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Shannon Information Entropy Sum of a Free Particle in Three Dimensions Using Cubical and Spherical Symmetry

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Abstract

In this paper, the plane wave solutions of a free particle in three dimensions for Cubical and Spherical Symmetry have been considered. The coordinate space wave functions for the Cubical and Spherical Symmetry are obtained by solving the Schrödinger differential equation. The momentum space wave function is obtained by using the operator form of an observable in the case of Cubical Symmetry. For Spherical Symmetry, the same is obtained by taking the Fourier transform of the respective coordinate space wave function. The wave functions have been used to constitute probability densities in coordinate and momentum space for both the symmetries. Further, the Shannon information entropy has been computed both in coordinate and momentum space respectively for $L = 1, 2,3,4, \dots ,10$ (L is the length of the side of the cubical box) values for Cubical Symmetry and for $L = 1, 2,3,4,5$ values in Spherical Symmetry keeping $k = 2p$ (k is the wave vector and p is the momentum of the free particle) constant. The values obtained for the Shannon information entropies are found to satisfy the Bialynicki-Birula and Myceilski (*BBM*) inequality at larger L values ($L \geq 9$) in case of Cubical Symmetry and for values of $L = 1, 2,3,4$ and 5 in Spherical Symmetry.

Keywords: Bialynicki-Birula and Myceilski inequality; Cubical symmetry; Spherical symmetry; Operator form; Shannon information entropy.

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1. Introduction

Information theory has its primary roots in two classic papers by Claude E. Shannon in 1948 [1]. It should come as no surprise that information theory provides a way to measure uncertainty. It has subsequently been applied to areas ranging from the calculation of the ability of a material to be penetrated by charged particles [2] to analyzing binding sites on nucleotide sequences [3]. Shannon's purpose was to develop a mathematical theory to quantitatively analyze the passage of information from a source through an information channel to a receiver. A key measure in information theory is 'entropy'. Entropy quantifies the amount of uncertainty involved in the value of a random variable or the outcome of a random process. Intuitively, uncertainty could be equated with a lack of

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information. Simply, entropy is the amount of information contained in a system. This is a term that reveals the amount of disorderliness in the system. A plain hypothetical system with no disorder or in perfect order has no information; only when the disorder sets into the system, it starts having information that is proportional to the disorder in the system. Information entropy is typically measured in ‘bits’ alternatively called "Shannon’s". There are different types of entropy measures, namely Shannon information entropy *(S)*, Fisher information entropy *(I)*, R*é*nyi entropy *(R)*, Tsallis entropy *(T)* etc. [4-8]. In this paper, the interest is concentrated only on the Shannon information entropy (*S*). Information entropy is subject characterized by the charge density [9] or the probability density of the system corresponding to changes in some observable such that the higher the probability density lower is the information. So, the lower the entropy is, the more concentrated is the wave function. Shannon information entropy (*S*) is very insensitive to changes in the distribution over a small-sized region and thus possesses a global character. The coordinate space Shannon information entropy (s_ρ) [10] for a normalized wave function $\psi(\vec{r})$ is written by

$$s_\rho = -\iiint \rho(\vec{r}) ln\, \rho(\vec{r}) d^3r \tag{1}$$

where,

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

The probability density $\rho(\vec{r})$ is also normalized to unity.
Correspondingly, the momentum space Shannon information entropy (s_γ) is defined as

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

Here $\gamma(\vec{p}) = \emptyset^*(\vec{p})\emptyset(\vec{p}) = |\emptyset(\vec{p})|^2$ is the probability density of the particle, where the momentum space wave function $\phi(\vec{p})$ is obtained by taking the Fourier transform [11] of the coordinate space wave function $\psi(\vec{r})$. The coordinate and momentum space information entropies [12], as defined by Eq. (1) and (3), allowed Bialynicki-Birula and Mycielski [13] to introduce another version of the uncertainty relation, which for a three-dimensional system reads as follows:

