average position densities evaluated above for the single electron ions. These ratios are presented in Fig. 4. This observation must be a manifestation that the relativistic effect on the measure of disequilibrium is dominated by the effect on the innermost orbital.

VII. SCALE INVARIANT ENTROPIES

A. Residual position and momentum entropies

The Kullback-Leibler relative/residual information measure of a given probability density is defined with respect to a prior density and it determines the extra information contained in the given density relative to the prior. Such a residual entropy for the relativistic density over the nonrelativistic density as the prior can be defined in both the position and the momentum space. In position space this can be done analytically, yielding

$$
\begin{aligned}
S_r^{R/NR} &= \int_0^\infty 4\pi r^2 \rho_R(r) \log\left(\frac{\rho_R(r)}{\rho_{NR}(r)}\right) dr \\
&= \log\left(\frac{2}{\Gamma(2\gamma+1)}\right) + (\gamma-1)\left(2\Psi(2\gamma)+\frac{1}{\gamma}\right) \\
&\approx 0.197467(\alpha Z)^4 + 0.150105(\alpha Z)^6 + 0.115104(\alpha Z)^8 + \cdots
\end{aligned} \tag{35}
$$

The Taylor series for $S_r^{R/NR}$ was obtained by evaluating its first six derivatives with respect to Z, using maple. The values of $S_r^{R/NR}$ for $Z < 25$ were calculated using the three-term Taylor series, since evaluating the analytic expression involves cancellation errors. We note that for $Z = 25$ the analytic expression and the three-term expansion practically coincide.

The extreme relativistic value is obtained from eq. (35) by evaluating its limit as $\gamma \to 0$. It is found that $S_r^{R/NR} = \log(2) + 2C \approx 1.847579$.

The residual momentum entropy $S_p^{R/NR} = \int_0^\infty 4\pi p^2 \Pi_R(p) \log\left(\frac{\Pi_R(p)}{\Pi_{NR}(p)}\right) dp$ was evaluated numerically. Differentiating the integrand four times with respect to Z and integrating numerically we obtained the leading term in the power series expansion $S_p^{R/NR} \approx 0.572467(\alpha Z)^4 + \cdots$.

The value of $\frac{S_p^{R/NR}}{(\alpha Z)^4}$ at $Z = \frac{1}{\alpha}$ was obtained using the extreme relativistic momentum density, eq. (20).

Since $S_r^{R/NR}$ and $S_p^{R/NR}$ are pure (dimensionless) quantities, they do not measure position or momentum widths or uncertainties. They do measure the (somewhat slow) onset of relativistic effects upon increase of the nuclear charge.

B. Average Measures of relative distance

The average measure of relative distance [28, 50] of the position densities is the sum of the two relative entropies

$$
S_r^{R/NR} = \int_0^\infty 4\pi r^2 \rho_R(r) \log\left(\frac{\rho_R(r)}{\rho_{NR}(r)}\right) dr
$$

and

$$
S_r^{NR/R} = \int_0^\infty 4\pi r^2 \rho_{NR}(r) \log\left(\frac{\rho_{NR}(r)}{\rho_R(r)}\right) dr \ .
$$

It can be written in the form

$$\tilde{S}_r = \int_0^\infty 4\pi r^2 \Big(\rho_R(r) - \rho_{NR}(r)\Big) \log\left(\frac{\rho_R(r)}{\rho_{NR}(r)}\right) dr \ .$$

The measure of relative distance of the momentum densities is defined in an analogous manner.

