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A Theoretical Study on Wave Packet Dynamics Using Information Theory

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Abstract

The article intertwines the study of wave packet dynamics with information-theoretic measurements in one dimensional ($D = 1$) system. A localized wave packet at time $t = 0$ has been considered here and its change at later instant of time t is calculated for the position space wave function. The momentum space wave function is obtained by taking the Fourier transform of the position space wave function at time $t = 0$. These wave functions are then employed to construct the wave packet's respective probability densities in position and momentum space, and later have been used to compute the corresponding position and momentum space Shannon (S) and Fisher information (I) entropies. It has been observed that although the Shannon and Fisher information entropies explicitly depend on the standard deviation, neither the Shannon entropy sum nor the product of Fisher information entropies is. Moreover, for D dimensional systems, the computed values of the Shannon and Fisher entropies are found to satisfy the lower bounds of the Bialynicki-Birula and Myceilski (*BBM*) inequality relation and the Stam-Cramer-Rao inequalities better known as the Fisher based uncertainty relation. Thus, our theoretical study explores the validation of information-theoretic measurements for wave packet dynamics using the basic formulations of information theory.

Keywords: Bialynicki-Birula and Myceilski (*BBM*) inequality; Fisher information entropy; Fisher-based uncertainty relation; Information theory; Shannon information entropy; Wave packet dynamics.

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1. Introduction

Erwin Schrödinger introduced the concept of wave packets that follow a classical trajectory in order to reduce the gap between the classical and quantum descriptions of nature [1]. This approach has culminated in Ehrenfest's theorem, which states that in the classical limit, the quantum mechanical expectation values behave classically [2]. The wave packets had no practical use for a long time because their preparation seemed impossible. However, recent advances in the physics and chemistry of laser interactions with atoms and molecules have brought wave packets and their dynamics into the limelight. Wave packets are being utilized in other areas of physics too. For example, the

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low temperatures achieved in laser cooling lead to cold collisions of atoms, which require a wave packet treatment. The strong possibility of laser-induced excitation and subsequent spontaneous decay during such a collision makes it difficult to use any time-independent methods [3]. Wave packets are also proving useful in atom optics, where the packet represents an atomic matter-wave, and in semiconductor physics. A localized wave function is called a wave packet. A wave packet, therefore, comprises a group of waves of slightly different wavelengths, with phases and amplitudes so chosen such that they interfere constructively over a small region of space, outside of which they produce amplitude that reduces to zero rapidly as a result of destructive interference.

Not only is the wave packet useful in the description of 'isolated' particles confined to certain spatial regions, but they also play a key role in understanding the connection between quantum mechanics and classical mechanics. Therefore, the wave packet concept represents a unifying mathematical tool that can cope with and embody nature's particle-like behavior and its wave-like behavior [4]. In all natural sciences, measurements play a fundamental role. Every measurement has some uncertainty, so the mathematical and 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',which can be termed 'uncertainty'. Since Bohr and Heisenberg formulated, the uncertainty relations have become the landmark of quantum theory. Information theory is primarily rooted in two classic papers by Claude E. Shannon in 1948 [5]. A key measure in information theory is 'entropy'. Entropy is the amount of information contained in a system. It should come as no surprise that information theory provides a way to measure uncertainty. The position–momentum uncertainty principle is likely to be the most prominent difference between classical and quantum physics. The information entropy fits perfectly with the statistical nature of quantum mechanical measurements. The first mathematical realization of this principle was proposed by Heisenberg [6] and Kennard [7] in terms of the standard deviations (σ) of the quantum mechanical probability densities $\rho(\vec{r})$ and $\gamma(\vec{p})$ of the particle in position and momentum spaces. Quantum-mechanical uncertainty relations state that probability distributions of canonically conjugate variables of a physical system cannot be simultaneously localized sharply. The standard uncertainty relation is the variance-based Heisenberg principle given by the expression

$$V_\rho V_\gamma \geq \frac{1}{4} \tag{1}$$

where, V_ρ and V_γ denote the variances of the probability densities $\rho(\vec{r})$ and $\gamma(\vec{p})$ respectively in position and momentum space. The probability densities are assumed to be normalized to unity. This inequality is relevant in quantum mechanics, not because of its accuracy (generally, very small) but because it indicates that refined single-particle position measurements require large indeterminations for the single-particle momentum. This principle and its momentum-based generalizations [8] reflect the essential inadequacy of the classical concepts of single-particle position and momentum to describe real systems. There are different types of entropy measures, namely Shannon information entropy (*S*), Fisher information entropy (*I*), Rényi entropy (*R*) Tsallis entropy (*T*) [9-13]. The use of information-theoretic quantities as uncertainty measures has led to deriving uncertainty relations that improve the standard uncertainty relation. This is the case of the celebrated entropic uncertainty relation,

$$S_T = S_\rho + S_\gamma \geq D(1 + ln\pi) \quad (2)$$

where, *D* represents the spatial dimension of the system and

$$S_\rho = -\int \rho(\vec{r}) ln\rho(\vec{r})\, d^3r \quad (3)$$

that describes the Shannon information entropy of the probability density in three-dimensional position space [14], whereas,

