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Some features of the statistical complexity, Fisher–Shannon information and Bohr-like orbits in the quantum isotropic harmonic oscillator

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Abstract

The Fisher–Shannon information and a statistical measure of complexity are calculated in position and momentum spaces for the wavefunctions of the quantum isotropic harmonic oscillator. We show that these quantities are independent of the strength of the harmonic potential. Moreover, for each level of energy, it is found that these two indicators take their minimum values on the orbitals that correspond to the classical (circular) orbits in the Bohr-like quantum image, just those with the highest orbital angular momentum.

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In recent years, the study of statistical quantities on quantum systems has been increasing in interest [1, 2]. Different indicators that have been developed in the framework of information and complexity theories, for instance, Fisher and Shannon information [3–5], and statistical measures of complexity [6, 8] have been calculated for several systems under different approaches [9–15]. The probability densities characterizing the state of a quantum system are defined in position and momentum spaces [16, 17]. From here, the calculation of all those statistical indicators can be performed with a low computational cost.

The dependence of these quantities on the quantum numbers of the system can reflect the hierarchical organization of that quantum system. Even for states with the same energy it is possible to have different values of these statistical quantities. Take, for instance, the H-atom. It has been shown [18] that for a given energy the minimum values of the Fisher–Shannon information and statistical complexity are reached for the highest allowed orbital angular momentum for that energy. This means that a variational process on these statistical measures can select just those orbitals that in the pre-quantum image are the Bohr-like orbits.

Following this insight, it is our aim in the present work to analyze if the above described behavior of these statistical measures can also be found in the case of the isotropic quantum harmonic oscillator.

Let us start by recalling the three-dimensional non-relativistic wavefunctions of this system when the potential energy is written as $V(r) = \lambda^2 r^2/2$, where λ is a positive real constant expressing the potential strength. Atomic units are used through the text. The wavefunctions in position space ($\vec{r} = (r, \Omega)$, with r being the radial distance and Ω the solid angle) are:

$$\Psi_{n,l,m}(\vec{r}) = R_{n,l}(r)Y_{l,m}(\Omega), \quad (1)$$

where $R_{n,l}(r)$ is the radial part and $Y_{l,m}(\Omega)$ is the spherical harmonic of the quantum state determined by the quantum numbers (n, l, m) . The radial part is expressed as [10]

$$R_{n,l}(r) = \left[\frac{2n!\lambda^{l+3/2}}{\Gamma(n+l+3/2)} \right]^{1/2} r^l e^{-\frac{\lambda}{2}r^2} L_n^{l+1/2}(\lambda r^2), \quad (2)$$

where $L_\alpha^\beta(t)$ are the associated Laguerre polynomials. The levels of energy are given by

$$E_{n,l} = \lambda(2n+l+3/2) = \lambda(e_{n,l}+3/2), \quad (3)$$

where $n = 0, 1, 2, \dots$ and $l = 0, 1, 2, \dots$. Let us observe that $e_{n,l} = 2n+l$. Thus, different pairs of (n, l) can give the same $e_{n,l}$, and then the same energy $E_{n,l}$.

The wavefunctions in momentum space ($\vec{p} = (p, \hat{\Omega})$, with p being the momentum modulus and $\hat{\Omega}$ the solid angle) are:

$$\hat{\Psi}_{n,l,m}(\vec{p}) = \hat{R}_{n,l}(p)Y_{l,m}(\hat{\Omega}), \quad (4)$$

where the radial part $\hat{R}_{n,l}(p)$ is now given by the expression [10]

$$\hat{R}_{n,l}(p) = \left[\frac{2n!\lambda^{-l-3/2}}{\Gamma(n+l+3/2)} \right]^{1/2} p^l e^{-\frac{p^2}{2\lambda}} L_n^{l+1/2}(p^2/\lambda). \quad (5)$$

