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(Dedicated to Professor G. C. Sharma on His 85^{th} Birth Anniversary Celebrations)

FISHER-SHANNON ENTROPIC UNCERTAINTY RELATIONS AND THEIR POWER-PRODUCTS AS A MEASURE OF ELECTRONIC CORRELATION

[1]Sudin Singh and [2]Aparna Saha
[1]Department of Physics, Bolpur College, Bolpur, Birbhum, West Bengal, India-731204
[2]Department of Physics, Visva-Bharati University, Santiniketan, West Bengal, India-731235
[1]Corresponding Author
Email: skyalpha731204@gmail.com, aparnasaha1507@gmail.com

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Abstract

In this paper, we have presented an analytical model of two electron systems consisting of a many particle correlated wave function with some variational parameters α, λ and μ and used it to quantify the electron-electron correlation described by the wave function containing explicitly r_{12} (inter atomic distance between two electrons) dependent term. The single particle wave functions and the charge densities have been extracted from the said correlated wave function both for the uncorrelated and correlated systems in coordinate space and its momentum analogs have been obtained by taking the Fourier transform of the coordinate analogs. We have computed and presented the results of the numerical values of the theoretic information entropies of the Shannon entropy, Fisher information entropy, Shannon power and the FisherShannon product. The numerical values are consistently found to satisfy the Beckner, Bialynicki-Birula and Mycielski (BBM) inequality relation; Stam-Cramer-Rao inequalities or Fisher based uncertainty relation and Fisher-Shannon product relation for the uncorrelated and correlated systems in both the coordinate and momentum spaces.

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Keywords and Phrases: Coordinate and momentum space; uncorrelated and correlated system; Shannon information entropy; Fisher information entropy; uncertainty relations; Fisher-Shannon product.

1 Introduction

The electron correlation is a major problem in physics of atoms, molecules, and clusters as a consequence of the electronelectron repulsion. The correlation effect has a major influence on measureable quantities in atomic systems. The correlation energy (E_{corr}) [9] of a many-electron system is defined by the difference between the exact total energy (the exact non-relativistic energy) and Hartree-Fock energy, as well as by some statistical correlation coefficients [15] which assess radial and angular correlation in both the coordinate and momentum density distributions. The correlation energy had been used as a guide [16] for the amount of correlation in a given system. Recently, some information-theoretic measures of the electron correlation in atomic systems have been proposed: the so-called correlation entropy [30] which is the information entropy of the one-particle density matrix, and the sum of the Shannon information entropies of the electron density in coordinate and momentum spaces [20]. The entropic uncertainty relation has many applications both in physics and chemistry [27, 28] and because of their many applications in different areas of physics and chemistry, there have been a growing interest by many researchers in studying Shannon entropy and Fisher information in recent years. The two most important measures of the information theories are the Shannon entropy(S) [25] and Fisher information entropy(I) [10]. 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 [14, 17]. On one hand, the Shannon entropic uncertainty relation in coordinate and momentum spaces satisfy the Beckner, Bialynicki-Birula and Mycielski (BBM) inequality relation as [4, 6],

$$S_T = (S_\rho + S_\gamma) \geqslant D(1 + ln\pi), \tag{1.1}$$

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 and S_T is the Shannon entropy sum. The entropies

S_ρ and S_γ are defined as [4,6,21,22],

$$S_\rho = -\int \rho(\vec{r}) ln[\rho(\vec{r})] d^3r, \tag{1.2}$$

$$S_\gamma = -\int \gamma(\vec{p}) ln[\gamma(\vec{p})] d^3p, \tag{1.3}$$

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 $\psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)$ being the normalized wave function in the spatial coordinate, $\rho(\vec{r}) = \int |\psi(\vec{r}, \vec{r}_2, ..., \vec{r}_N)|^2 d^3r_2...$
d^3r_N is the single particle charge density in the spatial coordinate and $\gamma(\vec{p}) = \int |\phi(\vec{p}, \vec{p}_2, ..., \vec{p}_N|^2$
$d^3p_2...d^3p_N$ is the single particle charge density in momentum space. The Shannon information entropy is usually regarded as the measure of the spatial spread of the wave function for different states [12]. One of the consequences of the BBM inequality is that represents the lower bound values of the Shannon entropy sum [4,6] 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 [2,18], and conversely, the smaller the uncertainty the higher the accuracy in predicting the localization of the particles [2,18]. 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 [1,19]

$$I_\rho = \int \frac{1}{\rho(\vec{r})} [\vec{\nabla}\rho(\vec{r})]^2 d^3r, \tag{1.4}$$

$$I_\gamma = \int \frac{1}{\gamma(\vec{p})} [\vec{\nabla}\gamma(\vec{p})]^2 d^3p. \tag{1.5}$$

