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A Theoretical Study on the Information Theoretic Inequalities and Fisher-Shannon Product of a Free Particle

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Author's contribution

The work is carried out solely by the author beginning from the literature review, design, analysis, the numerical calculations and the preparation of the manuscript.

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ABSTRACT

In this article, the plane wave solution for a free particle in three dimensions is considered and the wave function is normalized in an arbitrarily large but finite cube. The momentum space wave function is obtained by taking the Fourier transform of the coordinate space wave function. The probability densities are employed to compute the numerical values of the information theoretic quantities such as Shannon information entropy (S), Fisher information entropy (I), Shannon power (J) and the Fisher–Shannon product (P) both in coordinate and momentum spaces for different values of the length (L) of the cubical box. Numerical values so found satisfy the Beckner, Bialynicki-Birula and Myceilski (*BBM*) inequality relation; Stam-Cramer-Rao inequalities (better known as the Fisher based uncertainty relation) and Fisher-Shannon product relation. This establishes the validity of the information theoretic inequalities in respect of the motion of a free particle.

Keywords: Beckner, Bialynicki-Birula and Myceilski (BBM) inequality; Fisher information entropy; Fisher-Shannon product; Shannon information entropy; uncertainty relations.

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1. INTRODUCTION

Information theory has its primary roots in two classic papers written by Claude E. Shannon in 1948 [1]. In all natural sciences measurements play a fundamental role. Every measurement has some uncertainty, so the theoretical tools are to be directly correlated with the knowledge of that uncertainty. Here the term ‘uncertainty’ is used as a measure of missing information. It can be interpreted in a different way by reversing its sign. The ‘lack of information’ can be associated with ‘negative information’ and such negative information can be termed as the ‘uncertainty’. The uncertainty relations have become the landmark of quantum theory since they were formulated by Bohr and Heisenberg. It should come as no surprise that information theory provides a way to measure uncertainty. The uncertainty principle is likely to be the most prominent difference between classical and quantum physics. The use of the information entropy fits perfectly with the statistical nature of quantum mechanical measurements. The first mathematical realization of this principle was proposed by Heisenberg [2] and Kennard [3] in terms of the standard deviations of the quantum mechanical probability densities of the particle in position and momentum spaces. However, the so-called Heisenberg uncertainty relation is neither the most appropriate nor the most stringent [4-6]. Indeed, the standard deviation is a measure of separation of the region(s) of concentration of the probability cloud from the centroid (a particular point of the distribution), rather than a measure of the extent to which the distribution is in fact concentrated [5-7]. Shannon connected the measure of the information content with probability density. It is necessary to mention that both Shannon information entropy (*S*) and Fisher information entropy (*I*) [8] are characterized by probability density corresponding to changes in some observable. Because of their many applications in different areas of physics and chemistry, there has been a growing interest by many researchers in studying Shannon entropy and Fisher information in recent years. These two information entropies carry out a vital role in different areas of physics and chemistry. The entropic uncertainty relations in quantum information theory have been proved to be an alternative to the Heisenberg uncertainty relation in quantum mechanics [9-11]. On one hand, the Shannon entropic uncertainty relation in coordinate and momentum spaces satisfy the Beckner, Bialynicki-Birula (*BBM*) inequality relation as [12-13],

$$S_T = S_\rho + S_\gamma \geq D(1 + ln\pi) \tag{1}$$

where *D* represents the spatial dimension, s_ρ is the Shannon entropy in the coordinate space, s_γ is the corresponding Shannon entropy in the momentum space. In case of three dimensions (*D = 3*) the *BBM* inequality relation takes the form as, $S_\rho + S_\gamma \geq 6.434$. The entropies s_ρ and s_γ are defined as [12-15],