$$S_\gamma = -\int \gamma(\vec{p}) ln\gamma(\vec{p}) d^3p \quad (4)$$

denotes the corresponding momentum space Shannon entropy of the system; with $d^3r = r^2\, dr\, d\Omega$, $d^3p = p^2\, dp\, d\Omega$ and $d\Omega = sin\theta\, d\theta\, d\varphi$ is the solid angle with $\psi(\vec{r})$ being the normalized wave function in position space. The relation in Eq. (2) was conjectured by Hirschman [15] in 1957 and proved by Beckner [16] and Bialynicki-Birula and Mycielski [17]. Shannon connected the measure of the information content with probability density. It is necessary to mention that Shannon information entropy (*S*) and Fisher information entropy (*I*) [18] are both characterized by probability density or the charge density corresponding to changes in some observables [19]. The two most important entropic measures of the information theories are the Shannon information entropy (*S*) and Fisher information entropy (*I*) [20,21]. 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 proven to be an alternative to the Heisenberg uncertainty relation in quantum mechanics [22-25].

On the one hand, the Shannon entropic uncertainty relation in position and momentum space satisfies the Bialynicki-Birula and Mycielski (*BBM*) inequality relation $S_T = S_\rho + S_\gamma \geq D(1 + ln\pi)$. The Shannon information entropy is usually regarded as the measure of the spatial spread of the wave function for different states [26]. One of the consequences of the *BBM* inequality is that it represents the lower bound values of the Shannon entropy sum. If the position entropy increases, then the momentum entropy will decrease in such a way that their sum bounds above (*BBM*) inequality. The most important information theoretic alternative to the Shannon entropy as an uncertainty measure is the Fisher information, [27] given by in position and momentum space as follows:

$$I_\rho = \int \frac{1}{\rho(\vec{r})} [\vec{\nabla}\rho(\vec{r})]^2\, d^3r \quad (5)$$

and

$$I_\gamma = \int \frac{1}{\gamma(\vec{p})} [\vec{\nabla}\gamma(\vec{p})]^2\, d^3p \quad (6)$$

The above-mentioned expressions in Eqs. (5) and (6) for Fisher information entropies in position and momentum space can also be written in equivalent forms [28] as

$$I_\rho = 4 \int |\vec{\nabla} \psi(\vec{r})|^2 d^3 r \tag{7}$$

and

$$I_\gamma = 4 \int |\vec{\nabla} \varphi(\vec{p})|^2 d^3 p \, . \tag{8}$$

Working with eqs. (7) and (8) for computational purposes will be profitable. The Shannon entropy represents a global measure of the spreading of the density because it is a logarithmic function, whereas the Fisher information has a locality property as it is a gradient function of the density. The higher this quantity, the more localized the density. Meanwhile, when the uncertainty becomes smaller, the accuracy in predicting particle localization becomes higher [29,30].

On the other hand, the Fisher information is the basic variable of the principle extreme physical information in the same manner as the Shannon entropy is the cornerstone of the maximum entropy method [31,32]. Moreover, it has been used (a) to describe some macroscopic quantities such as the kinetic [33] and the Weiszäcker [34,35] energies, (b) to characterize correlation properties in atomic systems [36], and (c) to identify the most distinctive nonlinear phenomena (the avoided crossings) of the energy spectra of atomic and molecular systems in strong external fields [37]. Other quantum-mechanical uses of the Fisher information are available in literature [29,38,39].

Unlike the Shannon entropy that satisfies the *BBM* inequality, the Fisher information fulfills the Stam inequalities [40], $I_\rho \leq 4 \langle p^2 \rangle$, $I_\gamma \leq 4 \langle r^2 \rangle$ and the Cramer–Rao inequalities [41] $I_\rho \geq \frac{9}{\langle r^2 \rangle}$, $I_\gamma \geq \frac{9}{\langle p^2 \rangle}$.

It has been shown by E. Romera *et al.* see Ref. [40] that the Fisher information of single-particle systems with a central potential in D-dimensional ($D \geq 3$) position and momentum space satisfy the following uncertainty relation,

$$I_\rho I_\gamma \geq 4 D^2 \left(1 - \frac{(2l+D-2)|m|}{2l(l+D-2)}\right)^2 (l > 0), \tag{9}$$

where 'l' and 'm' represent the hyper-angular quantum numbers and magnetic quantum numbers.

When $l = 0$ and $m = 0$, the inequality of Eq. (9) reduces to

$$I_\rho I_\gamma \geq 4 D^2, \tag{10}$$

and when $D = 2$, it gives the trivial inequality as

$$I_\rho I_\gamma \geq 0. \tag{11}$$

Our present work aims to theoretically study wave packet dynamics using information theory. The study intertwines the dynamics of wave packets with the information-theoretic measurements for the numerical values of the Shannon ($S_\rho$and S_γ) and Fisher information entropies (I_ρ and I_γ) in position and momentum space satisfying the entropic uncertainty relations.