$$S_\rho + S_\gamma \geq 3(1 + ln\pi) \tag{4}$$

This relation was conjectured independently in 1957 by Everett [14] and Hirschman [15] and proved in 1975 by Beckner [16] and Bialynicki-Birula and Mycielski. It provides a strict improvement on the standard Heisenberg relation [17]. Eq. (4) is known as the *BBM* inequality. Because the information entropy measures the localization of a distribution, Eq. (4) places a limit on the simultaneous localization of the coordinate and momentum distributions. If one of the entropies becomes small, then the other must become large enough to preserve the inequality. This is philosophically consistent with the Heisenberg uncertainty principle. *BBM* also showed that the Heisenberg inequality could be derived from their entropic uncertainty relation. The *BBM* entropic uncertainty relation has a constant lower bound and thus overcomes one of the limitations of the Heisenberg inequality. These entropic uncertainty relations have recently received considerable interest in the literature. The interested reader is referred to Majerník and Richterek [18], Yáñez *et al*. [19], Majerník and Majerníková [20], and references therein. A few years ago, Montgomery [21] considered an infinite square well of length L, centered at the origin and confined to the interval $-L/2 \leq x \leq L/2$. The system is symmetric about $x = 0$, and for a quantum mechanical particle defined by this system, the solution is given by the wave function described by $\psi_n(x) = \sqrt{\frac{2}{L}}\cos(\frac{(2n-1)\pi x}{L})$, where $n = 1,2,3$ .... In his work, he found that the sum of the Shannon information entropies $(S_\rho + S_\gamma)$ in one dimension ranged from 2.2120 to 3.0175, which satisfies *BBM* inequality and which is a quantitative relation between the coordinate space and momentum space uncertainties. This inequality is independent of the value of n. Henry E. Montgomery, Jr. compared his work to work done by Majerník *et al*., where they showed that the limiting value for the sum of the Shannon information entropies is $(S_\rho + S_\gamma) \approx 2.6564$. In his paper, Henry E. Montgomery Jr. used the wave function to treat the Shannon information entropy in one dimension and examined the entropic uncertainty relation. This paper examines the same uncertainty relation (BBM inequality) using the cubical and spherical symmetric plane wave solutions in three dimensions.

The Materials and Method section shows how the wave functions are obtained in coordinate and momentum space both for the Cubical and Spherical Symmetry, along with some specific assumptions and brief derivation. The coordinate space wave functions for the Cubical and Spherical Symmetry are obtained by solving the Schrödinger differential equation, whereas the momentum space wave function is obtained by using the operator form of an observable in the case of Cubical Symmetry, and the same is found by taking the Fourier transform of the respective coordinate space wave function in the case of Spherical Symmetry. Then these wave functions have been used to constitute the probability densities both in coordinate and momentum space for both the symmetries. The length of the side of the cubical box is taken as L, and the value of the momentum of the free particle is taken as

$$\begin{aligned} p &= \hbar k \\ &= \frac{2\pi\hbar}{\lambda} \\ &\approx \frac{2\pi\hbar}{2L} \\ &\approx \pi\hbar/L \end{aligned}$$
(assuming the wavelength, $\lambda \approx 2L$, where k is the wave vector).

Next, in the Results section, the Shannon information entropy has been computed using the respective probability densities for Cubical Symmetry for $L = 1, 2,3,4 \ldots 10$ values both in coordinate and momentum space. The same is computed for Spherical Symmetry for $L = 1, 2,3,4,$ and 5 values in both spaces keeping $k = 2p$ constant. Thereafter the computed values of the Shannon information entropies for both symmetries are put into tabular forms separately. Further, the values of the Shannon information entropies presented in Table 1 and Table 2 have been represented graphically. The graphical representation shows the variations of the Shannon entropy in coordinate space and momentum space along with the Shannon entropy sum depending upon the different values of the length of the box (L). The numerical values obtained for the Shannon information entropies are found to satisfy the Bialynicki-Birula and Myceilski (*BBM*) inequality at larger L values ($L \geq 9$) in the case of the Cubical Symmetry and for values of $L = 1, 2,3,4$ and 5 in Spherical Symmetry. It is to remember that we have used the atomic units ($m = \hbar = e = 1$) throughout our entire calculations.

Finally, an outlook on the present work has been summarized with some concluding remarks.