$$s_\rho = -\int \rho(\vec{r}) ln\, \rho(\vec{r})\, d^3r \tag{2}$$

$$s_\gamma = -\int \gamma(\vec{p}) ln\, \gamma(\vec{p}) d^3p \tag{3}$$

where $d^3r = r^2\, dr\, d\Omega$, $d^3p = p^2\, dp\, d\Omega$ and $d\Omega = sin\theta\, d\theta\, d\varphi$ is the solid angle with $\psi(\vec{r})$ being the normalized wave function in the spatial coordinate, $\rho(\vec{r})$ and $\gamma(\vec{p})$ are the probability densities in coordinate and momentum space. The Shannon information entropy is usually regarded as the measure of the spatial spread of the wave function for different states [16]. One of the consequences of the *BBM* inequality is that it represents the lower bound values of the Shannon entropy sum such that if the coordinate entropy increases, then the momentum entropy will decrease in such a way that their sum bounds above (*BBM*) inequality. On the other hand, Fisher information is a local measure since it is sensitive to local rearrangement of the density. It has been reported that the higher the Fisher information, the more localized is the charge density [17-18] and conversely, the smaller the uncertainty the higher the accuracy in predicting the localization of the particles. The Fisher information is defined as the gradient functional of the charge density of the system and is given in the coordinate and momentum spaces as [19-20]

$$I_\rho = \int \frac{1}{\rho(\vec{r})} [\vec{\nabla}\rho(\vec{r})]^2\ d^3r \tag{4}$$

$$I_\gamma = \int \frac{1}{\gamma(\vec{p})} [\vec{\nabla}\gamma(\vec{p})]^2\, d^3p. \tag{5}$$

The disorder aspect of Fisher information entropy has been studied in some length by Frieden [21]. The uncertainty properties are clearly delineated by the Stam inequalities [22]. The product $I_\rho I_\gamma$ has been conjectured to exhibit a nontrivial lower bound [23] such that for three-dimensional systems it reads as

$$I_\rho I_\gamma \geq 36. \tag{6}$$

Unlike, the Shannon entropy that satisfy the *BBM* inequality, the Fisher information fulfills the Stam inequalities [24], $I_\rho \leq 4\langle p^2\rangle$, $I_\gamma \leq 4\langle r^2\rangle$ and the Cramer–Rao inequalities [25] $I_\rho \geq \frac{9}{\langle r^2\rangle}$, $I_\gamma \geq \frac{9}{\langle p^2\rangle}$. Generally, for an arbitrary angular momentum quantum number '*l*' of any central potential model, the two products of the Fisher information must satisfy the relation [26],

$$I_\rho I_\gamma \geq 4\langle r^2\rangle\langle p^2\rangle\,[\,2-\frac{2l+1}{l(l+1)}|m|]^2 \tag{7}$$

where m = 0,±1,±2 . . . is the magnetic quantum number. With the help of the definitions of Eq. (1) to Eq. (5), the Shannon power (*J*) in coordinate and momentum space can be defined as:

$$J_\rho = \frac{1}{2\pi e} e^{\frac{2S_\rho}{D}} \tag{8}$$

$$J_\gamma = \frac{1}{2\pi e} e^{\frac{2S_\gamma}{D}} \tag{9}$$

and the Fisher–Shannon product(*P*) in coordinate and momentum space are defined as

$$P_\rho = \frac{I_\rho J_\rho}{D} \tag{10}$$

and

$$P_\gamma = \frac{I_\gamma J_\gamma}{D} \tag{11}$$

which must satisfy the following relation

$$P_{\rho\gamma} = P_\rho P_\gamma \geq 1 \tag{12}$$

where *D* is the spatial dimensions [27]. It is necessary to mention that throughout all the calculations, the values are taken for $D = 3$ and $m = \hbar = e = 1$.

In this article, the solution of the Schrödinger differential equation of a free particle of mass m for the wave functions $\psi(\vec{r})$ for the potential, $V(\vec{r}) = 0$ is obtained by using the method of separation of variables. The momentum space wave function of the solution is obtained by taking the Fourier transform [28] of the coordinate space wave function. Then the wave functions are used to constitute the probability densities both in coordinate and momentum space, which play a vital role for the computation of the numerical values for the Shannon information entropy (*S*), Fisher entropy (*I*) and Fisher-Shannon product (*P*). The aim of this article is to explore the validity of the entropic uncertainty relations such as the Beckner, Bialynicki-Birula and Myceilski (*BBM*) inequality, Stam-Cramer-Rao inequalities (Fisher based uncertainty relation) and Fisher-Shannon product relations of a free particle in three dimensions.