The article is organized as follows:

The materials and method Section has been focused on obtaining the expression of the position space wave function for a localized wave packet of a free particle. The change of minimum wave packet with time and the dynamical changes of the wave packet's spread have been mathematically delineated [42,43]. It can be observed that the amplitude factor of the wave function of the initial wave packet depends on the standard deviation (σ), but at a later instant of time t when the wave packet starts spreading, the amplitude factor no longer remains dependent on the standard deviation (σ). Later the momentum space wave function $\varphi(p_x, 0) \equiv \varphi(p_x)$ is obtained by the recourse of the Fourier transform [44] of the position space wave function $\psi(x, 0) \equiv \psi(x)$.

In the results and discussion Section, the constructions of the position and momentum space probability densities [$\rho(x, 0) \equiv \rho(x)$ and $\gamma(p_x, 0) \equiv \gamma(p_x)$] for the wave functions $\psi(x)$ and $\varphi(p_x)$ at $t = 0$ i.e. $\langle x\rangle = \langle p_x\rangle = 0$; have been described respectively. These probability densities have been used to compute the numerical values of the position and momentum space Shannon ($S_\rho$and S_γ) and Fisher information entropies (I_ρ and I_γ). Later, the numerical values so obtained (in the case of a one-dimensional system) have been found to satisfy the *BBM* inequality relation $(S_\rho + S_\gamma) \geq 2.1447$ for the Shannon entropy sum$(S_\rho + S_\gamma)$ [45] and the Fisher-based inequality relation $I_\rho I_\gamma \geq 4$ for the product of Fisher information entropies ($I_\rho I_\gamma$) respectively in the position and momentum space.
Finally, the conclusion Section has been devoted to summarizing the present work with some concluding remarks.

2. Materials and Method

Let us take for simplicity that the wave packet centered at the origin at time $t = 0$ has the form with $\langle x\rangle$ [or $\langle p_x\rangle$]. In terms of standard deviation (σ), we have the position space wave function as below:

$$\psi(x, 0) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} e^{[-\frac{x^2}{2\sigma^2}]} e^{[\frac{i}{\hbar}\langle p_x\rangle x]}. \tag{12}$$

Its Fourier transform at $t = 0$ gives the momentum space wave function $\varphi(p_x)$ and it can be expressed as follows:

$$\varphi(p_x, 0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x, 0)\, e^{[-\frac{i}{\hbar}p_x x]}\, dx$$

$$\text{Or, } \varphi(p_x, 0) = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \int_{-\infty}^{\infty} e^{[-\frac{x^2}{2\sigma^2}]}\, e^{[\frac{i}{\hbar}\langle p_x\rangle x]} e^{[-\frac{i}{\hbar}p_x x]}\, dx$$

$$\text{Or, } \varphi(p_x) = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\sigma^2}}\, e^{-\frac{i}{\hbar}(p_x - \langle p_x\rangle)x}\, dx$$

$$\text{Or, } \varphi(p_x) = \sqrt{\frac{\sigma}{\hbar\sqrt{\pi}}}\, e^{-\frac{\sigma^2}{2\hbar^2}(p_x - \langle p_x\rangle)^2}. \tag{13}$$

Therefore, the wave packet at a later instant of time 't' has the form given by the Fourier transform:

$$\psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \varphi(p_x)\, e^{\frac{i}{\hbar}(p_x x - E_x t)}\, dp_x\,, \tag{14}$$

where, $E_x = \frac{p_x^2}{2m}$ for a free particle wave function.

$$\therefore \psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\sqrt{\frac{\sigma}{\hbar\sqrt{\pi}}}\int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}(p_x - \langle p_x\rangle)^2}\, e^{\frac{i}{\hbar}(p_x x - \frac{p_x^2}{2m}t)}dp_x$$

$$= \sqrt{\frac{\sigma}{2\pi\hbar\cdot\hbar\sqrt{\pi}}}\int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}(p_x - \langle p_x\rangle)^2}\, e^{\frac{i}{\hbar}(p_x x - \frac{p_x^2}{2m}t)}dp_x$$

$$= C\int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}(p_x - \langle p_x\rangle)^2}\, e^{\frac{i}{\hbar}(p_x x - \frac{p_x^2}{2m}t)}dp_x$$

where, $C = \sqrt{\frac{\sigma}{2\pi\hbar\cdot\hbar\sqrt{\pi}}}$. (15)

$$\therefore \psi(x,t) = C\int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}(p_x - \langle p_x\rangle)^2}\, e^{\frac{i}{\hbar}(p_x x - \frac{p_x^2}{2m}t)}dp_x. \quad (16)$$

Let, $p_x - \langle p_x\rangle = k$ (17)

$\therefore p_x = k + \langle p_x\rangle$ (18)

and $(p_x - \langle p_x\rangle)^2 = k^2$ (19)

Also, $p_x x = kx + \langle p_x\rangle x$ (20)

and

$dp_x = dk.$ (21)