$S_r^{R/NR}$ was evaluated above, *cf.* eq. (35). $S_r^{NR/R}$ can be evaluated in a similar way, yielding

$$S_r^{NR/R} = \log\left(\frac{\Gamma(2\gamma+1)}{2}\right) + (1-\gamma)(3-2C) \ .$$

Hence,

$$\tilde{S}_r = (1-\gamma)\left(3 - 2C - 2\Psi(2\gamma) - \frac{1}{\gamma}\right) \ .$$

The Taylor series for $\tilde{S}_r$ can be obtained analytically. The first three terms are given by

$$\begin{aligned}
\tilde{S}_r \ &\approx \ \left(\frac{\pi^2}{6} - \frac{5}{4}\right)(\alpha Z)^4 + \left(\frac{\pi^2}{12} + \zeta(3) - \frac{7}{4}\right)(\alpha Z)^6 \\
&+ \ \left(\frac{\pi^4}{90} + \frac{5\pi^2}{96} + \frac{3}{4}\zeta(3) - \frac{147}{64}\right)(\alpha Z)^8 + \cdots \\
&\approx \ 0.394934(\alpha Z)^4 + 0.27452(\alpha Z)^6 + 0.20103(\alpha Z)^8 + \cdots
\end{aligned}$$

$\tilde{S}_p$ was evaluated numerically.

The residual (relativistic vs. nonrelativistic) position and momentum entropies, and the average measures of the distances of the corresponding position and momentum distributions, are presented in Table 1, all normalized via division by $(\alpha Z)^4$. We note that $\frac{\tilde{S}_r}{(\alpha Z)^4}$ is a monotonic function of Z, but $\frac{\tilde{S}_p}{(\alpha Z)^4}$ is not.

VIII. CONCLUSIONS

The characterization of inherent quantum mechanical uncertainties has become a rich field of study with direct relevance to emerging technologies. In the present article we examine the application of widely used information measures to the ground state of the relativistic hydrogen-like atoms, clearly bringing out the dependence on Z due to the relativistic effects. Further, we point out and illustrate the well-established but largely ignored difficulties associated with the most common quantum mechanical formulation of the uncertainty principle, that arise as a consequence of the fact that the radial momentum is not self-adjoint. Several information measures exhibit singularities at particular nuclear charges, notably $Z = \frac{\sqrt{3}}{2\alpha} \approx 118.68$ and $Z = \frac{\sqrt{15}}{4\alpha} \approx 132.68$, whose significance remains to be elucidated. In the coordinate representation *all* the information measures considered allowed analytic evaluation of the integrals involved. This has not been the case for the corresponding momentum space quantities. What we find particularly puzzling in this context is the fact that the closed analytic expression for the position-space expectation value of the Laplacian agrees, as expected, with the numerically evaluated average over p^2, in momentum space, and still we failed to evaluate the latter analytically. These, and many other issues such as uncertainty and information measures for excited states as well as for many-electron atoms, suggest that the study of information measures for relativistic systems is a widely open field.

Acknowledgements: It is a great pleasure to dedicate this work to Jesus Dehesa on the ocassion of his sixtieth birthday. We consider it as an extension of his pioneering contribution [6] on the information entropy of non-relativistic hydrogen atom.One of the authors (JK) wishes to thank Professor Ady Mann for a helpful discussion. This author also wishes to thank the School of Chemistry, University of Hyderabad, for its hospitality.KDS acknowledges the financial support received from the Department of Science and Technology, New Delhi.

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TABLE I: Residual entropies and average measures of relative distance.

Z	$\frac{S_r^{R/NR}}{(\alpha Z)^4}$	$\frac{S_p^{R/NR}}{(\alpha Z)^4}$	$\frac{\tilde{S}_r}{(\alpha Z)^4}$	$\frac{\tilde{S}_p}{(\alpha Z)^4}$
1	0.19748		0.39495	1.14237
2	0.19750	0.57129	0.39499	1.13967
5	0.19767	0.56733	0.39530	1.13122
10	0.19827	0.56329	0.39640	1.11703
25	0.20259	0.55744	0.40430	1.08183
50	0.21973	0.57582	0.43545	1.06601
75	0.25602	0.64370	0.50071	1.12751
100	0.33489	0.81215	0.63971	1.33467
$\frac{1}{\alpha}$	1.84758	4.03749	3.000000	5.485774

