Rigorous bounds for Rényi entropies of spherically symmetric potentials

Pablo Sánchez-Moreno[*,†], Steeve Zozor[**] and Jesús S. Dehesa[*,‡]

[*]*Instituto Carlos I de Física Teórica y Computacional, Univ. de Granada, 18071-Granada, Spain*
[†]*Departamento de Matemática Aplicada, Univ. de Granada, 18071-Granada, Spain*
[**]*GIPSA-Lab, Domaine universitaire, 38402 St martin d'Hères, France*
[‡]*Departamento de Física Atómica, Molecular y Nuclear, Univ. de Granada, 18071-Granada, Spain*

Abstract. The Rényi and Shannon entropies are information-theoretic measures which have enabled to formulate the position-momentum uncertainty principle in a much more adequate and stringent way than the (variance-based) Heisenberg-like relation. Moreover, they are closely related to various energetic density-functionals of quantum systems. Here we find sharp upper bounds to these quantities in terms of the second order moment $\langle r^2 \rangle$ for general spherically symmetric potentials, which substantially improve previous results of this type, by means of the Rényi maximization procedure with a covariance constraint due to Costa, Hero and Vignat [1]. The contributions to these bounds coming from the radial and angular parts of the physical wavefunctions are explicitly given.

Keywords: Rényi entropy, Shannon entropy, spherically symmetric potentials, variational upper bounds
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INTRODUCTION

The Shannon and Rényi entropies of a normalized probability distribution $\rho(\mathbf{x})$, $\mathbf{x} = (x_1, \ldots, x_d) \in \mathbb{R}^d$, are information-theoretic measures which quantify the spread of $\rho(\mathbf{x})$ all over the d-dimensional space in different, but complementary, ways. They have been used not only to study the statistical properties of multifractals [2], and to derive entanglement criteria for continuous variable systems [3], but also to set up more adequate and stringent mathematical formulations [4, 5, 6] of the position-momentum quantum-mechanical uncertainty principle than the Heisenberg-like uncertainty relation. Moreover, although they are not physical observables because they cannot be expressed as expectation values of any Hermitian operator of a quantum system, they are closely related with various macroscopic properties of the system; particularly, with energy functionals of various types [7]. These are some physical reasons to motivate the search for sharp upper bounds to these two entropies in terms of the power moment of order 2, $\langle r^2 \rangle$, where $r^2 = \|\mathbf{x}\|^2 = \sum_{i=1}^{d} x_i^2$. This is because the power moments are not only important by their own, but also they represent fundamental and/or experimentally accessible quantities of the system (see e.g. the recent review [7]).

Extending previous three-dimensional results [8, 9], it was variationally shown [10, 11] that the Shannon entropy defined as

$$S[\rho] = -\int_{\mathbb{R}^d} \rho(\mathbf{x}) \ln \rho(\mathbf{x}) \, d\mathbf{x} \tag{1}$$

is bounded from above by

$$S[\rho] \leq \frac{d}{2} \ln \left(2\pi e \frac{\langle r^2 \rangle}{d} \right) \qquad (2)$$

in terms of $\langle r^2 \rangle$. Moreover, the Rényi entropy defined as [10, 12, 13]

$$H_\lambda[\rho] = \frac{1}{1-\lambda} \ln \int_{\mathbb{R}^d} [\rho(\mathbf{x})]^\lambda \, d\mathbf{x}; \; \lambda > 0, \; \lambda \neq 1, \qquad (3)$$

has shown to be bounded in terms of $\langle r^2 \rangle$ [1, 7, 14, 15] as follows:

$$H_\lambda[\rho] \leq \mathscr{B}_d(\lambda) + \frac{d}{2} \ln \left(\frac{\langle r^2 \rangle}{d} \right), \qquad (4)$$