The disorder aspect of Fisher information entropy has been studied in some length by Frieden [11]. The uncertainty properties are clearly delineated by the Stam inequalities [26]. The product $I_\rho I_\gamma$ has been conjectured to exhibit a nontrivial lower bound [7] such that for three-dimensional systems it reads as:

$$I_\rho I_\gamma \geqslant 36. \tag{1.6}$$

Unlike, the Shannon entropy that satisfy the BBM inequality, the Fisher information fulfills the Stam inequalities [23], $I_\rho \leqslant 4 < p^2 >$, $I_\gamma \leqslant 4 < r^2 >$ and the Cramer-Rao inequalities [8] $I_\rho \geqslant \frac{9}{<r^2>}$, $I_\gamma \geqslant \frac{9}{<p^2>}$. Generally, for an arbitrary angular momentum quantum number *'l'* of any central potential model, the two products of the Fisher information must satisfied the relation [24],

$$I_\rho I_\gamma \geqslant 4 < r^2 >< p^2 > [2 - \frac{2l+1}{l(l+1)}|m|]^2, \tag{1.7}$$

where $m = 0, \pm1, \pm2$ . . . is the magnetic quantum number. With the help of the definitions of equations (1.1) to (1.5), we can define the Shannon power (J) in coordinate and momentum space as

$$J_\rho = \frac{1}{2\pi e} e^{\frac{2S_\rho}{D}}, \tag{1.8}$$

$$J_\gamma = \frac{1}{2\pi e} e^{\frac{2S_\gamma}{D}}, \tag{1.9}$$

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

$$P_\rho = \frac{I_\rho J_\rho}{D}, \tag{1.10}$$

and

$$P_\gamma = \frac{I_\gamma J_\gamma}{D}, \tag{1.11}$$

which must satisfy the following relation

$$P_{\rho\gamma} = P_\rho P_\gamma \geqslant 1, \tag{1.12}$$

where D is the spatial dimensions [29]. It is necessary to mention that throughout our all calculations, we shall use D=3 and m=$\hbar$=e=1. In this paper, we are going to study an analytical model of two electron system consisting of 'Hartree and Ingman(1933)' [13] type correlated wave function with some variational parameters α, λ and μ. The aim of our present work is to use the derived analytical model to quantify the correlation in two electron systems described by wave function containing explicitly r_{12} (inter atomic distance between two electrons) dependent term and thereafter present the results of our numerical analysis for the theoretic information entropies such as the Shannon entropy, Fisher information entropy and the Fisher-Shannon product. To begin with, we shall take an account of the effect of correlation on two electron systems using the 'Hartree and Ingman (1933)' [13] type trial wave function which can be written as

$$\psi(\vec{r}_1, \vec{r}_2, r_{12}) = ce^{-\alpha(r_1+r_2)}\chi(r_{12}), \tag{1.13}$$

where, $r_{12} = (\vec{r}_1 - \vec{r}_2)$, *'c'* is the normalization constant and the correlated function $\chi(r_{12})$ is written as

$$\chi(r_{12}) = (1 - \lambda e^{-\mu r_{12}}). \tag{1.14}$$

A few years ago, attempts were made by Bhattacharyya *et al* [5] to find out the ground-state energy of the two-electron system working with the 'Hartree and Ingman(1933)'[13] type trial wave function, $\psi(\vec{r}_1, \vec{r}_2, r_{12})$ = $e^{-\alpha(r_1+r_2)}$ (1 - $\lambda e^{-\mu r_{12}}$) with the variation parameters α, λ and μ. After minimizing the Hamiltonian with respect to the variations in the parameters of $\psi(\vec{r}_1, \vec{r}_2, r_{12})$, they obtained the values, $\alpha = 1.8395$, $\lambda = 0.586$ and $\mu = 0.379$. It is necessary to mention that we shall use these standard values for our computational purposes. It is to note that when $\lambda = 1$ and $r_{12} = 0$, the wave function takes the form as $\psi(\vec{r}_1, \vec{r}_2, r_{12}) = 0$ and the system becomes explicitly r_{12} dependent which is then referred to as the correlated system. Physically, this implies that two electrons in the atom cannot occupy the same position. And, when $\lambda = 1$ and $r_{12} = \infty$, the wave function leads to $\psi(\vec{r}_1, \vec{r}_2, r_{12}) = c\ e^{-\alpha(r_1+r_2)}$. Mechanistically, this implies when the inter-electronic separation is very large, the system becomes uncorrelated. The subscripts marked with *'uc'* and *'c'* has been used to indicate the 'uncorrelated' and 'correlated' systems respectively in all the sections of this paper. We shall use our model to compute the uncorrelated and correlated Shannon, Fisher information entropies and the Fisher-Shannon product both in the coordinate and momentum spaces for the uncorrelated and correlated systems. In applicative context it will, therefore, be quite interesting to examine how Shannon (S) and Fisher (I) information entropies along with the Fisher-Shannon product respond to important physical effects like the electron-electron correlation which plays an important role in the physics of many electron systems. To the best of our knowledge, the Shannon entropy, Shannon information and Fisher-Shannon product of the 'Hartree and Ingman (1933)' [13] type trial wave function have not been reported before in the literature.