Taking the former expressions, the probability density in position and momentum spaces,

$$\rho_{n,l,m;\lambda}(\vec{r}) = |\Psi_{n,l,m}(\vec{r})|^2, \quad \gamma_{n,l,m;\lambda}(\vec{p}) = |\hat{\Psi}_{n,l,m}(\vec{p})|^2, \quad (6)$$

can be explicitly calculated. From these densities, the statistical complexity and the Fisher-Shannon information are computed. We find that these quantities are independent of λ , the potential strength. This non-trivial property is proved in appendix A. For this reason, we drop the λ subindex in the densities from now and on. Also, for the sake of simplicity, the quantum numbers (n, l, m) are omitted in the notation.

First, the measure of complexity C recently introduced by Lopez-Ruiz, Mancini and Calbet [6–8], the so-called LMC complexity, is defined as

$$C = H \cdot D, \quad (7)$$

where H represents the information content of the system and D gives an idea of how much concentrated is its spatial distribution. Let us recall at this point that C has been quantified in different contexts (see [19] and references therein). It has been shown to be an useful indicator to successfully discern many situations regarded as complex in systems out of equilibrium [19]. Thus, C identifies the entropy or information H stored in a system and its disequilibrium D , that in the discrete case is the distance from its actual state to the probability distribution of equilibrium, as the two basic ingredients for calculating the complexity of a system. In consequence, this quantity vanishes both for completely ordered and for completely random systems giving then the correct asymptotic properties required for a well-behaved measure of complexity.

For our purpose, in order to calculate C for the present continuous system, we take a version used in [8] as a quantifier of H . This is the simple exponential Shannon entropy, that in position and momentum spaces takes the form, respectively,

$$H_r = e^{S_r}, \quad H_p = e^{S_p}, \quad (8)$$

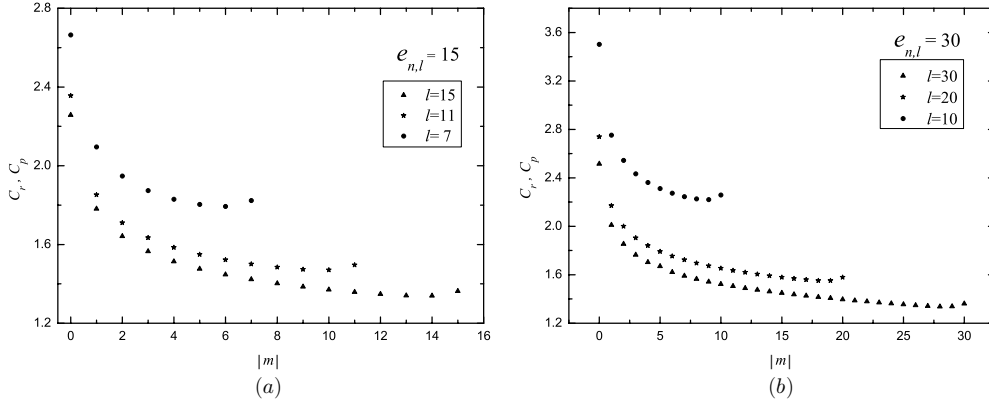


Figure 1. Statistical complexity in position space, C_r , and momentum space, C_p , versus $|m|$ for different energy $e_{n,l}$ -values in the quantum isotropic harmonic oscillator for (a) $e_{n,l} = 15$ and (b) $e_{n,l} = 30$. Recall that $C_r = C_p$. All values are in atomic units.

where S_r and S_p are the Shannon information entropies [4],

$$S_r = - \int \rho(\vec{r}) \log \rho(\vec{r}) d\vec{r}, \quad S_p = - \int \gamma(\vec{p}) \log \gamma(\vec{p}) d\vec{p}. \quad (9)$$

We keep for the disequilibrium the form originally introduced in [6, 8], that is,

$$D_r = \int \rho^2(\vec{r}) d\vec{r}, \quad D_p = \int \gamma^2(\vec{p}) d\vec{p}. \quad (10)$$

In this manner, the final expressions for C in position and momentum spaces are:

$$C_r = H_r \cdot D_r, \quad C_p = H_p \cdot D_p. \quad (11)$$

The form of the wavefunctions, due to the harmonic interaction, allows us to show in appendix A that these quantities, C_r and C_p , are the same.