2. Materials and Method

2.1. *The wave function and probability density in cubical symmetry*

The exact solutions of Schrödinger wave equation plays an important role in solving and understanding some of the complicated systems in physics. Such solutions can be used as valuable tools in checking, solving, and improving models for the systems involving potentials like 'the Eckart potential', the Rosen-Morse potential, etc. [22]. Now, the Schrödinger differential equation for a free particle of mass m for the wave functions $\psi_k(\vec{r})$ with the potential varying as $V(\vec{r}) = 0$ everywhere in space can be written as

$$-\frac{\hbar^2}{2m}\nabla^2\psi_k(\vec{r}) = E\psi_k(\vec{r}) \tag{5}$$

The solutions for this equation can be expressed using the separation of variables as

$$\psi_k(\vec{r}) = A(\vec{k})e^{i\vec{k}.\vec{r}} \tag{6}$$

These solutions represent plane waves or the momentum eigenfunctions, and they are infinite in number since values of k_x , k_y , k_z are not restricted along with the condition $k_x^2 + k_y^2 + k_z^2 = K^2 = \frac{2mE}{\hbar^2}$. The momentum wave functions $A(\vec{k})$ are the amplitudes of the possible momentum eigenfunctions that superimpose to form the wave functions $\psi_k(\vec{r})$. The wave functions $\psi_k(\vec{r})$ sometimes have a continuous range of eigenvalues and sometimes discrete eigenvalues. In the latter case, normalization of the wave functions is carried out by defining the wave function on an arbitrarily large but finite cubical box of side L centered at the origin.

Taking the complex conjugate of the wave function obtained in Eq. (6), we have

$$\psi_k^*(\vec{r}) = A^*(\vec{k})e^{-i\vec{k}.\vec{r}} \tag{7}$$

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

$$\iiint_{-\infty}^{\infty} \psi_k^*(\vec{r})\,\psi_k(\vec{r})d^3r = 1 \tag{8}$$

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

Then by normalization condition,

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

$$\therefore\ |A|^2 \int_0^L dx \int_0^L dy \int_0^L dz = 1$$

$$\therefore\ A = \frac{1}{L^{3/2}}$$

Thus giving, $A(\vec{k}) = L^{-3/2}$

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

$$\psi(\vec{r}) = L^{-3/2}\, e^{i\vec{k}.\vec{r}} \tag{9}$$

and the complex conjugate wave function in coordinate space is given by

$$\therefore\ \psi^*(\vec{r}) = L^{-3/2}\, e^{-i\vec{k}.\vec{r}} \tag{10}$$

The probability density in coordinate space is

$$\rho(\vec{r}) = \psi^*(\vec{r})\psi(\vec{r}) = \frac{1}{L^3} \tag{11}$$

The momentum space wave function is obtained by using the operator form of an observable $\varphi(p_x)$ and the eigenfunctions are given by

$$\hat{x}_p\varphi(p_x) = x_0\varphi(p_x) \tag{12}$$

$$\therefore\ i\hbar\frac{\partial}{\partial p_x}\varphi(p_x) = x_0\varphi(p_x)$$

Where the operator $\hat{x}_p = i\hbar\frac{\partial}{\partial p_x}$,

$$\therefore\ \frac{\partial\varphi(p_x)}{\varphi(p_x)} = \frac{x_0}{i\hbar}$$

$$\therefore\ \varphi_x(p_x) = C\, e^{-\frac{ix_0p_x}{\hbar}} \tag{13}$$

The suffix $x\ to\ \varphi$ indicates that these are eigenfunctions of x in momentum space. The eigenvalues form a continuous set. The normalization constant '*C*' is found by Dirac-delta normalization:

$$\int_{-\infty}^{\infty}\varphi_{x_0}(p_x)\varphi^*_{x'_0}dp_x = \delta(x_0 - x'_0) \tag{14}$$

Now from the Eq. (14) we can write

$$L.H.S. = \int_{-\infty}^{\infty}\varphi_{x_0}(p_x)\varphi^*_{x'_0}dp_x$$

$$= \int_{-\infty}^{\infty} C\, e^{-\frac{ix_0p_x}{\hbar}}C^*e^{-\frac{ix'_0p_x}{\hbar}}\, dp_x$$

$$= |C|^2\int_{-\infty}^{\infty} e^{-\frac{i(x_0-x'_0)p_x}{\hbar}}\, dp_x$$

$$= |C|^2 2\pi\delta(\frac{x'_0-x_0}{\hbar})$$

$$= |C|^2 2\pi\hbar\, \delta(x'_0 - x_0) \tag{15}$$

and

$$R.H.S. = \delta(x'_0 - x_0) \tag{16}$$

Now, from Eq. (15) and Eq. (16) we have

$$\therefore\ |C|^2 2\pi\hbar\,\delta(x_0' - x_0) = \delta(x_0' - x_0)$$

Thus giving,

$$C = \frac{1}{(2\pi\hbar)^{1/2}} \tag{17}$$

In p-representation, for a particle localized at x_0 , the x-wave functions are

$$\varphi_x(p_x) = \frac{1}{(2\pi\hbar)^{1/2}}\ e^{-\frac{ix_0 p_x}{\hbar}} \tag{18}$$