with

$$\mathscr{B}_d(\lambda) = \begin{cases} \frac{d}{2} \log \left(\frac{\pi((2+d)\lambda-d)}{\lambda-1} \right) + \log \left(\left(\frac{(2+d)\lambda-d}{2\lambda} \right)^{\frac{1}{1-\lambda}} \frac{\Gamma\left(\frac{\lambda}{\lambda-1}\right)}{\Gamma\left(\frac{(2+d)\lambda-d}{2(\lambda-1)}\right)} \right), & \lambda > 1 \\[3mm] \frac{d}{2} \log \left(\frac{\pi((2+d)\lambda-d)}{1-\lambda} \right) - \log \left(\left(\frac{(2+d)\lambda-d}{2\lambda} \right)^{\frac{\lambda}{1-\lambda}} \frac{\Gamma\left(\frac{\lambda}{1-\lambda}\right)}{\Gamma\left(\frac{(2+d)\lambda-d}{2(1-\lambda)}\right)} \right), & \lambda \in \left(\frac{d}{d+2}, 1\right) \\[3mm] \frac{d}{2} \log(2\pi e), & \lambda = 1 \end{cases} \qquad (5)$$

Note that the bounds (4)-(5) to Rényi entropies boil down to the bound (2) to Shannon entropy, in accordance to the known limit $\lim_{\lambda \to 1} H_\lambda[\rho] = S[\rho]$.

On the other hand let us highlight the fundamental relevance and utility of the spherically symmetric potentials in the quantum-mechanical description of the natural systems. Indeed, the central-field model of the atom is, together with the Pauli exclusion principle, the theoretical basis of the Aufbau principle of the Mendeleev atomic periodic table. Moreover, the spherically symmetric potentials have been used as prototypes for many other purposes and systems not only in the three-dimensional world but also in non-relativistic and relativistic d-dimensional physics.

The goal of this paper is to improve the upper bounds (2) and (4) to the Shannon and Rényi entropies in terms of $\langle r^2 \rangle$ for quantum systems with spherically symmetric potentials. Briefly, we use the following three-step methodology. First, we separate out the radial and angular contributions to the physical entropies by making an appropriate change of variable which involves the covariance matrix of the system. Then, we use the maximization procedure of Costa et al [1] for the Rényi entropy under a covariant matrix constraint. Finally, we take into account the spherical symmetry in the evaluation of the bound previously found.

The structure of the paper is the following. First, we formulate the quantum-mechanical d-dimensional problem for spherically symmetric potentials, indicating the probability density of the system $\rho(\mathbf{x})$, and we separate out the Rényi entropy of $\rho(\mathbf{x})$ into a radial and an angular part. Then, we obtain an upper bound to the radial Rényi entropy by means of the maximization procedure of Costa et al subject to a covariance-matrix constraint, and we calculate the angular Rényi entropy in terms of the generalized quantum numbers $\{\mu\}$ of the system. Finally, some conclusions and open problems are given.

THE QUANTUM PROBLEM FOR d-DIMENSIONAL SPHERICALLY SYMMETRIC POTENTIALS

The Schrödinger equation of a particle moving in a d-dimensional spherically symmetric potential $V_d(r)$, i.e. that only depends on the distance to the origin $r = \|\mathbf{x}\|$, $\mathbf{x} \in \mathbb{R}^d$, can be written as

$$\left[-\frac{1}{2}\nabla_d^2 + V_d(r) \right] \Psi(\mathbf{x}) = E\Psi(\mathbf{x}), \tag{6}$$

where $\Psi(\mathbf{x})$ is the wavefunction describing a quantum-mechanical stationary bound state of the particle. The symbol $\mathbf{x}$ denotes the d-dimensional position vector having the Cartesian coordinates $\mathbf{x} = (x_1, x_2, \ldots, x_d)$ and the hyperspherical coordinates $(r, \theta_1, \theta_2, \ldots, \theta_{d-1}) \equiv (r, \Omega_{d-1})$, where naturally $\|\mathbf{x}\|^2 = r^2 = \sum_{i=1}^{d} x_i^2$; they are mutually related by

$$\begin{cases} x_1 & = & r\cos\theta_1 \\ & \vdots & \\ x_k & = & r\sin\theta_1 \ldots \sin\theta_{k-1}\cos\theta_k \\ & \vdots & \\ x_{d-1} & = & r\sin\theta_1 \ldots \sin\theta_{d-2}\cos\theta_{d-1} \\ x_d & = & r\sin\theta_1 \ldots \sin\theta_{d-2}\sin\theta_{d-1} \end{cases} \tag{7}$$

where $r \in [0\,;\,+\infty)$, $\theta_i \in [0\,;\,\pi)$, $i < d-1$ and $\theta_{d-1} \in [0\,;\,2\pi)$.