The article is organized as follows: Section-2, the theoretical background has been focused on obtaining the expressions for the free particle wave functions [$\psi(\vec{r})$, $\phi(\vec{p})$] and the probability densities [$\rho(\vec{r})$, $\gamma(\vec{p})$] using the coordinate space wave function and its momentum analog both in coordinate and momentum space.

In Section-3, the expressions for the probability densities [$\rho(\vec{r})$, $\gamma(\vec{p})$] have been used to calculate the numerical values of the Shannon entropy (*S*), Fisher entropy(*I*) and Fisher-Shannon product (*P*) both in coordinate and momentum space for different values of *L* by keeping the linear relation $k = 2p$ throughout the entire calculations. Further the numerical values computed for the Shannon entropy (*S*), Fisher entropy (*I*) and Fisher-Shannon products (*P*) have been put into tabular forms with their respective table numbers.

Finally, Section-4 has been devoted for summarizing the present work with relevant inferences.

2. MATERIALS AND METHODS

Consider a free particle of mass m for which the potential varying as $V(\vec{r}) = 0$ everywhere in space for all values of $\vec{r}$. So, the Hamiltonian is:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2. \tag{13}$$

Thus, its time-independent Schrödinger equation can be written as

$$\hat{H}\psi(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) = E\,\psi(\vec{r}) \tag{14}$$

The expression for the free particle solution can be obtained as the following:

$$\psi(\vec{r}) = A\, e^{i\vec{k}.\vec{r}} \tag{15}$$

where *A* is the normalization constant.

$$\therefore\ \psi^*(\vec{r}) = A^* e^{-i\vec{k}.\vec{r}} \tag{16}$$

In the latter case, normalization of the wave functions is carried out by defining the domain of the wave function $\psi(\vec{r})$ to an arbitrarily large but finite cubical box of side L centered at the origin.

The wave function $\psi(\vec{r})$ is said to be normalized if

$$\iiint_{-\infty}^{\infty} \psi^*(\vec{r})\, \psi(\vec{r}) d^3r = 1 \tag{17}$$

In this case, the box is considered to be of finite length *L*.

Then by normalization condition,

$$A^*A \iiint_0^L e^{-i\vec{k}.\vec{r}}\, e^{i\vec{k}.\vec{r}}\, d^3r = 1$$

Thus giving, $A = L^{-3/2}$.

In three dimensional representations, the normalized wave function can be expressed as

$$\psi(\vec{r}) = L^{-3/2}\, e^{i\vec{k}.\vec{r}} \tag{18}$$

To find the momentum representation of the coordinate space wave function it needs the use of the Fourier transform pair given below

$$f(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \iiint_{-\infty}^{\infty} g(\vec{k})\, e^{i\vec{k}.\vec{r}} d^3k \tag{19}$$

where,

$$g(\vec{k}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \iiint_{-\infty}^{\infty} f(\vec{r})\, e^{-i\vec{k}.\vec{r}} d^3r. \tag{20}$$

Accordingly, the momentum space wave function, $\phi(\vec{p})$ of the particle is obtained by taking Fourier transform of the coordinate space wave function $\psi(\vec{r})$ as

$$\phi(\vec{p}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \iiint_{-\infty}^{\infty} \psi(\vec{r}) e^{-i\vec{p}.\vec{r}} d^3r\ . \tag{21}$$

The momentum representation of the coordinate space wave function $\psi(\vec{r})$ can be written as $\phi(\vec{p}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \iiint_{-\infty}^{\infty} \psi(\vec{r}) e^{-i\vec{p}.\vec{r}} d^3r$

$$= \frac{1}{(2\pi)^{\frac{3}{2}}} L^{-3/2} \iiint_0^L e^{i\vec{k}.\vec{r}}\, e^{-i\vec{p}.\vec{r}}\, d^3r$$

$$= \frac{1}{(2\pi)^{\frac{3}{2}}} L^{-3/2} \iiint_0^L e^{i\vec{k}.\vec{r} - i\vec{p}.\vec{r}}\, d^3r$$