Then the momentum space wave function in three dimensions can be written as

$$\varphi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{-i\,\vec{p}.\vec{r}/\hbar} \tag{19}$$

Taking the complex conjugate of the Eq. (19) we have

$$\therefore\ \varphi^*(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\,\vec{p}.\vec{r}/\hbar} \tag{20}$$

The probability density in momentum space is

$$\gamma(\vec{p}) = \varphi^*(\vec{p})\varphi(\vec{p})$$

$$= [\frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}.\vec{r}/\hbar}\ \frac{1}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}.\vec{r}/\hbar}]$$

$$= \frac{1}{(2\pi\hbar)^3}$$

$$\therefore\ \gamma(\vec{p}) = \frac{1}{(2\pi\hbar)^3} \tag{21}$$

2.2. *The wave function and probability density in spherical symmetry*

Considering the plane wave solutions, the wave function in coordinate space can be written as

$$\psi(\vec{r}) = N\ e^{i\vec{k}.\vec{r}} \tag{22}$$

where 'N' is the normalization constant, and for a spherically symmetric space, the value of 'N' is obtained as follows,

$$|N|^2 \iint_0^L r^2 dr \iint_0^\pi Sin\theta\ d\theta \iint_0^{2\pi} d\varphi = 1$$

$$\therefore\ N = [\frac{3}{4\pi L^3}]^{1/2}$$

The normalized wave function is thus obtained as

$$\therefore\ \psi(\vec{r}) = [\frac{3}{4\pi L^3}]^{1/2}\ e^{i\vec{k}.\vec{r}} \tag{23}$$

Again, the complex conjugate wave function for Eq. (23) we can write,

$$\psi^*(\vec{r}) = [\frac{3}{4\pi L^3}]^{1/2}\ e^{-i\vec{k}.\vec{r}} \tag{24}$$

The probability density in coordinate space is

$$\rho(\vec{r}) = \psi^*(\vec{r})\psi(\vec{r})$$

$$= [\frac{3}{4\pi L^3}]^{1/2}\, e^{-i\vec{k}.\vec{r}} [\frac{3}{4\pi L^3}]^{1/2}\, e^{i\vec{k}.\vec{r}}$$

$$= \frac{3}{4\pi L^3}$$

$$\therefore\ \rho(\vec{r}) = \frac{3}{4\pi L^3} \tag{25}$$

To find the momentum representation of the coordinate space wave function, we use the generalized expressions as given below,

$$f(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \iiint_{-\infty}^{\infty} g(\vec{k})\, e^{i\,\vec{k}\,.\vec{r}} d^3k \tag{26}$$

where

$$g(\vec{k}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \iiint_{-\infty}^{\infty} f(\vec{r})\, e^{-i\,\vec{k}\,.\vec{r}} d^3r. \tag{27}$$

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

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

As, $\psi(\vec{r}) = N\, e^{i\vec{k}.\vec{r}}$

Now the momentum space wave function can be obtained as,

$$\varphi(\vec{p}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \iiint_{-\infty}^{\infty} N\, e^{i\vec{k}.\vec{r}}\, e^{-i\,\vec{p}\,.\vec{r}}\, d^3r \tag{28}$$

Using the spherically symmetric property of the wave function we have,

$$\varphi(\vec{p}) = N\sqrt{\frac{2}{\pi}}\, \frac{(\,L(-k+p)Cos[L(k-p)]+Sin[L(k-p)]\,)}{(k-p)^3} \tag{29}$$

Substituting the values of wave vector $k = 2p$ and putting $L = 1$ in Eq. (29) we get,

$$\varphi(\vec{p}) = N\sqrt{\frac{2}{\pi}}\, \frac{(\,-p\;Cos[p]+Sin[p]\,)}{(p)^3} \tag{30}$$

Using the normalization condition for a spherically symmetric wave function from Eq. (30), we get the value of the normalization constant as

$$N = \frac{1}{2}\sqrt{\frac{3}{2\pi}}\,.$$

Thus we get the normalized momentum space wave function as

$$\varphi(\vec{p}) = \sqrt{\frac{3}{2}}\, \frac{(\,-p\;Cos[p]+Sin[p]\,)}{(p)^3\pi} \tag{31}$$

and the complex conjugate momentum space wave function can be written as,

$$\therefore\ \varphi^*(\vec{p}) = \sqrt{\frac{3}{2}}\, \frac{(\,-p\;Cos[p]+Sin[p]\,)}{(p)^3\pi} \tag{32}$$