Now, substituting the values of Eqs. (17) to (21) for the expression of $\psi(x,t)$ in Eq. (16), we have,

$$\psi(x,t) = C\int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i}{\hbar}[kx + \langle p_x\rangle x - \frac{(k+\langle p_x\rangle)^2}{2m}t]}dk \quad (22)$$

$$= C\int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i}{\hbar}kx} e^{\frac{i}{\hbar}\langle p_x\rangle x} e^{-\frac{i}{\hbar}[\frac{(k+\langle p_x\rangle)^2}{2m}t]}dk$$

$$= C\int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i}{\hbar}kx} e^{\frac{i}{\hbar}\langle p_x\rangle x} e^{-\frac{i}{\hbar}\frac{[(k)^2 + 2k\langle p_x\rangle + (\langle p_x\rangle)^2]t}{2m}}dk$$

$$= C\, e^{\frac{i}{\hbar}\langle p_x\rangle x} e^{-\frac{i}{\hbar}\frac{\langle p_x\rangle^2 t}{2m}}\int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i}{\hbar}kx} e^{-\frac{i}{\hbar}\frac{(k^2 + 2k\langle p_x\rangle)t}{2m}}dk. \quad (23)$$

Let, $A = C\, e^{\frac{i}{\hbar}\langle p_x\rangle x} e^{-\frac{i}{\hbar}\frac{\langle p_x\rangle^2 t}{2m}}$ (24)

and $I = \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i}{\hbar}kx} e^{-\frac{i}{\hbar}\frac{(k^2 + 2k\langle p_x\rangle)t}{2m}}dk,$ (25)

such that

$\psi(x,t) = A\cdot I.$ (26)

Let us calculate 'I':

$$I = \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i}{\hbar}kx} e^{-\frac{i}{\hbar}\frac{(k^2 + 2k\langle p_x\rangle)t}{2m}}dk$$

$$= \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i}{\hbar}kx} e^{-\frac{i}{\hbar}\frac{(k^2 + 2k\langle p_x\rangle)t}{2m}} dk$$

$$= \int_{-\infty}^{\infty} e^{-\frac{\sigma^2}{2\hbar^2}k^2}\, e^{\frac{i2\hbar\sigma^2}{2\hbar^2\sigma^2}kx} e^{-\frac{i\hbar\sigma^2}{2\hbar^2 m\sigma^2}(k^2\, t + 2\, k\, \langle p_x\rangle t)}\, dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\sigma^2}{2\hbar^2}[-k^2 + \frac{2i\hbar}{\sigma^2}kx - \frac{i\hbar}{m\sigma^2}(k^2\, t + 2\, k\, \langle p_x\rangle t)]}\, dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\sigma^2}{2\hbar^2}[\left(-k^2 - \frac{i\hbar}{m\sigma^2}k^2\, t\right) + \left(\frac{2i\hbar}{\sigma^2}kx - \frac{i\hbar}{m\sigma^2}2\, k\, \langle p_x\rangle t\right)]}\, dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\sigma^2}{2\hbar^2}[-k^2\left(1 + \frac{i\hbar t}{m\sigma^2}\right) + \frac{2i\hbar k}{\sigma^2}(x - \frac{\langle p_x\rangle t}{m})]}\, dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\sigma^2}{2\hbar^2}[\frac{-k^2\sigma^2\left(1 + \frac{i\hbar t}{m\sigma^2}\right) + 2i\hbar k\,(x - \frac{\langle p_x\rangle t}{m})}{\sigma^2}]}\, dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\sigma^2}{2\hbar^2}[\frac{-k^2\left(\sigma^2 + \frac{i\hbar t}{m}\right) + 2i\hbar k\,(x - \frac{\langle p_x\rangle t}{m})}{\sigma^2}]}\, dk \tag{27}$$

Now, let the term: $\gamma^2 = \left(\sigma^2 + \frac{i\hbar t}{m}\right)$ (28)

Now the expression for 'I' from Eq. (27) can be rewritten as follows:

$$I = \int_{-\infty}^{\infty} e^{\frac{\sigma^2}{2\hbar^2}[\frac{-k^2\gamma^2 + 2i\hbar k\,(x - \frac{\langle p_x\rangle t}{m})}{\sigma^2}]}\, dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\sigma^2}{2\hbar^2}[\frac{\gamma^2}{\sigma^2}(-k^2 + \frac{2i\hbar k\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2})]}\, dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\gamma^2}{2\hbar^2}\cdot[-k^2 + 2\cdot k\cdot\frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2} + \{\frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2}\}^2 - \{\frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2}\}^2]}\, dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\gamma^2}{2\hbar^2}\cdot[(\frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2})^2 - \{(k)^2 - 2\cdot k\cdot\frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2} + (\frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2})^2\}]}\, dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\gamma^2}{2\hbar^2}\cdot[(\frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2})^2 - \{k - \frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2}\}^2]}\, dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\gamma^2}{2\hbar^2}\cdot(\frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2})^2} \cdot e^{-\frac{\gamma^2}{2\hbar^2}\cdot\{k - \frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2}\}^2}\, dk$$

$$= \int_{-\infty}^{\infty} e^{\frac{\gamma^2}{2\hbar^2}\cdot\frac{i^2\hbar^2}{\gamma^4}(x - \frac{\langle p_x\rangle t}{m})^2} \cdot e^{-\frac{\gamma^2}{2\hbar^2}\cdot\{k - \frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2}\}^2} dk$$

$$= \int_{-\infty}^{\infty} e^{-\frac{1}{2\gamma^2}(x - \frac{\langle p_x\rangle t}{m})^2} \cdot e^{-\frac{\gamma^2}{2\hbar^2}\cdot\{k - \frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2}\}^2} dk \quad (29)$$