It is known [16, 17] that the wave function can be separated out into a radial, $R_{El}(r)$, and an angular, $\mathscr{Y}_{\{\mu\}}(\Omega_{d-1})$, part as

$$\Psi_{E,\{\mu\}}(\mathbf{x}) = R_{E,l}(r)\mathscr{Y}_{\{\mu\}}(\Omega_{d-1}). \tag{8}$$

Note that the angular part, which is common to any spherically symmetric potential, is given by the hyperspherical harmonics [16, 17] $\mathscr{Y}_{\{\mu\}}(\Omega_{d-1})$, which satisfy the eigenvalue equation

$$\Lambda_{d-1}^2 \mathscr{Y}_{l,\{\mu\}}(\Omega_{d-1}) = l(l+d-2)\mathscr{Y}_{l,\{\mu\}}(\Omega_{d-1}),$$

associated to the generalized angular momentum operator given by

$$\Lambda_{d-1}^2 = -\sum_{i=1}^{d-1} \frac{(\sin\theta_i)^{i+1-d}}{\left(\prod_{j=1}^{i-1}\sin\theta_j\right)^2} \frac{\partial}{\partial\theta_i} \left[(\sin\theta_i)^{d-i-1}\frac{\partial}{\partial\theta_i} \right].$$

The quantum angular numbers $(l \equiv \mu_1, \mu_2, \ldots, \mu_{d-1} \equiv m)$ satisfy the chain of inequalities $l \equiv \mu_1 \geq \mu_2 \geq \cdots \geq \mu_{d-2} \geq |\mu_{d-1}| \equiv |m|$.

These mathematical functions can be expressed (see e.g. [16, 17, 18]) as

$$\mathscr{Y}_{\{\mu\}}(\Omega_{d-1}) = \frac{e^{im\theta_{d-1}}}{\sqrt{2\pi}} \prod_{j=1}^{d-2} \frac{1}{\sqrt{Z(\lambda_j,n_j)}} C_{n_j}^{\lambda_j}(\cos\theta_j)\,(\sin\theta_j)^{\mu_{j+1}}, \tag{9}$$

with

$$n_j = \mu_j - \mu_{j+1}, \quad \lambda_j = \frac{d-1-j}{2} + \mu_{j+1}. \tag{10}$$

and the normalization constant [19, eq. 8.939-8]

$$Z(\lambda,n) = \int_0^\pi \left(C_n^\lambda(\cos\theta)(\sin\theta)^\lambda \right)^2 d\theta = \frac{\pi 2^{1-2\lambda}\Gamma(n+2\lambda)}{(\lambda+n)n!(\Gamma(\lambda))^2}, \tag{11}$$

where $C_n^\lambda(x)$ are the Gegenbauer polynomials. Taking the Ansatz (8) into (6), one obtains that the radial part $R_{El}(r)$ fulfils the second order differential equation

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} - \frac{d-1}{2r}\frac{d}{dr} + \frac{l(l+d-2)}{2r^2} + V_d(r) \right] R_{E,l}(r) = E R_{E,l}(r),$$

which only depends on the energy E, the dimensionality d and the angular quantum number $l = \mu_1$.

Then, the quantum-mechanical probability density is given by

$$\rho_{E,\{\mu\}}(\mathbf{x}) = |\Psi_{E,\{\mu\}}(\mathbf{x})|^2 = |R_{E,l}(r)|^2 |\mathcal{Y}_{\{\mu\}}(\Omega_{d-1})|^2. \tag{12}$$

Let us note that the second-order moment $\langle r^2 \rangle$ of the d-dimensional density $\rho_{E,\{\mu\}}(\mathbf{x})$ has the expression

$$\langle r^2 \rangle = \int_{\mathbb{R}^d} \|\mathbf{x}\|^2 \rho_{E,\{\mu\}}(\mathbf{x}) d\mathbf{x} = \int_0^{+\infty} r^2 |R_{El}(r)|^2 r^{d-1} dr,$$

which only depends on the radial wave function $R_{El}(r)$ of the particle because the angular contribution is equal to the unity due to the normalization of the hyperspherical harmonics. Taking into account bounds (2) and (4) to the Shannon and Rényi entropies, it seems natural to think that to improve such bounds we have to use a variational method with constraints which involve not only the radial part but also the angular part of the wave function. A way to do that is to consider the whole covariance matrix $R_x = \langle \mathbf{x}\mathbf{x}^t \rangle$, which has the components $\langle x_i x_j \rangle$, not only the second order moment.