The probability density in momentum space for $k = 2p$ and $L = 1$ is

$$\gamma(\vec{p}) = \varphi^*(\vec{p})\varphi(\vec{p}) = \frac{3}{2}\frac{(-p\,Cos[p]+Sin[p])^2}{(p)^6\pi^2} \tag{33}$$

It is necessary to follow that the value of 'N' is different for different L values while $k = 2p$ remains constant. When $L = 2$; the value of the normalization constant obtained is as $N = \frac{1}{2}\sqrt{\frac{3}{2\pi}}$ and for $L = 3, 4,5, \dots$ the values of the normalization constant 'N' are obtained respectively as follows

$N = \frac{1}{6}\sqrt{\frac{1}{\pi}}, \frac{1}{16}\sqrt{\frac{3}{\pi}}, \frac{1}{10}\sqrt{\frac{3}{5\pi}}$ and so on. Then the corresponding wave functions can be written with their respective values of the normalization constant 'N'.

3. Results and Discussion

In this section, the numerical values for the Shannon information entropies (S), both in coordinate and momentum space of the free particle for Cubical and Spherical Symmetry, are calculated. To obtain these values, the expressions of the respective probability densities in coordinate and momentum space are employed. In the following cases, the values of $L = 1$ and $k = 2p$ have been considered only, and the rest of the calculations have been computed using all other respective values of L and k accordingly.

3.1. *Shannon information entropies for cubical symmetry case*

The probability density in coordinate space obtained is given by

$$\rho(\vec{r}) = \psi^*(\vec{r})\psi(\vec{r})$$
$$= \frac{1}{L^3}$$

The coordinate space Shannon entropy is obtained as

$$s_\rho = -\iiint \rho(\vec{r})ln\,\rho(\vec{r})d^3r$$
$$= -\int_0^L \left(\frac{1}{L^3}\right) ln\left[\frac{1}{L^3}\right] dx \int_0^L dy \int_0^L dz$$
$$= -\frac{1}{L^3}\, ln\left[\frac{1}{L^3}\right].L^3$$
$$= 3\,ln[L]$$
$$\therefore\ s_\rho = 3\,ln[L] \tag{34}$$

The probability density in momentum space for the wave function $\varphi(\vec{p})$ obtained from the Eq. (31) is given by

$$\gamma(\vec{p}) = \varphi^*(\vec{p})\varphi(\vec{p})$$
$$= \frac{1}{(2\pi\hbar)^3}$$

To calculate the momentum space Shannon entropy, the dimension of the wavelength is considered to be approximately equal to the length of the cubical box, i.e., $\lambda \approx 2L$, and the momentum of the free particle will then be written as

$$p = \hbar k$$
$$= \frac{2\pi\hbar}{\lambda}$$
$$\approx \frac{2\pi\hbar}{2L}$$
$$\therefore p \approx \frac{\pi\hbar}{L} \quad (35)$$

Using Eq. (21) and Eq. (35) the momentum space Shannon entropy is computed as

$$s_\gamma = -\iiint \gamma(\vec{p}) ln\, \gamma(\vec{p})\, d^3p$$
$$= -\iiint_0^{\frac{\pi\hbar}{L}} \frac{1}{(2\pi\hbar)^3} ln(\frac{1}{(2\pi\hbar)^3})\, d^3p$$
$$= -\frac{1}{(2\pi\hbar)^3} ln(\frac{1}{(2\pi\hbar)^3}) \int_0^{\frac{\pi\hbar}{L}} dp_x \int_0^{\frac{\pi\hbar}{L}} dp_y \int_0^{\frac{\pi\hbar}{L}} dp_z$$
$$= -\frac{1}{(2\pi\hbar)^3} ln\left(\frac{1}{(2\pi\hbar)^3}\right) (\frac{\pi\hbar}{L}) (\frac{\pi\hbar}{L}) (\frac{\pi\hbar}{L})$$
$$= \frac{1}{8L^3} ln[(2\pi\hbar)^3]$$
$$= \frac{3\, ln(2\pi)}{8L^3} \qquad [\because m = \hbar = e = 1]$$
$$\therefore\ s_\gamma = \frac{3\, ln(2\pi)}{8L^3} \quad (36)$$

Further, the numerical values for the Shannon information entropies, in this case, both in coordinate and momentum space, have been calculated for different values of L keeping $k = 2p$ constant, and the obtained values have been put into a tabular form as follows.