In figure 1, C_r (or C_p) is plotted as a function of the modulus of the third component m , $-l \leq m \leq l$, of the orbital angular momentum l for different l values with a fixed energy. That is, according to expression (3), the quantity $e_{n,l} = 2n + l$ is constant in each figure. Figure 1(a) shows C_r for $e_{n,l} = 15$ and figure 1(b) shows C_r for $e_{n,l} = 30$. In both figures, it can be observed that C_r splits into different sets of discrete points. Each one of these sets is associated with a different l value. It is worth noting that the set with the minimum values of C_r corresponds just to the highest l , that is, $l = 15$ in figure 1(a) and $l = 30$ in figure 1(b).

Other types of statistical measures that maintain the product form of C can be defined. Let us take, for instance, the Fisher–Shannon information, P , that has been also applied in [11, 15, 18] to quantum systems. This quantity, in position and momentum spaces, is given respectively by

$$P_r = J_r \cdot I_r, \quad P_p = J_p \cdot I_p, \quad (12)$$

where the first factor

$$J_r = \frac{1}{2\pi e} e^{2S_r/3}, \quad J_p = \frac{1}{2\pi e} e^{2S_p/3}, \quad (13)$$

is a version of the exponential Shannon entropy [5], and the second factor

$$I_r = \int \frac{[\vec{\nabla} \rho(\vec{r})]^2}{\rho(\vec{r})} d\vec{r}, \quad I_p = \int \frac{[\vec{\nabla} \gamma(\vec{p})]^2}{\gamma(\vec{p})} d\vec{p}, \quad (14)$$

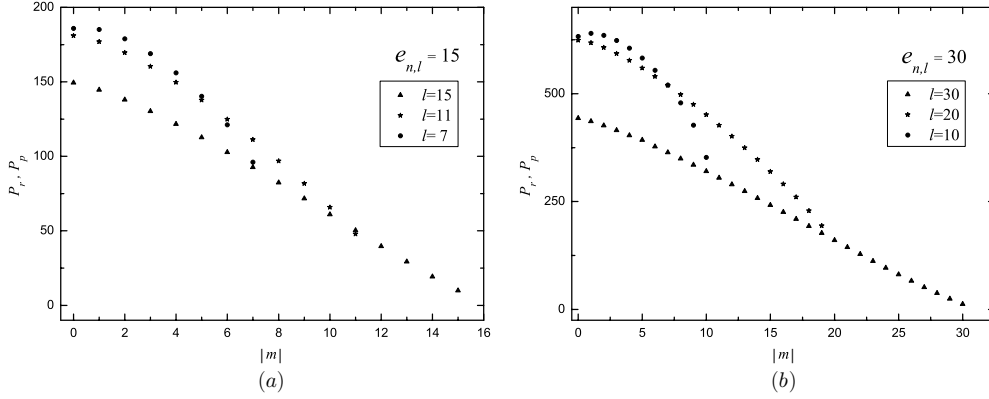


Figure 2. Fisher–Shannon information in position space, P_r , and momentum space, P_p , versus $|m|$ for different energy $e_{n,l}$ -values in the quantum isotropic harmonic oscillator. for (a) $e_{n,l} = 15$ and (b) $e_{n,l} = 30$. Recall that $P_r = P_p$. All values are in atomic units.

is the so-called Fisher information measure [3] that quantifies the narrowness of the probability density. Similar to the behavior of C_r and C_p , we also show in appendix A that $P_r = P_p$.