RÉNYI ENTROPY AND COVARIANCE MATRIX

Let us now initiate the determination of the upper bound to the Shannon and Rényi entropies of the probability density $\rho_{E,\{\mu\}}(\mathbf{x})$ given by eq. (12), by separating out the radial and angular contributions to these quantities. To do that we use, for mathematical convenience, a more appropriate, statistical notation.

Consider a column vector $\mathbf{x} \in \mathbb{R}^d$, a d-dimensional position described by the wave function $\Psi(\mathbf{x})$, and interpret such a vector as a random vector of probability density function $\rho_x(\mathbf{x}) = |\Psi(\mathbf{x})|^2$. Without loss of generality, assume that the vector $\mathbf{x}$ is centered, i.e. $\langle \mathbf{x} \rangle = 0$. In general, the statistical second order moment (or second order ensemble average) $\langle r^2 \rangle$ does not describe entirely the second order statistics of vector $\mathbf{x}$ and it is common to consider all the second order statistics via the covariance matrix $R_x = \langle \mathbf{x}\mathbf{x}^t \rangle$, of components $\langle x_i x_j \rangle$. Note that these two statistical quantities are linked by $\langle r^2 \rangle = \text{Tr}(R_x)$, where Tr denotes the trace of a matrix (i.e. the sum of its diagonal components).

Let us now consider the "modified" position vector $\mathbf{y} = R_x^{-1/2}\mathbf{x}$, where $R_x^{1/2}$ is the unique symmetric positive definite matrix that is the "square-root" of R_x [20, th. 7.2.6]. From the properties of covariance matrices [21], this is equivalent to consider a stretched and rotated version of the position vector $\mathbf{x}$. Clearly the covariance matrix of $\mathbf{y}$ is the identity matrix I_d, meaning that the transformation of $\mathbf{x}$ is so that the position $\mathbf{y}$ is isotropic in terms of the second order statistics.

Then, the Rényi entropy of $\mathbf{x}$ (or ρ_x), given by eq. (3), and that of $\mathbf{y}$ (or ρ_y) are mutually related by

$$H_\lambda[\rho_x] = H_\lambda[\rho_y] + \frac{1}{2}\log|R_x| \tag{13}$$

(see e.g. [10, 12, 13]). To obtain this well known result, one uses the change of variable $\mathbf{x} = R_x^{1/2}\mathbf{y}$ in $H_\lambda(\rho_x)$, and one realizes that $\rho_y(\mathbf{y}) = |R_x|^{1/2}\rho_x(R_x^{1/2}\mathbf{y})$. Notice that since $H_1[\rho] = S[\rho]$, eq. (13) is also valid for the Shannon entropies of $\mathbf{x}$ and $\mathbf{y}$ (see e.g. [10, eq. (9.67)] in the Shannon context or [13, eq. (22)]). Let us also keep in mind that the trace of the covariance matrix is the expectation value of the square norm of the vector; then, $\mathbf{y}$ verifies that its expectation value $\langle\|\mathbf{y}\|^2\rangle = d$.

Now, we can extract the "variance" term $\langle r^2\rangle$, where $r = \|\mathbf{x}\|$, from the covariance matrix remembering that $\langle r^2\rangle = \mathrm{Tr}(R_x)$, and writing

$$R_x = \frac{\langle r^2\rangle}{d} d\, C_x \quad \text{where} \quad C_x = \frac{R_x}{\mathrm{Tr}(R_x)}. \tag{14}$$

Matrix C_x contains only the correlation structure of $\mathbf{x}$, regardless its strength. $C_{x,i,i}$ represents the relative strength of component x_i relatively to the total power. Obviously, as $|R_x| = (\langle r^2\rangle/d)^d\, d^d\, |C_x|$, we have from (13) that

$$H_\lambda(\rho_x) = H_\lambda(\rho_y) + \frac{d}{2}\log\frac{\langle r^2\rangle}{d} + \mathscr{L}(\Omega_{d-1}), \tag{15}$$

where the symbol

$$\mathscr{L}(\Omega_{d-1}) = \frac{1}{2}\log|C_x| + \frac{d}{2}\log d. \tag{16}$$

represents the contribution to the entropy coming from the hyperspherical harmonics. Indeed, for a spherically symmetric density $\rho_x(\mathbf{x})$ the covariance matrix is $R_x = \frac{\langle r^2\rangle}{d}I_d$ (so, $C_x = \frac{1}{d}I_d$) and then its Rényi entropy is $H_\lambda[\rho_y] + \frac{d}{2}\log\frac{\langle r^2\rangle}{d}$.