Let, $x = cos\theta$, $d^3r = r^2\, dr\, d\Omega$ and $d\Omega = sin\theta\, d\theta\, d\varphi$

Substituting these values, the above expression for the momentum space wave function becomes as under:

$$\phi(\vec{p}) = \frac{1}{(2\pi\, L)^{\frac{3}{2}}} \int_0^L r^2 dr \int_0^{\pi} e^{i(k-p)r\, cos\theta} sin\theta d\theta \int_0^{2\pi} d\varphi$$

$$= \frac{4\pi}{(2\pi\, L)^{\frac{3}{2}}} \int_0^L r^2 \frac{\sin(k-p)r}{(k-p)r}\, dr$$

Thus giving,

$$\emptyset(\vec{p}) = \frac{\sqrt{\frac{2}{\pi}}\,(L(-k+p)\cos[L(k-p)] + \sin\,[L(k-p)]}{L^{3/2}\,(k-p)^3}\ . \tag{22}$$

The probability densities of the particle in coordinate and momentum spaces are denoted respectively by the following expressions

$$\rho(\vec{r}) = \psi^*(\vec{r})\, \psi(\vec{r}) = |\psi(\vec{r})|^2 \tag{23}$$

and

$$\gamma(\vec{p}) = \phi^*(\vec{p})\phi(\vec{p}) = |\phi(\vec{p})|^2. \tag{24}$$

3. RESULTS AND DISCUSSION

In this section the numerical values for the Shannon information entropy (*S*) and Fisher information entropy (*I*), Shannon powers (*J*) and Fisher-Shannon products(*P*) both in coordinate and momentum space for the particle are calculated.

In view of Eq.(18), we obtain

$$\psi(\vec{r}) = L^{-3/2}\, e^{i\vec{k}.\vec{r}}\ .$$
$$\therefore \psi^*(\vec{r}) = L^{-3/2}\, e^{-i\vec{k}.\vec{r}}\ .$$

The coordinate space and momentum space probability density are obtained by using the expressions of the Eq. (23) and Eq. (24) respectively as follows:

$$\rho(\vec{r}) = \psi^*(\vec{r})\, \psi(\vec{r}) = |\psi(\vec{r})|^2 = \frac{1}{L^3} \tag{25}$$

and

$$\gamma(\vec{p}) = \phi^*(\vec{p})\phi(\vec{p}) = |\phi(\vec{p})|^2 = \left[\frac{2(L(-k+p)\cos\,[L(k-p)] + \sin\,[L(k-p)])^2}{L^3\,(k-p)^6\,\pi}\right]. \tag{26}$$

The numerical values of the coordinate space Shannon entropy ($\boldsymbol{s_\rho}$) and the momentum space Shannon entropy (s_γ) have been computed with the help of the Eq. (2) and Eq. (3) for different values of *L* by keeping $k = 2p$. These computed values along with the Shannon entropy sums ($s_\rho + s_\gamma$) have been put into a tabular form and the same has been denoted by 'Table 1'.

It can be observed from Table 1 that the numerical values computed for the Shannon information entropies are satisfying the Beckner, Bialynicki-Birula and Myceilski (*BBM*) inequality relation, $S_\rho + S_\gamma \geq D(1 + ln\pi)$ i.e. $S_\rho + S_\gamma \geq 6.434$.

Table 1. The numerical values for the Shannon entropies in coordinate and momentum space along with the Shannon entropy sum

L	s_ρ	s_γ	$(s_\rho + s_\gamma)$
1	0	22.4242	22.4242
2	8.7103	13.6678	22.3781
3	13.8055	8.6201	22.4256
4	17.4206	4.9956	22.4162
5	20.2247	2.1967	22.4214
6	22.5159	-0.1134	22.4025
7	24.4530	-2.0441	22.4089
8	26.1310	-3.7176	22.4134
9	27.6111	-5.2118	22.3993
10	28.9351	-6.5222	22.4129

Similarly, the coordinate space Fisher information entropy (I_ρ) and the momentum space Fisher information entropy (I_γ) have been calculated by employing the Eq. (4) and Eq. (5) and the calculated values have been put into a tabular form along with their Fisher information product ($I_\rho\, I_\gamma$). Accordingly, the same has been denoted as 'Table 2'.