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

L	s_ρ	s_γ	$(s_\rho + s_\gamma)$
1	0	0.6892	0.6892
2	2.0794	0.0862	2.1656
3	3.2958	0.0255	3.3213
4	4.1588	0.0107	4.1695
5	4.8283	0.0055	4.8336
6	5.3752	0.0032	5.3784
7	5.8377	0.0020	5.8397
8	6.2383	0.0013	6.2396
9	6.5916	0.0009	6.5925
10	6.9077	0.0006	6.9083

3.2. *Shannon information entropies for spherical symmetry case*

The probability density in coordinate space is

$$\rho(\vec{r}) = \psi^*(\vec{r})\psi(\vec{r})$$
$$= [\frac{3}{4\pi L^3}] \quad (37)$$

The coordinate space Shannon entropy is obtained as

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

$$= -\int_0^L [\frac{3}{4\pi L^3}]\, ln\left[\frac{3}{4\pi L^3}\right] r^2\, dr \int_0^\pi Sin\theta\, d\theta \int_0^{2\pi} d\varphi$$

$$= -\, ln\left[\frac{3}{4\pi L^3}\right]$$

$$= ln\left[\frac{4\pi}{3}\right] + 3\, ln[L]$$

$$\therefore s_\rho = 1.432 + 3\, ln[L] \quad (38)$$

The probability density in momentum space for $k = 2p$ and $L = 1$ is given by

$$\gamma(\vec{p}) = \varphi^*(\vec{p})\varphi(\vec{p})$$

$$= \frac{3}{2}\frac{(-p\, Cos[p] + Sin[p])^2}{(p)^6\pi^2} \quad (39)$$

The momentum space Shannon entropy is calculated as

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

$$= -\int_0^\infty p^2\, dp\, \left[\frac{3}{2}\frac{(-p\, Cos[p]+Sin[p])^2}{(p)^6\pi^2}\right] ln\left[\frac{3}{2}\frac{(-p\, Cos[p]+Sin[p])^2}{(p)^6\pi^2}\right] \int_0^\pi Sin\theta d\theta \int_0^{2\pi} d\varphi$$

$$= -4\pi \int_0^\infty p^2 \left[\frac{3}{2}\frac{(-p\, Cos[p]+Sin[p])^2}{(p)^6\pi^2}\right] ln\left[\frac{3}{2}\frac{(-p\, Cos[p]+Sin[p])^2}{(p)^6\pi^2}\right] dp$$

$= 6.78594$ for $k = 2p$ and $L = 1$.

$$\therefore s_\gamma = 6.78594 \quad (40)$$

Further, the numerical values for the Shannon information entropies, in this case, both in coordinate and momentum space, have been calculated for different normalization constant 'N' with different associated L values keeping $k = 2p$ constant and the obtained values have been put into a tabular form as follows.

Table 2. The numerical values for the Shannon information entropies for Spherical Symmetry in coordinate and momentum space along with the Shannon entropy sum.

L	s_ρ	s_γ	$(s_\rho + s_\gamma)$
1	1.4320	6.7859	8.2179
2	3.5114	4.6944	8.2058
3	4.7278	3.4905	8.2183
4	5.5908	2.6250	8.2158
5	6.2603	1.9572	8.2175

3.3. *Graphical representation of the tabular data in case of cubical and spherical symmetry*

The following graphs labeled as Fig. 1. (A), (B), (C), and (D) have been plotted with the help of the data obtained from Table 1 considering the values of the Shannon information entropies in the case of Cubical Symmetry. The graphs represent the variations of the values of the coordinate and momentum space Shannon information entropy values along with the Shannon entropy sum for different values of the box lengths in Cubical Symmetry.