Section 2 has been focused on obtaining the expressions for single particle wave functions [$\psi(\vec{r})$, $\phi(\vec{p})$] and single particle charge densities [$\rho(\vec{r})$,$\gamma(\vec{p})$] both in coordinate and momentum space for the uncorrelated and correlated systems.

In Section 3, we have used the expressions for single particle charge densities in both coordinate and momentum space to calculate uncorrelated [$S_{\rho_{uc}}$,$S_{\gamma_{uc}}$] and correlated [S_{ρ_c},S_{γ_c}] Shannon entropies. Similarly we have calculated uncorrelated [$I_{\rho_{uc}}$,$I_{\gamma_{uc}}$] and correlated [I_{ρ_c},I_{γ_c}] Fisher entropies. Consequently, the Fisher-Shannon products both in coordinate and momentum space for the uncorrelated and correlated systems have also been computed. We have also shown that the sum of correlated Shannon entropies is greater than that of the sum of the uncorrelated Shannon entropies in coordinate and momentum space i.e. (S_{ρ_c} + S_{γ_c}) >($S_{\rho_{uc}}$ + $S_{\gamma_{uc}}$). Each of the sums also satisfies the *BBM* inequality i.e. (S_ρ + S_γ)$\geqslant 3(1+ln\pi)$. In case of Fisher information entropies, it has been observed that the product of correlated Fisher information entropies in coordinate and momentum space $I_{\rho_c}I_{\gamma_c}$ is greater than that of the product of the uncorrelated Fisher entropies in coordinate and momentum space $I_{\rho_{uc}}I_{\gamma_{uc}}$. Both the products $I_{\rho_{uc}}I_{\gamma_{uc}}$ and $I_{\rho_c}I_{\gamma_c}$ also satisfy the Fisher based uncertainty relation $I_\rho\ I_\gamma \geqslant 36$. The inequality relation for the Fisher-Shannon products for the uncorrelated and correlated systems is $P_{\rho\gamma} = P_\rho\ P_\gamma \geqslant 1$ and the corresponding numerical results along with the verification of the relation are presented in the Table 3.5.

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

2 Extraction of single particle wave function and single particle charge density from the correlated wave function

In this Section, we shall extract the expressions for the single particle wave function from the expression of the many particle correlated wave function expressed in equation (1.13) and equation (1.14) involving some adjustable parameters in coordinate and momentum spaces for both the correlated and uncorrelated systems and hence the single particle charge density. In this purpose, the many particles correlated trial wave function i.e. the 'Hartree and Ingman (1933)' [13] type wave function can be written as follows:

$$\psi(\vec{r}_1, \vec{r}_2, r_{12}) = ce^{-\alpha(r_1+r_2)}(1 - \lambda e^{-\mu r_{12}}). \tag{2.1}$$

Now integrating the wave function of equation (2.1) over $d\vec{r}_2$ we have,

$$\int \psi(\vec{r}_1, \vec{r}_2, r_{12}) d\vec{r}_2 = ce^{-\alpha r_1} \int e^{-\alpha r_2} d\vec{r}_2 - c\lambda e^{-\alpha r_1} \int e^{-\alpha r_2} e^{-\mu r_{12}} d\vec{r}_2.$$