From Table 2, it can be found that the values obtained for the Fisher information entropy are satisfying the Stam-Cramer-Rao inequalities or the Fisher based uncertainty relation and also exhibiting a nontrivial lower bound [23] such that $I_\rho I_\gamma \geq 36$.

Table 2. The numerical values for the Fisher information entropies in coordinate and momentum space along with the Fisher information product

L	I_ρ	I_γ	$I_\rho\, I_\gamma$
1	12.5663	8.3775	105.2741
2	3.1416	33.5103	105.2759
3	1.3962	75.3982	105.2709
4	0.7854	134.0412	105.2759
5	0.5026	209.4395	105.2642
6	0.3491	301.5929	105.2860
7	0.2565	410.5014	105.2936
8	0.1963	536.1651	105.2492
9	0.1551	678.5840	105.2483
10	0.1257	837.7580	105.3062

The values of the Shannon power (J_ρ and J_γ) in coordinate and momentum space have been computed by employing the Eq. (8) and Eq. (9) with the help of the values of the Shannon entropies (s_ρ and s_γ) obtained from Table 1. Thereafter, the computed values of the coordinate and momentum space Shannon powers (J_ρ and J_γ) have been put into a tabular form as below:

Table 3. The numerical values for the Shannon power in coordinate and momentum space

L	J_ρ	J_γ
1	0.1592	494643.8517
2	52.9312	1442.2984
3	1580.9691	49.8433
4	17599.9843	4.4484
5	114148.2466	0.6884
6	525824.7656	0.1476
7	1912885.3052	0.04074
8	5854922.3406	0.01335
9	15705527.7000	0.0049
10	37988471.5407	0.0021

Further, the numerical values obtained from Table 2 for the Fisher information entropies (I_ρ and I_γ) and for the Shannon powers (J_ρ and J_γ) from Table 3 have been used respectively to compute the corresponding Fisher–Shannon products ($P_\rho$and P_γ) in coordinate and momentum space with the help of the Eq. (10) and Eq. (11). And then these computed values for the coordinate and momentum space Fisher–Shannon products (P_ρ and P_γ) have been put into a tabular form and is denoted by 'Table 4'.

It can be verified from the Table 4 that the numerical values obtained for the Fisher–Shannon products (P_ρ and P_γ) in coordinate and momentum space are validating the relation expressed in Eq. (12), $P_{\rho\gamma} = P_\rho\, P_\gamma \geq 1$.

Table 4. The numerical values for the Fisher-Shannon product in coordinate and momentum space

L	P_ρ	P_γ
1	0.6667	1381292.9560
2	55.4296	16110.6174
3	735.7830	1252.6974
4	4607.6759	198.7541
5	19123.6362	48.0579
6	61181.4642	14.8344
7	163519.8122	5.5743
8	383185.1508	2.3858
9	812185.1891	1.1151
10	1591210.4446	0.0575