Let us denote by $\lambda_{x,i} \geq 0$ the eigenvalues of C_x. We have $\sum_i \lambda_{x,i} = \mathrm{Tr}(C_x) = 1$ and thus they can be viewed as probabilities. Let us denote by $\lambda_x = \{\lambda_{x,1}, \ldots, \lambda_{x,d}\}$ the discrete density of eigenvalues and by $u_d = \{1/d, \ldots, 1/d\}$ the uniform density. Hence, we obtain that

$$\mathscr{L}(\Omega_{d-1}) = -\frac{d}{2}\sum_{i=1}^d \frac{1}{d}\log\left(\frac{1/d}{\lambda_{x,i}}\right) = -\frac{d}{2}D_{\mathrm{kl}}(u_d\|\lambda_x) \leq 0. \tag{17}$$

The symbol $D_{\mathrm{kl}}(v\|w)$ denotes the Kullback-Leibler (KL, in short) divergence between the distributions v and w as defined by $D_{\mathrm{kl}}(v\|w) = \sum_{i=1}^d v_i\log(v_i/w_i)$, which is always

positive unless the two distributions are equal, in which case it vanishes [10, th. 2.6.3]. Then, the KL-divergence $D_{\mathrm{kl}}(u_d \| \lambda_x)$ between the uniform distribution u_d and the counting density of eigenvalues of C_x, which is controlled by the hyperspherical harmonics only, quantifies the loss of entropy, $\mathscr{L}(\Omega_{d-1})$. Note now that the loss of entropy vanishes if and only if the eigenvalues of C_x are uniformly distributed, what implies that $D_{\mathrm{kl}}(u_d \| \lambda_x) = 0$, and thus that matrix C_x is diagonal and equals to $\frac{1}{d} I_d$. Reciprocally, for $C_x = \frac{1}{d} I_d$, one has $\mathscr{L}(\Omega_{d-1}) = 0$.

Therefore, according to eq. (15), the Rényi entropy $H_\lambda[\rho_x]$ of the quantum probability density $\rho(\mathbf{x})$ of a particle in a spherically symmetric potential can be separated out into two parts: one which contains the contribution of the radial wavefunction of the system, and another one ($\mathscr{L}(\Omega_{d-1})$) which only depends on the angular wavefunction, that is on the hyperspherical harmonics. The radial Rényi entropy cannot be calculated unless we know the specific analytical form of the spherically symmetric potential, but the angular Rényi entropy can be explicitly determined via eq. (16). These two issues are tackled in the next Section.

UPPER BOUNDS TO THE RÉNYI ENTROPY

In this Section we bound from above the Rényi entropy of the isotropic density $\rho_y(\mathbf{y})$, $H_\lambda[\rho_y]$, and then we determine the loss of entropy $\mathscr{L}(\Omega_{d-1})$ due to the hyperspherical entropy; so, obtaining together with eq. (15) a sharp upper bound to the total Rényi and Shannon entropies of a particle moving in a spherically symmetric potential.

Let us begin with the use of the extremization procedure of Costa et al [1] to bound the Rényi entropy $H_\lambda[\rho_y]$ subject to the covariance-matrix constraint $R_y = I_d$. It straightforwardly yields the upper bound

$$H_\lambda(\rho_y) \leq \mathscr{B}_d(\lambda) \tag{18}$$

where $\mathscr{B}_d(\lambda)$ is given by (5).