The above integral can be written as

$$\int \psi(\vec{r}_1, \vec{r}_2, r_{12}) d\vec{r}_2 = ce^{-\alpha r_1} I_1 - c\lambda e^{-\alpha r_1} I_2 \tag{2.2}$$

where

$$I_1 = \int e^{-\alpha r_2} d\vec{r}_2 \tag{2.3}$$

and

$$I_2 = \int e^{-\alpha r_2} e^{-\mu r_{12}} d\vec{r}_2. \tag{2.4}$$

Here 'c' is the normalization constant.
Finally, the complete coordinate space wave function $\psi(\vec{r})$ can be written as follows

$$\begin{aligned} \psi(\vec{r}) &= \psi_1(\vec{r}) + \psi_2(\vec{r}) \\ &= ce^{-\alpha r_1} I_1 - c\lambda e^{-\alpha r_1} I_2 \\ &= \frac{8e^{-r\alpha} c\pi}{\alpha^3} + [\frac{4\pi c\lambda e^{-r\alpha}[\frac{8(e^{-r\alpha}-e^{-r\mu})\alpha\mu}{(-\alpha^2+\mu^2)^3} - \frac{2(e^{-r\mu})r\alpha}{(-\alpha^2+\mu^2)^2} - \frac{2(e^{-r\alpha})r\mu}{(-\alpha^2+\mu^2)^2}]}{r}], \end{aligned} \tag{2.5}$$

where

$$\psi_1(\vec{r}) = \frac{8e^{-r\alpha} c\pi}{\alpha^3} \tag{2.6}$$

and

$$\psi_2(\vec{r}) = [\frac{4\pi c\lambda e^{-r\alpha}[\frac{8(e^{-r\alpha}-e^{-r\mu})\alpha\mu}{(-\alpha^2+\mu^2)^3} - \frac{2(e^{-r\mu})r\alpha}{(-\alpha^2+\mu^2)^2} - \frac{2(e^{-r\alpha})r\mu}{(-\alpha^2+\mu^2)^2}]}{r}]. \tag{2.7}$$

We have used the standard values of the variational parameters (λ, α and μ) throughout our all calculations as $\lambda = 0.586$, $\alpha = 1.8395$ and $\mu = 0.379$.

The uncorrelated and correlated wave functions in coordinate-space are represented as

$$\psi_{uc}(\vec{r}) = \psi_1(\vec{r}) = \frac{8e^{-r\alpha} c\pi}{\alpha^3}, \tag{2.8}$$

with normalization constant $c = 0.3486$
and

$$\psi_c(\vec{r}) = \psi(\vec{r}) = \frac{8e^{-r\alpha} c\pi}{\alpha^3} + [\frac{4\pi c\lambda e^{-r\alpha}[\frac{8(e^{-r\alpha}-e^{-r\mu})\alpha\mu}{(-\alpha^2+\mu^2)^3} - \frac{2(e^{-r\mu})r\alpha}{(-\alpha^2+\mu^2)^2} - \frac{2(e^{-r\alpha})r\mu}{(-\alpha^2+\mu^2)^2}]}{r}], \tag{2.9}$$

with normalization constant $c = 0.5031$.

To study the properties of Shannon information entropy (S) and Fisher information entropy (I) in the momentum space, the Fourier transform of the coordinate space wave function is taken. For analytically calculating the required transformations the following standard integrals [3] have been used,

$$\int e^{-\gamma\xi} e^{i\vec{\mu}\cdot\vec{\xi}} = \frac{8\pi\gamma}{(\gamma^2+\mu^2)^2}, \tag{2.10}$$

$$\int \frac{1}{\xi} e^{-\gamma\xi} e^{i\vec{\mu}\cdot\vec{\xi}} = \frac{4\pi}{(\gamma^2+\mu^2)^2}. \tag{2.11}$$

Taking recourse of the Fourier transform of the coordinate space wave function $\psi(\vec{r})$, the momentum space wave function $\phi(\vec{p})$ can be written as $\phi(\vec{p}) = \phi_1(\vec{p}) + \phi_2(\vec{p})$.

The complete momentum space wave function $\phi(\vec{p})$ can be written as follows:

$$\begin{aligned} \phi(\vec{p}) &= \phi_1(\vec{p}) + \phi_2(\vec{p}) \\ &= \frac{64\pi^2\tilde{c}}{(2\pi)^{\frac{3}{2}}\alpha^2(\alpha^2+p^2)^2} + \frac{128\pi^2\tilde{c}\lambda\alpha\mu}{(2\pi)^{\frac{3}{2}}(-\alpha^2+\mu^2)^3}[\frac{1}{(4\alpha^2+p^2)} - \frac{1}{((\alpha+\mu)^2+p^2)}] - \frac{64\pi^2\tilde{c}\lambda\alpha(\alpha+\mu)}{(2\pi)^{\frac{3}{2}}(-\alpha^2+\mu^2)^2((\alpha+\mu)^2+p^2)^2} \end{aligned}$$

$$-\frac{128\pi^2\tilde{c}\lambda\alpha\mu}{(2\pi)^{\frac{3}{2}}(-\alpha^2+\mu^2)^2(4\alpha^2+p^2)^2} \quad (2.12)$$