4. CONCLUSION

In the present article, the plane wave solution for a free particle is considered in three dimensions and the momentum space wave function is obtained by using the Fourier transform of the coordinate space wave function. The coordinate and momentum space wave functions have been used to constitute the corresponding probability densities. Then the numerical values for the Shannon and Fisher information entropies for the different values of L have been computed both in coordinate and momentum space. All the quantities have been measured in atomic units ($m = \hbar = e = 1$) by keeping $k = 2p$ throughout the entire calculations. Further, the values of the Shannon and Fisher information entropies are used to calculate the corresponding Shannon powers (J_ρ and J_γ) and the Fisher-Shannon products (P_ρ and P_γ) in coordinate and momentum space. The calculated numerical values for Shannon powers (J_ρ and J_γ) and the Fisher-Shannon products (P_ρ and P_γ) can be observed from the Table 3 and Table 4 respectively. It is mentioned that Shannon entropy sum ($S_\rho + S_\gamma$) contains the entire information of the systems and it also obeys the well-known lower bound inequality $(S_\rho + S_\gamma) \geq D(1 + ln\pi)$. From Table 1 it can be noticed that the momentum space Shannon information entropy (s_γ) contains negative values. Negative values mean that Shannon entropy is highly localized. It is one of the consequences of the *BBM* inequality which represents the lower bound values of the Shannon entropy sum such that if the coordinate entropy increases then the momentum entropy will decrease in such a way that their sum bounds above (*BBM*) inequality. The other reason for this to happen is the confinement effect. In the region(s) where the confinement effect becomes rigorous there the values of the Shannon information entropy may assume negative values. This results has a simple explanation in quantum context, when the values of *L* (here considered in momentum space) are reasonably increasing, the probability densities then becoming smaller and smaller. In this situation, the quantity, $-\gamma \, ln \, \gamma$ becomes less than zero giving rises to the negative value(s) of s_γ. In Shannon's work, the continuous entropy was seen to be negative. The electron-electron correlation can, however, have major influence(s) on the information theoretic measures such as the Shannon and Fisher entropies in atomic and molecular systems. Here in this article, the correlation effect has not been considered. It can also be followed from Table 1 that the values ($S_\rho + S_\gamma$) are not only validating the *BBM* inequality but also satisfying the lower bound. Meanwhile the values of the entropic sum ($S_\rho + S_\gamma$) presented in Table 1 are higher than that of the value of the lower bound inequality in three dimensional systems. In general, the explicit derivations of information entropies are quite difficult. In particular, the derivations of analytical expressions of the information theoretic measures are almost impossible. To overcome such difficulties the numerical approach is proved to be a robust and effective instrument and it can be used in calculating the integrals containing probability densities and all that involve in such information theoretic measures. Accordingly, depending upon the numerical calculations, it can be found from the Table 2 that the numerical values obtained for the product of the Fisher information entropies ($I_\rho I_\gamma$) are greater than 105.2483. Thus, the computed values for $I_\rho I_\gamma$, however, much larger in this case, are validating the Stam-Cramer-Rao inequalities or Fisher based uncertainty relation $I_\rho I_\gamma \geq 36$. The Table 3 contains the values of the Shannon powers (J_ρ and J_γ) and the Table 4 contains the values of the Fisher–Shannon products (P_ρ and P_γ) in coordinate and momentum space. The values of the coordinate space Shannon powers (J_ρ) and the coordinate space Fisher-Shannon products (P_ρ) remain increasing with the increase of the length *L* while the opposite trend can be observed in case of the momentum space Shannon powers (J_γ) and the momentum space Fisher-Shannon products (P_γ). In both cases, the computed values of the Shannon power and the Fisher-Shannon product are found to be increasing in coordinate space and decreasing in momentum space rapidly with the increase of the value of *L*. The reason behind this, can be understood well from the definitions of Shannon powers mentioned in Eq. (8) and Eq. (9), where the numerical values of S_ρ and S_γ, used in the exponents, are responsible for obtaining such kind of increased or decreased values as outputs. The similar effect can be observed in case of the values obtained for the Fisher-Shannon product also and the same can be understood by the virtue of the Eq. (10) and Eq. (11) respectively. These increased or decreased values of the numerical outputs found in Table 3 and Table 4 turn out as the key factor in obtaining the huge numerical values for the Fisher-Shannon products ($P_\rho \, P_\gamma$). The Table 4 reveals that the values of the products ($P_\rho\, P_\gamma$) of the Fisher–Shannon products are also validating the relation $P_{\rho\gamma} = P_\rho\, P_\gamma \geq 1$. It can be realized that the values presented in Table 1, Table 2, Table 3 and Table 4 are very much dependent on the different values of the length of the cubical box *L* and the linear relation between the wave vector (*k*) and the momentum (*p*). In this work, the solution has been restricted to plane wave solutions only as the spherical wave solution involves sound mathematical knowledge of the spherical Bessel functions and the spherical Neumann functions. It remains an interesting curiosity to investigate the efficacy of this work to other global measures, such as Renyi entropy, Tsallis entropy and Onicescu information and some of these works may be undertaken in future.

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COMPETING INTERESTS

Author has declared that no competing interests exist.

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