Let, $\{k - \frac{i\hbar\left(x - \frac{\langle p_x\rangle t}{m}\right)}{\gamma^2}\} = z$ (30)

and the standard integral

$$\int_{-\infty}^{\infty} e^{-\alpha x^2}\, dx = \sqrt{\frac{\pi}{\alpha}} \quad (31)$$

Substituting the values of Eqs. (30) and (31) in Eq. (29) we have,

$$I = e^{-\frac{1}{2\gamma^2}(x - \frac{\langle p_x\rangle t}{m})^2} \int_{-\infty}^{\infty} e^{-\frac{\gamma^2}{2\hbar^2}z^2}\, dz$$

$$I = e^{-\frac{1}{2\gamma^2}(x - \frac{\langle p_x\rangle t}{m})^2} \cdot \sqrt{\frac{\pi}{\frac{\gamma^2}{2\hbar^2}}}$$

$$I = e^{-\frac{(x - \frac{\langle p_x\rangle t}{m})^2}{2\gamma^2}} \cdot \sqrt{\frac{\pi \cdot 2\hbar^2}{\gamma^2}} \quad (32)$$

Substituting the values of C, A, and I respectively, from Eqs. (15), (24), and (32) in Eq. (26), we have,

$$\psi(x,t) = A \cdot I$$

$$= C\, e^{\frac{i}{\hbar}\langle p_x\rangle x} e^{-\frac{i}{\hbar}\frac{\langle p_x\rangle^2 t}{2m}} \cdot e^{-\frac{(x - \frac{\langle p_x\rangle t}{m})^2}{2\gamma^2}} \cdot \sqrt{\frac{\pi \cdot 2\hbar^2}{\gamma^2}} \quad (33)$$

$$= \sqrt{\frac{\sigma}{2\pi\hbar\cdot\hbar\sqrt{\pi}}} \cdot e^{\frac{i}{\hbar}\langle p_x\rangle x} \cdot e^{-\frac{i}{\hbar}\frac{\langle p_x\rangle^2 t}{2m}} \cdot e^{-\frac{(x - \frac{\langle p_x\rangle t}{m})^2}{2\gamma^2}} \cdot \sqrt{\frac{\pi \cdot 2\hbar^2}{\gamma^2}}$$

$$= \sqrt{\frac{\sigma}{2\pi\hbar\cdot\hbar\sqrt{\pi}}\cdot\frac{\pi \cdot 2\hbar^2}{\gamma^2}} \cdot e^{\frac{i}{\hbar}\langle p_x\rangle x} \cdot e^{-\frac{i}{\hbar}\frac{\langle p_x\rangle^2 t}{2m}} \cdot e^{-\frac{(x - \frac{\langle p_x\rangle t}{m})^2}{2\gamma^2}}$$

$$= \sqrt{\frac{\sigma}{\gamma^2\sqrt{\pi}}} \cdot e^{\frac{i}{\hbar}\langle p_x\rangle\,(x - \frac{\langle p_x\rangle t}{2m})} \cdot e^{-\frac{(x - \frac{\langle p_x\rangle t}{m})^2}{2\gamma^2}}$$

$$= \sqrt{\frac{\sigma\,\cdot\,\sigma}{\sigma\,\cdot\,\gamma^2\sqrt{\pi}}} \cdot e^{\frac{i}{\hbar}\langle p_x\rangle\,(x - \frac{\langle p_x\rangle t}{2m})} \cdot e^{-\frac{\{x - \frac{\langle p_x\rangle t}{m}\}^2}{2\gamma^2}}$$

$$= \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \cdot \frac{\sigma}{\gamma} \cdot e^{-\frac{\{x - \frac{\langle p_x\rangle t}{m}\}^2}{2\gamma^2}} e^{\frac{i}{\hbar}\langle p_x\rangle\,(x - \frac{\langle p_x\rangle t}{2m})} \quad (34)$$

Finally the expression for the wave packet at a later instant of time t becomes

$$\therefore \psi(x,t) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \cdot \frac{\sigma}{\gamma} \cdot e^{-\frac{\{x - \frac{\langle p_x \rangle t}{m}\}^2}{2\gamma^2}} e^{\frac{i}{\hbar}\langle p_x \rangle (x - \frac{\langle p_x \rangle t}{2m})} \tag{35}$$

where, $\gamma^2 = \left(\sigma^2 + \frac{i\hbar t}{m}\right)$.