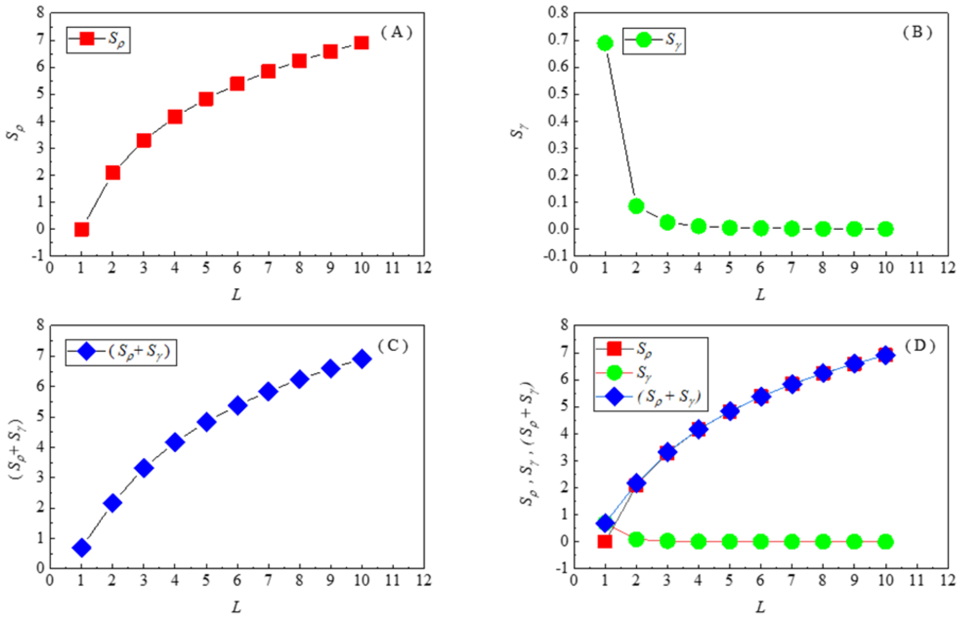

Fig. 1. (A) Shannon information entropy in coordinate space (s_ρ) versus the length of the box (*L*), (B) Shannon information entropy in momentum space (s_γ) versus the length of the box (*L*), (C) Shannon entropy sum ($s_\rho + s_\gamma$) versus the length of the box (*L*), (D) Shannon information entropy in coordinate space (s_ρ), Shannon information entropy in momentum space (s_γ), Shannon entropy sum ($s_\rho + s_\gamma$) versus the length of the box (*L*) for Cubical Symmetry.

In Fig. 1(A), the curve shows the increase in the values of coordinate space Shannon information entropies (s_ρ) with the increase of the length of the box, whereas the opposite nature of the curve for the values of the Shannon information entropies in momentum space (s_γ) is observed in Fig. 1(B). Fig. 1(C) shows the variation in the values of the Shannon entropy sum ($s_\rho + s_\gamma$) for different values of the length of the box. The composite nature of the curves of Fig. 1. (A), (B), and (C) can be observed in Fig. 1(D).

Similarly, the graphs labeled as Fig. 2. (A), (B), (C), and (D) have been plotted with the help of the data obtained from Table 2 considering the values of the Shannon information entropies in case of Spherical Symmetry. The graphs are depicted as follows:

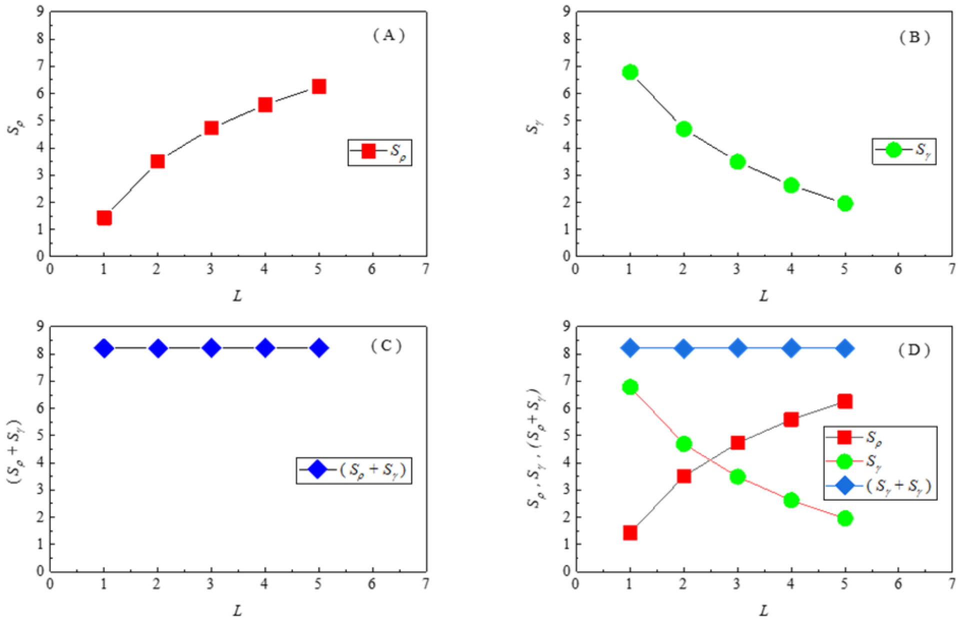

Fig. 2. (A) Shannon information entropy in coordinate space (s_ρ) versus the length of the box (L), (B) Shannon information entropy in momentum space (s_γ) versus the length of the box (L), (C) Shannon entropy sum ($s_\rho + s_\gamma$) versus the length of the box (L), (D) Shannon information entropy in coordinate space (s_ρ), Shannon information entropy in momentum space (s_γ), Shannon entropy sum ($s_\rho + s_\gamma$) versus the length of the box (L) for Spherical Symmetry.

The curve in Fig. 2(A) shows the increase in the values of Shannon information entropies in coordinate space (s_ρ) with the increase of the length of the box, whereas Fig. 2(B) shows the decrease in the values of the Shannon information entropies in momentum space (s_γ). Fig. 2(C) shows a linear variation for the values of the Shannon entropy sum ($s_\rho + s_\gamma$) for different lengths of the box and the same can be verified from the data obtained from Table 2. Moreover, Fig. 2(D) displays the composite nature of the curves of Fig. 2(A), (B), and (C). Thus it can be understood that Figs. 1 and 2 display the same nature of the curves for the values of the coordinate and momentum space Shannon information entropies along with the Shannon entropy sum for both cases of Cubical and Spherical Symmetry. It can be realized clearly that the values of the Shannon information entropies play a complementary role in coordinate and momentum space. When the values of Shannon information entropy augment in coordinate space with the increase of the length of the box, then on the other side, the values of the same diminish in the momentum space. This complementary nature of the Shannon information entropy has been observed consistently in the case of Cubical and Spherical Symmetry.

4. Conclusion

The characterization of information entropic uncertainty relations has become a rich field of study with direct relevance in the modern technological era. In the present work, the plane wave solutions of a free particle in three dimensions have been used. The coordinate space wave functions for the Cubical and Spherical Symmetry are obtained by solving the Schrödinger differential equation. The momentum space wave function is obtained by using the operator form of an observable in the case of Cubical Symmetry, and in the case of Spherical Symmetry, the same is obtained by taking the Fourier transform of the respective coordinate space wave function. These wave functions have been used to constitute the probability densities both in coordinate and momentum space for both the symmetries. Further, the Shannon information entropy has been computed for $L = 1, 2,3,4 \dots 10$ values in coordinate and momentum space for Cubical Symmetry. The same is computed for $L = 1, 2,3,4$ and 5 values in Spherical Symmetry both in coordinate and momentum space, keeping $k = 2p$ constant. The computed values of Shannon information entropy are then put into two Tables. From Table 1, it is noticed that the values obtained for the Shannon information entropies are found to satisfy the Bialynicki-Birula and Myceilski (*BBM*) inequality at larger L values ($L \geq 9$) in the case of the Cubical Symmetry while the Table 2 shows that the same inequality holds good for values of $L = 1, 2,3,4$ and 5 in case of Spherical Symmetry. It can be realized that all calculations regarding the values presented in Table 1 and Table 2 are very much dependent on the different values imposed on the length of the cubical box L and prominently dependent on the assumption of the linear value of wave vector k with the momentum p of the free particle also. The graphs presented in Figs. 1 and 2 have been plotted with the help of the data obtained from Tables 1 and 2, displaying the variations of the Shannon entropy values and Shannon entropy sums for the different values of L in coordinate and momentum space for both the symmetries considered in this work. The graphical representation shows that the values of the Shannon entropy augment in coordinate space, but in momentum space, just the opposite role for the same is observed. This complementary role of the Shannon information entropy is found consistent with the philosophy of the Heisenberg uncertainty principle in preserving the inequality relation such that when the values of Shannon entropy augmented in coordinate space, then the values of the same got diminished in momentum space. In this work, the solution is 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 is expected that this work will help the students and the researcher to acquire basic knowledge about the measures of information entropy and entropic uncertainty relations in the fields of quantum physics and quantum chemistry.

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