The expressions for the uncorrelated and correlated wave function in momentum space are given as follows:

$$\phi_{uc}(\vec{p}) = \phi_1(\vec{p}) = \frac{64\pi^2\tilde{c}}{(2\pi)^{\frac{3}{2}}\alpha^2(\alpha^2+p^2)^2}, \quad (2.13)$$

with the normalization constant $\tilde{c} = 0.3486$
and

$$\phi_c(\vec{p}) = \phi(\vec{p}) = \frac{64\pi^2\tilde{c}}{(2\pi)^{\frac{3}{2}}\alpha^2(\alpha^2+p^2)^2} + \frac{128\pi^2\tilde{c}\lambda\alpha\mu}{(2\pi)^{\frac{3}{2}}(-\alpha^2+\mu^2)^3}[\frac{1}{(4\alpha^2+p^2)} - \frac{1}{((\alpha+\mu)^2+p^2)}]$$
$$-\frac{64\pi^2\tilde{c}\lambda\alpha(\alpha+\mu)}{(2\pi)^{\frac{3}{2}}(-\alpha^2+\mu^2)^2((\alpha+\mu)^2+p^2)^2} - \frac{128\pi^2\tilde{c}\lambda\alpha\mu}{(2\pi)^{\frac{3}{2}}(-\alpha^2+\mu^2)^2(4\alpha^2+p^2)^2}, \quad (2.14)$$

with the normalization constant $\tilde{c} = 0.5031$.

Now we shall find the expressions for the single particle charge densities in coordinate and momentum spaces for both the correlated and uncorrelated systems. The uncorrelated and correlated single-particle charge densities in coordinate space can simply be expressed as follows:

$$\rho_{uc} = |\psi_{uc}(\vec{r})|^2, \quad (2.15)$$

and

$$\rho_c = |\psi_c(\vec{r})|^2. \quad (2.16)$$

Similarly the uncorrelated and correlated single particle charge densities in momentum space are written as follows:

$$\gamma_{uc} = |\phi_{uc}(\vec{p})|^2, \quad (2.17)$$

and

$$\gamma_c = |\phi_c(\vec{p})|^2. \quad (2.18)$$

3 Computation of Shannon entropy, Fisher information entropy and the Fisher-Shannon product

In this section we present the results for the Shannon information entropy (S), Fisher information entropy (I) and Fisher-Shannon product both in coordinate and momentum space for uncorrelated and correlated systems. The expressions of uncorrelated Shannon information entropies in coordinate space [$S_{\rho_{uc}}$] and momentum space [$S_{\gamma_{uc}}$] are computed using the expressions from the equation (1.2) and equation (1.3) respectively. Similarly the uncorrelated Fisher information entropies in coordinate space [$I_{\rho_{uc}}$] and momentum space [$I_{\gamma_{uc}}$] are computed using the expressions from the equation (1.4) and equation (1.5) respectively. Now for computing the expressions for correlated Shannon information entropies in coordinate space [S_{ρ_c}] and momentum space [S_{γ_c}] the corresponding correlated wave functions have been used in the expressions of equation (1.2) and equation (1.3) respectively. Similarly we have also done for the correlated Fisher information entropies in coordinate space [I_{ρ_c}] and momentum space [I_{γ_c}] respectively using the equation (1.4) and equation (1.5).

Moreover, the expressions for uncorrelated Fisher-Shannon product in coordinate space [$P_{\rho_{uc}}$] and momentum space [$P_{\gamma_{uc}}$] and correlated Fisher-Shannon product in coordinate space [P_{ρ_c}] and momentum space [P_{γ_c}] are computed from the equation (1.10) and equation (1.11) respectively with the help of the corresponding equation (1.8) and equation (1.9) for the Shannon power in coordinate space (J_ρ) and momentum space (J_γ) for the uncorrelated and correlated systems.