3. Results and Discussion

At time $t = 0$, $\langle x \rangle = \langle p_x \rangle = 0$, the position and momentum space wave functions are written as follows:

$$\psi(x,0) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} e^{[-\frac{x^2}{2\sigma^2}]} \text{ and } \varphi(p_{x,}0) = \sqrt{\frac{\sigma}{\hbar\sqrt{\pi}}} e^{-\frac{\sigma^2 p_x^2}{2\hbar^2}}.$$

The probability density in position space for the wave packet is expressed as

$$\rho(x,0) \equiv \rho(x) = \psi^*(x,0)\psi(x,0) = \frac{1}{\sigma\sqrt{\pi}} e^{-\frac{x^2}{\sigma^2}} \tag{36}$$

and in momentum space the same can be expressed as

$$\gamma(p_x,0) \equiv \gamma(p_x) = \varphi^*(p_x)\varphi(p_x) = \frac{\sigma}{\hbar\sqrt{\pi}} e^{-\frac{\sigma^2 p_x^2}{\hbar^2}}. \tag{37}$$

The Shannon entropies (S_ρ and S_γ) in position and momentum space which are defined in Eqs. (3) and (4) in three dimensions, can be expressed in one-dimension respectively as follows:

$$S_\rho = -\int_{-\infty}^{\infty} \rho \ln \rho \, dx \tag{38}$$

and

$$S_\gamma = -\int_{-\infty}^{\infty} \gamma \ln \gamma \, dp_x. \tag{39}$$

The Shannon entropy in position space (s_ρ) is

$$S_\rho = -\int_{-\infty}^{\infty} \rho \ln \rho \, dx$$

$$= -\int_{-\infty}^{\infty} \left(\frac{1}{\sigma\sqrt{\pi}} e^{-\frac{x^2}{\sigma^2}}\right) \ln\left(\frac{1}{\sigma\sqrt{\pi}} e^{-\frac{x^2}{\sigma^2}}\right) dx$$

$$= -\int_{-\infty}^{\infty} \left(\frac{1}{\sigma\sqrt{\pi}} e^{-\frac{x^2}{\sigma^2}}\right) [\ln\left(\frac{1}{\sigma\sqrt{\pi}}\right) + \ln\left(e^{-\frac{x^2}{\sigma^2}}\right)] dx$$

$$= -\frac{1}{\sigma\sqrt{\pi}} \ln\left(\frac{1}{\sigma\sqrt{\pi}}\right) \int_{-\infty}^{\infty} \left(e^{-\frac{x^2}{\sigma^2}}\right) dx - \frac{1}{\sigma\sqrt{\pi}} \int_{-\infty}^{\infty} \left(e^{-\frac{x^2}{\sigma^2}}\right) \ln\left(e^{-\frac{x^2}{\sigma^2}}\right)] dx$$

$$= -\frac{1}{\sigma\sqrt{\pi}}\ln\left(\frac{1}{\sigma\sqrt{\pi}}\right)\cdot\sigma\sqrt{\pi} - \frac{1}{\sigma\sqrt{\pi}}\left(-\frac{\sigma\sqrt{\pi}}{2}\right)$$

$$= \frac{1}{2} - \ln\left(\frac{1}{\sigma\sqrt{\pi}}\right)$$

$$= \frac{1}{2} - \ln(1) + \ln\left(\sigma\sqrt{\pi}\right)$$

$$= \frac{1}{2} + \ln(\sigma) + \ln\left(\sqrt{\pi}\right)$$

$$S_\rho = -\int_{-\infty}^{\infty}\rho\ln\rho\,dx = \frac{1}{2} + \ln(\sigma) + \ln\left(\sqrt{\pi}\right). \quad (40)$$

$$\therefore S_\rho = -\int_{-\infty}^{\infty}\rho\ln\rho\;dx$$

$$= -2\int_{0}^{\infty}\rho\ln\rho\;dx$$

$$= 2\left[\frac{1}{2} + \ln(\sigma) + \ln\left(\sqrt{\pi}\right)\right]$$

$$= 1 + 2\ln(\sigma) + 2\ln\left(\sqrt{\pi}\right). \quad (41)$$

The Shannon entropy in momentum space (S_γ) is

$$S_\gamma = -\int_{-\infty}^{\infty}\gamma\ln\gamma\,dp_x$$

$$= -\int_{-\infty}^{\infty}\left(\frac{\sigma}{\hbar\sqrt{\pi}}e^{-\frac{\sigma^2 p_x^2}{\hbar^2}}\right)\ln\left(\frac{\sigma}{\hbar\sqrt{\pi}}e^{-\frac{\sigma^2 p_x^2}{\hbar^2}}\right)dp_x$$

$$= -\int_{-\infty}^{\infty}\left(\frac{\sigma}{\hbar\sqrt{\pi}}e^{-\frac{\sigma^2 p_x^2}{\hbar^2}}\right)\left[\ln\left(\frac{\sigma}{\hbar\sqrt{\pi}}\right) + \ln\left(e^{-\frac{\sigma^2 p_x^2}{\hbar^2}}\right)\right]dp_x$$

$$= -\frac{\sigma}{\hbar\sqrt{\pi}}\ln\left(\frac{\sigma}{\hbar\sqrt{\pi}}\right)\int_{-\infty}^{\infty}\left(e^{-\frac{\sigma^2 p_x^2}{\hbar^2}}\right)dp_x - \frac{\sigma}{\hbar\sqrt{\pi}}\int_{-\infty}^{\infty}e^{-\frac{\sigma^2 p_x^2}{\hbar^2}}\ln\left(e^{-\frac{\sigma^2 p_x^2}{\hbar^2}}\right)dp_x$$