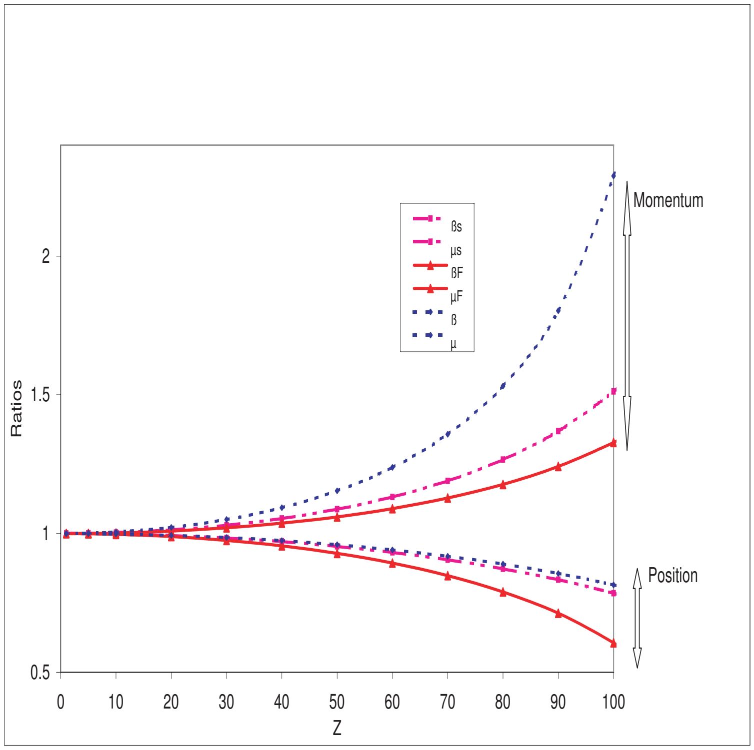

FIG. 1: Ratios between the relativistic and nonrelativistic Shannon and Fisher lengths (β_S, β_F) and impeti (μ_S, μ_F), and corresponding ratios for root mean square of position (β) and momentum (μ) as functions of Z .

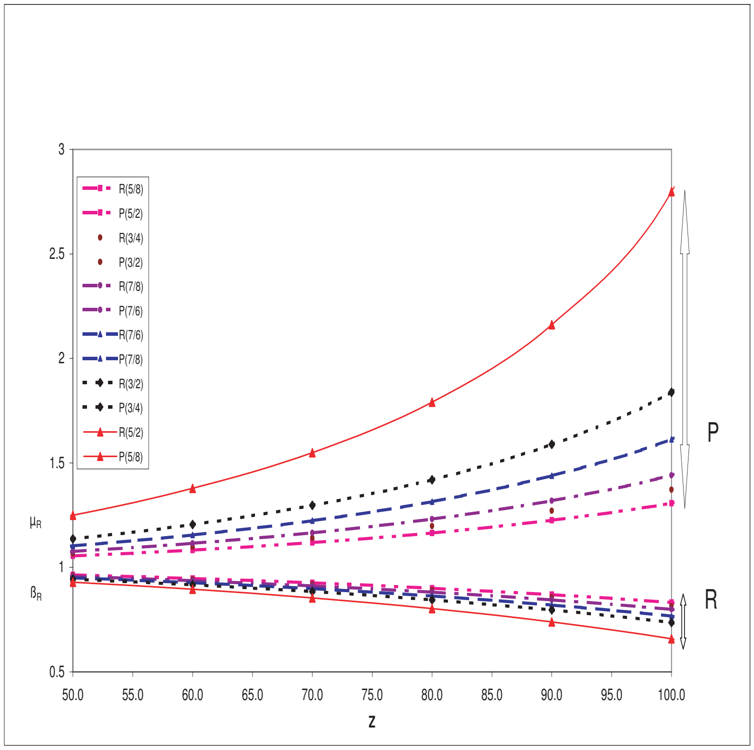

FIG. 2: Ratios between the relativistic and nonrelativistic Rényi lengths (β_R) and impeti (μ_R) as functions of Z.