The calculated values for the uncorrelated and correlated Shannon information entropies in coordinate and momentum space at different r and p values are presented in Table 3.1 respectively as follows:

***Table* 3.1:** Shannon information entropies in coordinate and momentum space for uncorrelated and correlated systems

Sl. No.	r varies from 0 to (in a.u.)	Coordinate space		p varies from 0 to (in a.u.)	Momentum space		$(S_{\rho_{uc}} + S_{\gamma_{uc}})$	$(S_{\rho_c} + S_{\gamma_c})$
		$S_{\rho_{uc}}$	S_{ρ_c}		$S_{\gamma_{uc}}$	S_{γ_c}		
1	5	2.316	2.442	5	4.134	4.024	6.450	6.466
2	10	2.316	2.442	10	4.243	4.123	6.559	6.565
3	100	2.316	2.442	100	4.250	4.130	6.566	6.572
4	1000	2.316	2.442	1000	4.250	4.130	6.566	6.572
5	5000	2.316	2.442	5000	4.250	4.130	6.566	6.572
6	10000	2.316	2.442	10000	4.250	4.130	6.566	6.572
7	100000	2.316	2.442	100000	4.250	4.130	6.566	6.572
8	1000000	2.316	2.442	1000000	4.250	4.130	6.566	6.572
9	5000000	2.316	2.442	5000000	4.250	4.130	6.566	6.572
10	Infinity	2.316	2.442	Infinity	4.250	4.130	6.566	6.572

From Table 3.1, it is observed that correlation augments the Shannon entropies in coordinate space as $S_{\rho_c} > S_{\rho_{uc}}$ and diminishes it in momentum space as $S_{\gamma_c} < S_{\gamma_u c}$. It is also evident that sum of correlated Shannon entropies i.e. $(S_{\rho_c} + S_{\gamma_c})$ is greater than the sum of uncorrelated Shannon entropies i.e. $(S_{\rho_{uc}} + S_{\gamma_{uc}})$. Thus we have verified the uncertainty relation,$(S_{\rho_c} + S_{\gamma_c}) > (S_{\rho_{uc}} + S_{\gamma_{uc}})$.

The calculated values for the uncorrelated and correlated Fisher information entropies for the coordinate and momentum space at different r and p values are presented in Table 3.2 respectively as follows:

***Table* 3.2:** Fisher information entropies in coordinate and momentum space for uncorrelated and correlated systems

Sl. No.	r varies from 0 to (in a.u.)	Coordinate space		p varies from 0 to (in a.u.)	Momentum space		$I_{\rho_{uc}}\ I_{\gamma_{uc}}$	$I_{\rho_c}\ I_{\gamma_c}$
		$I_{\rho_{uc}}$	I_{ρ_c}		$I_{\gamma_{uc}}$	I_{γ_c}		
1	5	13.535	12.588	5	3.539	3.862	47.901	48.615
2	10	13.535	12.588	10	3.546	3.868	47.995	48.690
3	100	13.535	12.588	100	3.546	3.822	47.995	48.111
4	1000	13.535	12.588	1000	3.546	3.868	47.995	48.690
5	5000	13.535	12.588	5000	3.546	3.868	47.995	48.690
6	10000	13.535	12.588	10000	3.546	3.868	47.995	48.690
7	100000	13.535	12.588	100000	3.546	3.867	47.995	48.678
8	1000000	13.535	12.588	1000000	3.546	3.861	47.995	48.602
9	5000000	13.535	12.588	5000000	3.546	3.831	47.995	48.225
10	Infinity	13.535	12.588	Infinity	3.546	3.869	47.995	48.703

From Table 3.2 it is observed that correlation diminishes the Fisher entropies in coordinate space and augments it in momentum space. We have also verified from Table 3.2 that the product of correlated $[I_{\rho_c} I_{\gamma_c}]$ and the product of uncorrelated $[I_{\rho_{uc}} I_{\gamma_{uc}}]$ Fisher entropies satisfy the inequality condition $I_{\rho_c}\ I_{\gamma_c} > I_{\rho_{uc}} I_{\gamma_{uc}}$. It is also verified in general that the products of Fisher entropies ($I_{\rho_c} I_{\gamma_c}$ and $I_{\rho_{uc}} I_{\gamma_{uc}}$) satisfy the Fisher-based uncertainty relation
$I_\rho\ I_\gamma \geqslant 36$.