Now, let us calculate the loss of entropy $\mathscr{L}(\Omega_{d-1})$. Starting from eq. (16) it is easily shown that all the non-diagonal matrix elements of C_x for spherically symmetric potentials vanish, what implies that the matrix C_x is diagonal, in which case

$$\mathscr{L}(\Omega_{d-1}) = \frac{1}{2} \sum_{i=1}^{d} \log C_{x,i,i} + \frac{d}{2} \log d \tag{19}$$

Then, keeping in mind eq. (7) we have that the diagonal elements $C_{x,i,i}$ of the matrix C_x are given by

$$C_{x,i,i} = \frac{\langle x_i x_i \rangle}{\langle r^2 \rangle} = \left(\prod_{k=1}^{i-1} \langle \sin^2 \theta_k \rangle \right) \langle \cos^2 \theta_i \rangle, \tag{20}$$

where the trigonometric expectation values are defined in terms of the partial hyperspherical harmonics, and where the non existing angle θ_d has to be removed from this expression (or to be chosen as $\theta_d = 0$ by convention).

Since $\langle\sin^2\theta_k\rangle = 1 - \langle\cos^2\theta_k\rangle$, we only need to evaluate $\langle\cos^2\theta_k\rangle$ for $k < d - 1$. The latter value can be obtained as follows

$$\langle\cos^2\theta_k\rangle = \frac{1}{Z(\lambda_k, n_k)}\int_0^\pi \left(\cos\theta\, C_{n_k}^{\lambda_k}(\cos\theta)\sin^{\lambda_k}\theta\right)^2 d\theta = \frac{n_k^2 + 2\lambda_k n_k + \lambda_k - 1}{2\,(n_k + \lambda_k + 1)(n_k + \lambda_k - 1)}$$

Replacing n_k and λ_k by their values (10) one obtains

$$\langle\cos^2\theta_k\rangle = \frac{2\mu_k(\mu_k + d - k - 1) - 2\mu_{k+1}(\mu_{k+1} + d - k - 2) + d - k - 3}{4\mu_k(\mu_k + d - k - 1) + (d - k + 1)(d - k - 3)}. \qquad (21)$$

For $k = d - 1$, and with the convention $\mu_d = 0$, one has $\lambda_{d-1} = 0$ and a direct computation shows that (21) holds also for $k = d - 1$, i.e. $\langle\cos^2\theta_{d-1}\rangle = \frac{1}{2}$.

Then, from eqs. (16), (19) the angular Rényi entropy or loss of entropy turns out to have the expression

$$\mathscr{L}(\Omega_{d-1}) = \frac{1}{2}\sum_{k=1}^{d-2}\left((d - k)\log\langle\sin^2\theta_k\rangle + \log\langle\cos^2\theta_k\rangle\right) - \log 2 + \frac{d}{2}\log d, \qquad (22)$$

where the trigonometric expectation values can be obtained by eq. (21).

Then, taking into account eq. (15) and ineq. (18) one finally has the sharp bound

$$H_\lambda[\rho_x] \leq \mathscr{B}_d(\lambda) + \frac{d}{2}\log\frac{\langle r^2\rangle}{d} + \mathscr{L}(\Omega_{d-1}), \qquad (23)$$

for d-dimensional single-particle systems in a spherically symmetric potential, where $\mathscr{L}(\Omega_{d-1})$ is obtained from eqs. (21) and (22).

CONCLUSIONS AND OPEN PROBLEMS

In this work we substantially improve the sharp upper bounds to the Shannon and Rényi entropies of the stationary quantum states of single-particle systems in a spherically symmetric potential, previously found in terms of the expectation value $\langle r^2\rangle$. This is done by taking into account the loss of entropy due to the explicit consideration of the angular part of the corresponding wavefunctions (i.e., the hyperspherical harmonics) into these physical entropies by means of the covariance matrix of the system. Briefly, we have decomposed the Rényi entropy into two parts: one depending on the radial wavefunction and another one on the angular wavefunction. Then, the radial Rényi entropy is upper bounded in terms of $\langle r^2\rangle$ and the angular part is explicitly calculated making profit of the the fact that the covariance matrix is diagonal for spherically symmetric potentials.

A natural and useful extension of this work is to use radial expectation values of order other than 2 as constraints, which would require the ideas and methodology of Refs. [1, 22]; or considering q-variances instead of classical variance by changing the pdf ρ by ρ^q in the statistical average. Another way of extending the work could be to look to the optimum structure of the correlation matrix that minimizes the bound.

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