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Complexity of D-dimensional hydrogenic systems in position and momentum spaces

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ABSTRACT

The internal disorder of a D-dimensional hydrogenic system, which is strongly associated to the non-uniformity of the quantum-mechanical density of its physical states, is investigated by means of the shape complexity in the two reciprocal spaces. This quantity, which is the product of the disequilibrium or averaging density and the Shannon entropic power, is mathematically expressed for both ground and excited stationary states in terms of certain entropic functionals of Laguerre and Gegenbauer (or ultraspherical) polynomials. We emphasize the ground and circular states, where the complexity is explicitly calculated and discussed by means of the quantum numbers and dimensionality. Finally, the position and momentum shape complexities are numerically discussed for various physical states and dimensionalities, and the dimensional and Rydberg energy limits as well as their associated uncertainty products are explicitly given. As a byproduct, it is shown that the shape complexity of the system in a stationary state does not depend on the strength of the Coulomb potential involved.

1. Introduction

The hydrogenic system (i.e., a negatively-charged particle moving around a positively-charged core which electromagnetically binds it in its orbit) with dimensionality $D \geq 1$, plays a central role in D-dimensional quantum physics and chemistry [1,2]. It includes not only a large variety of three-dimensional physical systems (e.g., hydrogenic atoms and ions, exotic atoms, antimatter atoms, Rydberg atoms) but also a number of nanoobjects so much useful in semiconductor nanostructures (e.g., quantum wells, wires and dots) [3,4] and quantum computation (e.g., qubits) [5,6]. Moreover it has a particular relevance for the dimensional scaling approach in atomic and molecular physics [1] as well as in quantum cosmology [7] and quantum field theory [8,9]. Let us also say that the existence of hydrogenic systems with non-standard dimensionalities has been shown for $D < 3$ [4] and suggested for $D > 3$ [10]. We should also highlight the use of D-dimensional hydrogenic wavefunctions as complete orthonormal sets for many-body problems [11,12] in both position and momentum spaces, explicitly for three-body Coulomb systems (e.g. the hydrogen molecular ion and the helium atom); generalizations are indeed possible in momentum-space orbitals as well as in their role as Sturmians in configuration spaces.

The internal disorder of this system, which is manifest in the non-uniformity quantum-mechanical density and in the so distinctive hierarchy of its physical states, is being increasingly investigated beyond the root-mean-square or standard deviation (also called Heisenberg measure) by various information-theoretic elements; first, by means of the Shannon entropy [13–15] and then, by other individual information and/or spreading measures as the Fisher information and the

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power and logarithmic moments [16], as is described in Ref. [17] where the information theory of D-dimensional hydrogenic systems is reviewed in detail. Just recently, further complementary insights have been shown to be obtained in the three-dimensional hydrogen atom by means of composite information-theoretic measures, such as the Fisher–Shannon and the shape complexity [18,19]. In particular, Sañudo and Lopez-Ruiz [18] have found some numerical evidence that, contrary to the energy, both the Fisher–Shannon measure and the shape complexity in the position space do not present any accidental degeneracy (i.e. they do depend on the orbital quantum number l); moreover, they take on their minimal values at the circular states (i.e., those with the highest l). In fact, the position Shannon entropy by itself has also these two characteristics as it has been numerically pointed out long ago [13], where the dependence on the magnetic quantum number is additionally studied for various physical states.

The shape complexity [20] occupies a very special position not only among the composite information-theoretic measures in general, but also within the class of measures of complexity. This is because of the following properties: (i) invariance under replication, translation and rescaling transformations, (ii) minimal value for the simplest probability densities (namely, e.g. uniform and Dirac's delta in one-dimensional case), and (iii) simple mathematical structure: it is given as the product of the disequilibrium or averaging density and the Shannon entropy power of the system.