I_r can be analytically obtained in both spaces (position and momentum). The results are [12]:

$$I_r = 4(2n + l + 3/2 - |m|)\lambda, \tag{15}$$

$$I_p = 4(2n + l + 3/2 - |m|)\lambda^{-1}. \tag{16}$$

Let us note that I_r and I_p depend on λ , although the final result for P_r and P_p are non- λ -dependent (see appendix A).

Figure 2 shows P as a function of the modulus of the third component m for different pairs of $(e_{n,l} = 2n + l, l)$ values. In figure 2(a), P_r (or P_p) is plotted for $e_{n,l} = 15$, and P_r is plotted for $e_{n,l} = 30$ in figure 2(b). Here, P_r also splits into different sets of discrete points, showing a behavior similar to that of C in figure 1. Each one of these sets is related to a different l value, and the set with the minimum values of P_r also corresponds just to the highest l , that is, $l = 15$ and $l = 30$, respectively.

Let us finish this paper with the conclusions. The statistical complexity and the Fisher–Shannon information have been shown to be independent of the potential strength, λ . It is the specific forms, (8), (10) and (13), (14), of the definitions of these two indicators that yield this property. This fact could be an indirect argument to justify the choice of these expressions. Then, these quantities have been calculated. We have taken advantage of the exact knowledge of the wavefunctions. Concretely, we put in evidence that, for a fixed level of energy, let us say $e_{n,l} = 2n + l$, these statistical quantities take their minimum values for the highest allowed orbital angular momentum, $l = e_{n,l}$. It is worth remembering at this point that the radial part of this particular wavefunction, that describes the quantum system in the $(n = 0, l = e_{n,l})$ orbital, has no nodes. This means that the spatial configuration of this state is, in some way, a spherical-like shell. In appendix B, the mean radius of this shell, $\langle r \rangle_{n,l,m}$, is found for the case $(n = 0, l = e_{n,l}, m)$. This is:

$$\langle r \rangle_{n=0,l=e_{n,l},m} \equiv \langle r \rangle_{n=0,l=e_{n,l}} \simeq \sqrt{\lambda^{-1}(e_{n,l} + 1)}(1 + \Theta(e_{n,l}^{-1})), \tag{17}$$

that tends, when $e_{n,l} \gg 1$, to the radius of the N th energy level, $r_N = \sqrt{\lambda^{-1}(N+1)}$, taking $N = e_{n,l}$ in the Bohr-like picture of the harmonic oscillator (see appendix B).

As it was remarked in [18], here we also obtain that the minimum values of the statistical measures calculated from the wavefunctions of the quantum isotropic harmonic oscillator select just those orbitals that in the pre-quantum image are the Bohr-like orbits. Therefore, we conclude that our intuition is enhanced when using these quantities to discern complexity at a quantum level.

Appendix A. Invariance of C and P under rescaling transformations

Here, we show that the statistical complexities C_r and C_p are equal and independent of the strength potential, λ , for the case of the quantum isotropic harmonic oscillator. Also, the same behavior is displayed by P_r and P_p .

For a fixed set of quantum numbers, (n, l, m) , let us define the normalized probability density $\hat{\rho}(\vec{r})$:

$$\hat{\rho}(\vec{r}) = \frac{2n!}{\Gamma(n+l+3/2)} t^{2l} e^{-t^2} [L_n^{l+1/2}(t^2)]^2 |Y_{l,m}(\Omega)|^2. \quad (\text{A.1})$$

From expressions (1), (2) and (6), it can be obtained that

$$\rho_\lambda(\vec{r}) = \lambda^{3/2} \hat{\rho}(\lambda^{1/2} \vec{r}), \quad (\text{A.2})$$

where ρ_λ is the normalized probability density of expression (6). Now, it is straightforward to find that

$$H_r(\rho_\lambda) = \lambda^{-3/2} H(\hat{\rho}), \quad (\text{A.3})$$

and that

$$D_r(\rho_\lambda) = \lambda^{3/2} D(\hat{\rho}). \quad (\text{A.4})$$

Then,

$$C_r(\rho_\lambda) = C(\hat{\rho}), \quad (\text{A.5})$$

and the non- λ -dependence of C_r is shown.