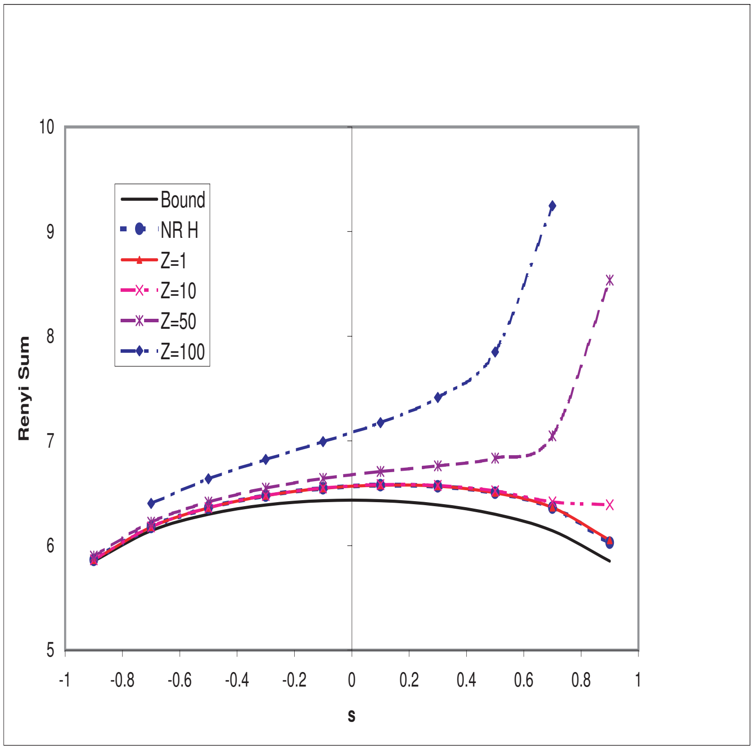

FIG. 3: Rényi sum vs s for the non-relativistic H atom and relativistic H-like atoms.

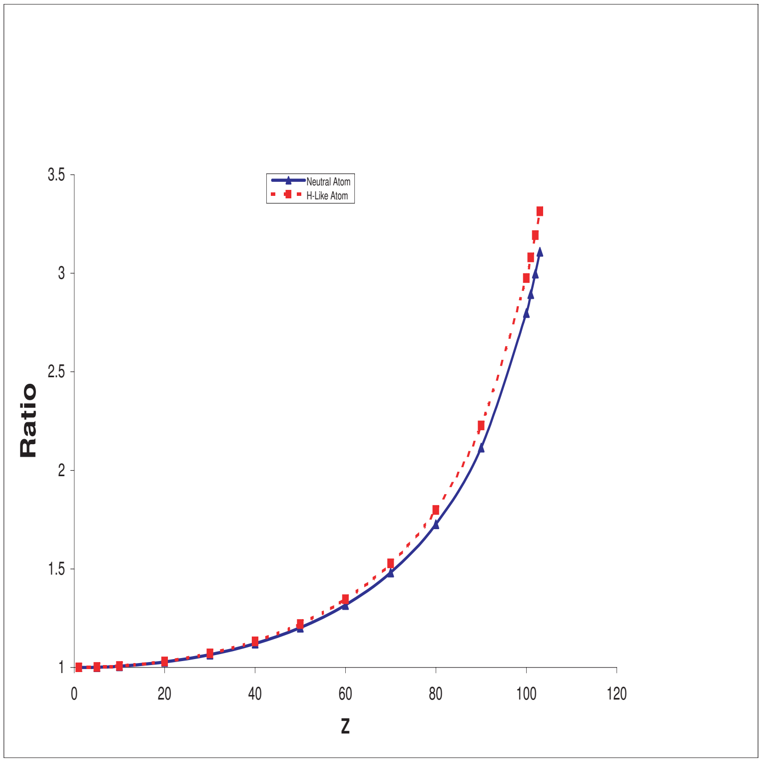

FIG. 4: Ratio of relativistic to non-relativistic estimates of the linear entropy for neutral atoms and H-like atoms.