In this work we provide the analytical methodology to calculate the shape complexity of the stationary states of the D-dimensional hydrogenic system in the two reciprocal position and momentum spaces and later we apply it to a special class of physical states which includes the ground state and the circular states (i.e. states with the highest hyperangular momenta allowed within a given electronic manifold). First, in Section 2, we briefly describe the known expressions of the quantum-mechanical density of the system in both spaces. In Section 3 we show that the computation of the two shape complexities for arbitrary D-dimensional hydrogenic stationary states boils down to the evaluation of some entropic functionals of Laguerre and Gegenbauer polynomials. To have the final expressions of these complexity measures in terms of the dimensionality D and the quantum numbers characterizing the physical state under consideration, we need to compute the values of these polynomial entropic functionals what is, in general, a formidable open task. However, in Section 4, we succeed to do it for the important cases of ground and circular states. It seems that for the latter ones the shape complexity has the minimal values, at least in the three-dimensional case as indicated above. It is also shown that our results always fulfil the uncertainty relation satisfied by the position and momentum shape complexities [19]. In Section 5, the shape complexities are numerically studied and their dimensionality dependence is discussed. Finally, some conclusions are given.

2. The D-dimensional hydrogenic quantum-mechanical densities

Let us consider an electron moving in the D-dimensional Coulomb ($D \geqslant 2$) potential $V(\vec{r}) = -\frac{Z}{r}$, where $\vec{r} = (r, \theta_1, \theta_2, \ldots, \theta_{D-1})$ denotes the electronic vector position in polar coordinates. The stationary states of this hydrogenic system are described by the wavefunctions

$$\Psi_{n,l,\{\mu\}}\left(\vec{r}, t\right) = \psi_{n,l,\{\mu\}}\left(\vec{r}\right) \exp\left(-\mathrm{i}E_n t\right),$$

where $\left(E_n, \Psi_{n,l,\{\mu\}}\right)$ denote the physical solutions of the Schrödinger equation of the system [1,2,17]. Atomic units ($\hbar = e = m_e = 1$) are used throughout the paper. The energies are given by

$$E = -\frac{Z^2}{2\eta^2}, \quad \text{with } \eta = n + \frac{D-3}{2}; n = 1, 2, 3, \ldots, \tag{1}$$

and the eigenfunctions can be expressed as

$$\Psi_{n,l,\{\mu\}}(\vec{r}) = R_{n,l}(r)\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}), \tag{2}$$

where $(l, \{\mu\}) \equiv (l \equiv \mu_1, \mu_2, \ldots, \mu_{D-1}) \equiv (l, \{\mu\})$ denote the hyperquantum numbers associated to the angular variables $\Omega_{D-1} \equiv (\theta_1, \theta_2, \ldots, \theta_{D-1} \equiv \varphi)$, which may have all values consistent with the inequalities $l \equiv \mu_1 \geq \mu_2 \geq \cdots \geq |\mu_{D-1}| \equiv |m| \geq 0$. The radial function is given by

$$R_{n,l}(r) = \left(\frac{\lambda^{-D}}{2\eta}\right)^{1/2} \left[\frac{\omega_{2L+1}(\hat{r})}{\hat{r}^{D-2}}\right]^{1/2} \tilde{\mathcal{L}}^{2L+1}_{\eta-L-1}(\hat{r}), \tag{3}$$

where $\tilde{\mathcal{L}}^{\alpha}_{k}(x)$ denotes the Laguerre polynomials of degree k and parameter α, orthonormal with respect to the weight function $\omega_\alpha(x) = x^\alpha \mathrm{e}^{-x}$, and the grand orbital angular momentum hyperquantum number L and the adimensional parameter $\hat{r}$ are

$$L = l + \frac{D-3}{2}, \quad l = 0, 1, 2, \ldots \quad \text{and} \quad \hat{r} = \frac{r}{\lambda}, \quad \text{with } \lambda = \frac{\eta}{2Z}. \tag{4}$$

The angular part $\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1})$ is given by the hyperspherical harmonics [2,21]

$$\mathcal{Y}_{l,\{\mu\}}(\Omega_{D-1}) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}m\varphi} \prod_{j=1}^{D-2} \tilde{C}^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(\cos\theta_j) \left(\sin\theta_j\right)^{\mu_{j+1}}, \tag{5}$$

with $\alpha_j = \frac{1}{2}(D - j - 1)$ and $\tilde{C}^{\lambda}_{k}(x)$ denotes the orthonormal Gegenbauer polynomials of degree k and parameter λ.