To show that C_r and C_p are equal, let us note that, from expressions (4)–(6), the normalized probability density $\gamma_\lambda(\vec{p})$ for the same set of quantum numbers (n, l, m) can be written as

$$\gamma_\lambda(\vec{p}) = \lambda^{-3/2} \hat{\rho}(\lambda^{-1/2} \vec{p}). \quad (\text{A.6})$$

Now, it is found that

$$H_p(\gamma_\lambda) = \lambda^{3/2} H(\hat{\rho}), \quad (\text{A.7})$$

and that

$$D_p(\gamma_\lambda) = \lambda^{-3/2} D(\hat{\rho}). \quad (\text{A.8})$$

Then,

$$C_p(\gamma_\lambda) = C(\hat{\rho}), \quad (\text{A.9})$$

and the equality of C_r and C_p , and their non- λ -dependence are shown.

Similarly, from expressions (12), (13), (15) and (16), it can be found that $P_r = P_p$, and that these quantities are also non- λ -dependent.

Appendix B. Bohr-like orbits in the quantum isotropic harmonic oscillator

Here, the mean radius of the orbital with the lowest complexity is calculated as a function of the energy. Also, the radii of the orbits in the Bohr picture are obtained.

The general expression of the mean radius of a state represented by the wavefunction $\Psi_{n,l,m}$ is given by

$$\langle r \rangle_{n,l,m} \equiv \langle r \rangle_{n,l} = \frac{n!}{\Gamma(n+l+3/2)} \frac{1}{\lambda^{1/2}} \int_0^\infty t^{l+1} e^{-t} [L_n^{l+1/2}(t)]^2 dt. \quad (\text{B.1})$$

For the case of the minimum complexity (see figure 1 or 2), the state has the quantum numbers ($n = 0, l = e_{n,l}$). The last expression (B.1) becomes:

$$\langle r \rangle_{n=0,l=e_{n,l}} = \frac{(e_{n,l} + 1)!}{\Gamma(e_{n,l} + 3/2)\lambda^{1/2}}, \quad (\text{B.2})$$

that, in the limit $e_{n,l} \gg 1$, simplifies to expression (17):

$$\langle r \rangle_{n=0,l=e_{n,l} \gg 1} \simeq \sqrt{\lambda^{-1}(e_{n,l} + 1)} (1 + \Theta(e_{n,l}^{-1})). \quad (\text{B.3})$$

We now proceed to obtain the radius of an orbit in the Bohr-like image of the isotropic harmonic oscillator. Let us recall that this image establishes the quantization of the energy through the quantization of the classical orbital angular momentum. So, the energy E of a particle of mass m moving with velocity v on a circular orbit of radius r under the harmonic potential $V(r) = m\lambda^2 r^2/2$ is:

$$E = \frac{1}{2}m\lambda^2 r^2 + \frac{1}{2}mv^2. \quad (\text{B.4})$$

The circular orbit is maintained by the central force through the equation:

$$\frac{mv^2}{r} = m\lambda^2 r. \quad (\text{B.5})$$

The angular momentum takes discrete values according to the condition

$$mvr = (N + 1)\hbar \quad (N = 0, 1, 2, \dots). \quad (\text{B.6})$$

Combining the last three equations (B.4)–(B.6), and taking atomic units, $m = \hbar = 1$, the radius r_N of a Bohr-like orbit for this system is obtained

$$r_N = \sqrt{\lambda^{-1}(N + 1)} \quad (N = 0, 1, 2, \dots). \quad (\text{B.7})$$

Let us observe that this expression coincides with the quantum-mechanical radius given by expression (B.3) when $e_{n,l} = N$ for $N \gg 1$.

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