$$= -\frac{\sigma}{\hbar\sqrt{\pi}}\ln\left(\frac{\sigma}{\hbar\sqrt{\pi}}\right)\frac{\sqrt{\pi}}{\sqrt{\frac{\sigma^2}{\hbar^2}}} - \frac{\sigma}{\hbar\sqrt{\pi}}\left(-\frac{1}{2}\cdot\frac{\sqrt{\pi}}{\sqrt{\frac{\sigma^2}{\hbar^2}}}\right)$$

$$= -\frac{\sigma}{\hbar\sqrt{\pi}}\frac{\hbar\sqrt{\pi}}{\sigma}\ln\left(\frac{\sigma}{\hbar\sqrt{\pi}}\right) + \frac{\sigma}{\hbar\sqrt{\pi}}\frac{\hbar\sqrt{\pi}}{2\sigma}$$

$$= -\ln\left(\frac{\sigma}{\hbar\sqrt{\pi}}\right) + \frac{1}{2}$$

$$= \frac{1}{2} + \ln(\hbar\sqrt{\pi}) - \ln(\sigma)$$

$$= \frac{1}{2} + \ln(\sqrt{\pi}) - \ln(\sigma) \quad [\therefore\ \hbar = 1]. \tag{42}$$

$$\therefore S_\gamma = -\int_{-\infty}^{\infty} \gamma \ln\gamma \; dp_x$$

$$= -2\int_{0}^{\infty} \gamma \ln\gamma \; dp_x$$

$$= 1 + 2\ln(\sqrt{\pi}) - 2\ln(\sigma). \tag{43}$$

Now, the Shannon entropy sum, i.e. $(S_\rho + S_\gamma)$ by using the values obtained from Eq. (41) and (43) becomes

$$\therefore S_\rho + S_\gamma$$

$$= \left\{1 + 2\ln(\sigma) + 2\ln\left(\sqrt{\pi}\right)\right\} + \left\{1 + 2\ln\left(\sqrt{\pi}\right) - 2\ln(\sigma)\right\}$$

$$= 2 + 4\ln\left(\sqrt{\pi}\right)$$

$$= 2 + 2.28945$$

$$= 4.28945. \tag{44}$$

Similarly, the position and momentum space Fisher information entropy ($I_\rho$andI_γ) defined in Eqs. (7) and (8) in three dimensions can be expressed in one-dimension respectively as follows:

$$I_\rho = 4\int |\vec{\nabla}\psi(x)|^2 dx \tag{45}$$

And

$$I_\gamma = 4\int |\vec{\nabla}\varphi(p_x)|^2 dp_x. \tag{46}$$

The Fisher information entropy (I_ρ) in position space is

$$I_\rho = 4\int |\vec{\nabla}\psi(x)|^2 dx$$

$$= \int_{0}^{\infty} 4\left(\frac{e^{-\frac{x^2}{\sigma^2}}x^2}{\sqrt{\pi}\,\sigma^5} - \frac{2e^{-\frac{x^2}{\sigma^2}}}{\sqrt{\pi}\,\sigma^3} + \frac{e^{-\frac{x^2}{\sigma^2}}}{\sqrt{\pi}\,x^2\,\sigma}\right)dx$$

$$= \int_0^\infty 4\left(\frac{e^{-\frac{x^2}{\sigma^2}}x^2}{\sqrt{\pi}\,\sigma^5} - \frac{2e^{-\frac{x^2}{\sigma^2}}}{\sqrt{\pi}\,\sigma^3}\right)dx + \int_0^\infty 4\left(\frac{e^{-\frac{x^2}{\sigma^2}}}{\sqrt{\pi}\,x^2\,\sigma}\right)dx \tag{47}$$

The second integral of Eq. (47) i.e. $\int_0^\infty 4\left(\frac{e^{-\frac{x^2}{\sigma^2}}}{\sqrt{\pi}x^2\,\sigma}\right)dx$ is an improper type integral. The integral of $\left(\frac{e^{-\frac{x^2}{\sigma^2}}}{x^2}\right)$ does not converge in the limit ($-\infty$ to ∞). But, it converges at all values of x, except at $x = 0$. Thus by ignoring the contribution of the said improper integral, we obtain the Fisher information entropy (I_ρ) in position space as follows:

$$I_\rho = \int_0^\infty 4\left(\frac{e^{-\frac{x^2}{\sigma^2}}x^2}{\sqrt{\pi}\sigma^5} - \frac{2e^{-\frac{x^2}{\sigma^2}}}{\sqrt{\pi}\sigma^3}\right)dx$$

$$= -\frac{3\sqrt{\frac{1}{\sigma^2}}}{\sigma}$$

$$= -\frac{3}{\sigma^2}. \tag{48}$$

The Fisher information entropy (I_γ) in momentum space is

$$I_\gamma = 4\int |\vec{\nabla}\varphi(p_x)|^2 dp_x$$

$$= \int_0^\infty 4\,\left(\frac{e^{-\frac{p_x^2\,\sigma^2}{\hbar^2}}p_x^2\sigma^5}{\sqrt{\pi}\hbar^5} - \frac{2e^{-\frac{p_x^2\,\sigma^2}{\hbar^2}}\sigma^3}{\sqrt{\pi}\hbar^3} + \frac{e^{-\frac{p_x^2\,\sigma^2}{\hbar^2}}\sigma}{p_x^2\sqrt{\pi}\hbar}\right)dp_x$$

$$= \int_0^\infty 4\,\left(\frac{e^{-\frac{p_x^2\,\sigma^2}{\hbar^2}}p_x^2\,\sigma^5}{\sqrt{\pi}\hbar^5} - \frac{2e^{-\frac{p_x^2\,\sigma^2}{\hbar^2}}\sigma^3}{\sqrt{\pi}\hbar^3}\right)dp_x + \int_0^\infty 4\,\left(\frac{e^{-\frac{p_x^2\,\sigma^2}{\hbar^2}}\sigma}{p_x^2\sqrt{\pi}\hbar}\right)dp_x \tag{49}$$