To calculate the values of the uncorrelated and correlated Shannon power in coordinate space ($J_{\rho_{uc}}$,J_{ρ_c}) and momentum space ($J_{\gamma_{uc}}$,J_{γ_c}) following equation (1.8) and equation (1.9), we have used the values for the Shannon information entropies of the Table 3.1 for different r and p values and presented them in Table 3.3 as follows:

***Table* 3.3:** Shannon information entropies, Shannon power in coordinate and momentum space for uncorrelated and correlated systems

Sl. No.	r and p varies from 0 to (in a.u.)	Shannon information entropies				Shannon Power			
		Coordinate space		Momentum space		Coordinate space		Momentum space	
		$S_{\rho_{uc}}$	S_{ρ_c}	$S_{\gamma_{uc}}$	S_{γ_c}	$J_{\rho_{uc}}$	J_{ρ_c}	$J_{\gamma_{uc}}$	J_{γ_c}
1	5	2.316	2.442	4.134	4.024	0.745	0.810	2.504	2.327
2	10	2.316	2.442	4.243	4.123	0.745	0.810	2.693	2.486
3	100	2.316	2.442	4.250	4.130	0.745	0.810	2.705	2.498
4	1000	2.316	2.442	4.250	4.130	0.745	0.810	2.705	2.498
5	5000	2.316	2.442	4.250	4.130	0.745	0.810	2.705	2.498
6	10000	2.316	2.442	4.250	4.130	0.745	0.810	2.705	2.498
7	100000	2.316	2.442	4.250	4.130	0.745	0.810	2.705	2.498
8	1000000	2.316	2.442	4.250	4.130	0.745	0.810	2.705	2.498
9	5000000	2.316	2.442	4.250	4.130	0.745	0.810	2.705	2.498
10	Infinity	2.316	2.442	4.250	4.130	0.745	0.810	2.705	2.498

Moreover, to calculate the values for the uncorrelated and correlated Fisher-Shannon product in coordinate space ($P_{\rho_{uc}}$,P_{ρ_c}) and momentum space ($P_{\gamma_{uc}}$,P_{γ_c}) at different r and p values following equation (1.10) and equation (1.11), we have used the values for the Fisher information entropies and Shannon power from Table 3.2 and Table 3.3 respectively and presented them in Table 3.4 as follows:

***Table* 3.4:** Fisher information entropies, Shannon power and Fisher-Shannon product in coordinate and momentum space for uncorrelated and correlated systems

Sl. No.	r and p varies from 0 to (in a.u.)	Fisher information entropies				Shannon power				Fisher-Shannon product			
		Coordinate space		Momentum space		Coordinate space		Momentum space		Coordinate space		Momentum space	
		$I_{\rho_{uc}}$	I_{ρ_c}	$I_{\gamma_{uc}}$	I_{γ_c}	$J_{\rho_{uc}}$	J_{ρ_c}	$J_{\gamma_{uc}}$	J_{γ_c}	$P_{\rho_{uc}}$	P_{ρ_c}	$P_{\gamma_{uc}}$	P_{γ_c}
1	5	13.535	12.588	3.539	3.862	0.745	0.810	2.504	2.327	3.361	3.399	2.954	4.283
2	10	13.535	12.588	3.546	3.868	0.745	0.810	2.693	2.486	3.361	3.399	3.183	3.205
3	100	13.535	12.588	3.546	3.822	0.745	0.810	2.705	2.498	3.361	3.399	3.197	3.446
4	1000	13.535	12.588	3.546	3.868	0.745	0.810	2.705	2.498	3.361	3.399	3.197	3.488
5	5000	13.535	12.588	3.546	3.868	0.745	0.810	2.705	2.498	3.361	3.399	3.197	3.488
6	10000	13.535	12.588	3.546	3.868	0.745	0.810	2.705	2.498	3.361	3.399	3.197	3.488
7	100000	13.535	12.588	3.546	3.867	0.745	0.810	2.705	2.498	3.361	3.399	3.197	3.487
8	1000000	13.535	12.588	3.546	3.861	0.745	0.810	2.705	2.498	3.361	3.399	3.197	3.481
9	5000000	13.535	12.588	3.546	3.831	0.745	0.810	2.705	2.498	3.361	3.399	3.197	3.454
10	Infinity	13.535	12.588	3.546	3.869	0.745	0.810	2.705	2.498	3.361	3.399	3.197	3.489

Let us now verify the values obtained in the Table 3.4 for the Fisher-Shannon product, as per the requirement of the equation (1.12) the Fisher-Shannon product must satisfy the inequality relation $P_{\rho\gamma} = P_\rho\ P_\gamma \geqslant 1$. Following is the Table of verification for the Fisher-Shannon product:

***Table* 3.5:** Verification Table for Fisher-Shannon product in coordinate and momentum space for uncorrelated and correlated systems