Similarly, the integral in Eq. (49) i.e. $\int_0^\infty 4\left(\frac{e^{-\frac{p_x^2\,\sigma^2}{\hbar^2}}\sigma}{p_x^2\sqrt{\pi}\hbar}\right)dp_x$ is an improper integral. The integral of $\left(\frac{e^{-\frac{p_x^2\,\sigma^2}{\hbar^2}}}{p_x^2}\right)$ does not converge in the limit ($-\infty$ to ∞). But, it converges at all values of p_x except at $p_x = 0$. Thus by ignoring the contribution of the said improper integral, we obtain the Fisher information entropy (I_γ) in momentum space as follows:

$$I_\gamma = \int_0^\infty 4\left(\frac{e^{-\frac{p_x^2\sigma^2}{\hbar^2}}p_x^2\sigma^5}{\sqrt{\pi}\hbar^5} - \frac{2e^{-\frac{p_x^2\sigma^2}{\hbar^2}}\sigma^3}{\sqrt{\pi}\hbar^3}\right)dp_x$$

$$= -\frac{3\sigma\sqrt{\frac{\sigma^2}{\hbar^2}}}{\hbar}$$

$$= -\frac{3\sigma^2}{\hbar^2}. \quad (50)$$

The product of the Fisher information entropies,

$$I_\rho I_\gamma = \left(-\frac{3}{\sigma^2}\right)\left(-\frac{3\sigma^2}{\hbar^2}\right) = \frac{9}{\hbar^2} = 9 \ [\because \ \hbar = 1]. \quad (51)$$

4. Conclusion

In the present article, the dynamics of wave packets and the entropic uncertainty relations for the Shannon and Fisher information entropies have been addressed mainly. Here, a wave packet localized in a very small region at time $t = 0$ has been considered. The change with time of the wave packet at a later instant of time t is calculated for the position space wave function so that it evolves the wave function $\psi(x, 0)$ to $\psi(x, t)$. It can be observed that although the amplitude of the wave function of the initial wave packet depends on the standard deviation (σ), but at a later instant of time t when the wave packet starts spreading, it doesn't. The momentum analog $\varphi(p_x)$ for the wave packet is obtained by the recourse of the Fourier transform of the position space wave function $\psi(x)$. The probability densities [$\rho(x)$ and $\gamma(p_x)$] in position space and momentum space have been constructed with the help of these wave functions [$\psi(x)$ and $\varphi(p_x)$]. Further, these probability densities [$\rho(x)$ and $\gamma(p_x)$] have been used to compute the corresponding Shannon (S) and Fisher information (I) entropies both in the position and momentum space. It has been observed that though the numerical values of the position and momentum space Shannon ($S_\rho$and S_γ) and Fisher information (I_ρ and I_γ) entropies explicitly depend on the standard deviation (σ) but neither the Shannon entropy sum ($S_\rho + S_\gamma$) nor the product of Fisher information entropies ($I_\rho I_\gamma$) is. By using Eq. (2) and (10) in one-dimension , one can find the numerical values for the Shannon entropy sum and the Fisher-based uncertainty relation respectively as $(S_\rho + S_\gamma) \geq 2.1447$ and $I_\rho I_\gamma \geq 4$. Herein, all our calculations, we have taken $D = 1$ and used the traditional atomic units ($m = \hbar = e = 1$). In our present work, the numerical values for Shannon entropy sum have been obtained as $(S_\rho + S_\gamma) = 4.28945$ and for the Stam-Cramer-Rao inequalities (Fisher based uncertainty relation) as $I_\rho I_\gamma = 9$. Therefore, the computed values for the Shannon and Fisher information entropies are found to satisfy the lower bound of the Bialynicki-Birula and Myceilski (*BBM*) inequality relation $(S_\rho + S_\gamma) \geq D(1 + ln\pi)$ and the Stam-Cramer-Rao inequalities, better known as the Fisher-based uncertainty relation $I_\rho I_\gamma \geq 4D^2$. Thus, our theoretical study explores the validation of the information-theoretic measurements for the wave packet dynamics in respect of the lower bounds for the *BBM* inequality and the Fisher-based uncertainty relation using the basic formulations of the information theory. Finally, this work finds a useful and different view of the problems and possibilities associated with the works of wave packet dynamics and the information theory exploring the broader applicability. We believe that our present work could be treated as a valuable reference and facilitate further research on 'wave packet dynamics using information theory' drawing more attention in the near future, giving a deeper insight into it.

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