Sl. No.	Fisher-Shannon product				Uncorrelated system	Correlated system	The inequality relation to verify $P_\rho\ P_\gamma \geqslant 1$
	Coordinate space		Momentum space				
	$P_{\rho_{uc}}$	P_{ρ_c}	$P_{\gamma_{uc}}$	$P_{\gamma_{uc}}$	$P_{\rho_{uc}}\ P_{\gamma_{uc}}$	$P_{\rho_c}\ P_{\gamma_c}$	$P_{\rho_{uc}}\ P_{\gamma_{uc}} \geqslant 1$ or $P_{\rho_c}\ P_{\gamma_c} \geqslant 1$
1	3.361	3.399	2.954	4.283	9.928	14.558	Yes
2	3.361	3.399	3.183	3.205	10.698	10.894	Yes
3	3.361	3.399	3.197	3.446	10.745	11.713	Yes
4	3.361	3.399	3.197	3.488	10.745	11.856	Yes
5	3.361	3.399	3.197	3.488	10.745	11.856	Yes
6	3.361	3.399	3.197	3.488	10.745	11.856	Yes
7	3.361	3.399	3.197	3.487	10.745	11.852	Yes
8	3.361	3.399	3.197	3.481	10.745	11.832	Yes
9	3.361	3.399	3.197	3.454	10.745	11.740	Yes
10	3.361	3.399	3.197	3.489	10.745	11.859	Yes

4 Concluding remarks

In the present work, we have used the r_{12}- dependent two electron 'Hartree and Ingman(1933)' type trial wave function to construct a single particle wave function $\psi(\vec{r})$. By taking the Fourier transform of $\psi(\vec{r})$, the wave function in momentum space i.e. $\phi(\vec{p})$ has been constructed. The wave functions $\psi(\vec{r})$ and $\phi(\vec{p})$ are used to evaluate the expressions for the single particle charge densities in coordinate and momentum spaces. These expressions have been further used to construct the analytical expressions for Shannon and Fisher entropies, Shannon power and the Fisher-Shannon product and hence to compute their values in both coordinate and momentum spaces. The expressions have been constructed by taking the correlation into account as well as without it. In Table 3.1 and Table 3.2 we have provided the values of Shannon and Fisher entropies for different values of r and p. In coordinate space, the correlation augments the values of Shannon entropies and in momentum space the correlation plays just the opposite role. In case of Fisher entropies, the correlation diminishes the values in coordinate space and augments in momentum space. Thus from the data of the two Tables we observe that correlation plays just the opposite roles in case of Shannon and Fisher information entropies. In addition to this, we have verified from Table 3.1 the uncertainty relation $(S_\rho + S_\gamma) \geqslant 3(1+ln\pi)$and the inequality condition $(S_{\rho_c} + S_{\gamma_c}) > (S_{\rho_{uc}} + S_{\gamma_{uc}})$ for Shannon entropy. Simultaneously, for Fisher entropies we have verified the relations from Table 3.2 that $I_{\rho_c} I_{\gamma_c} > I_{\rho_{uc}} I_{\gamma_{uc}}$ and $I_\rho\ I_\gamma \geqslant 36$. In Table 3.3 the numerical values relating to Shannon power for the uncorrelated and correlated systems in coordinate space ($J_{\rho_{uc}}$,J_{ρ_c}) and momentum space ($J_{\gamma_{uc}}$,J_{γ_c}) have been demonstrated. And Table 3.4 depicts altogether the numerical values of Fisher information entropies for the uncorrelated and correlated systems, Shannon power and Fisher-Shannon product in coordinate and momentum space. Moreover, the verification of Fisher-Shannon product has been checked and confirmed by the data presented in Table 3.5. Since our computed values of Shannon, Fisher information entropies and Fisher-Shannon product satisfy their respective uncertainty relationships; it validates our results obtained in a consistent way. Further the variation of information entropic measurements with coordinate (r) and momentum (p) values give us an insight into the dynamics of evolution of the system in the coordinate and momentum spaces respectively and that can easily be analyzed from the difference of numerical values computed separately for the Fisher-Shannon product in respect of the uncorrelated and correlated systems. It thus provides important evidence that the Fisher-Shannon product can be regarded as an appropriate measure of electron correlation. A more systematic and extensive analysis of this new correlation measure in many other N-electron systems is needed to get a deeper insight into it. It thus remains an interesting curiosity to investigate the efficacy of this method for studying higher electronic systems. In our further works we shall try to investigate such systems.

Conflict of Interest

The authors declare that there is no conflict of interests, financial or otherwise regarding the publication of this paper.

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