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Studying the Effect of Correlation on Two Electron Systems and Measurement of Information Entropies

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ABSTRACT: In this paper, a three parameter (α, λ, μ) 'Hartree and Ingman (1933)' type correlated wave function has been used to derive an analytical model to quantify the two electron systems. The model is used to construct the expressions for the single particle wave functions [$\psi(\vec{r})$, $\phi(\vec{p})$] in coordinate space and momentum space respectively with the subscripts marked as correlated (c) and uncorrelated (uc) ones. Further, the correlated and uncorrelated wave functions are used to form the single particle charge densities [$\rho(\vec{r})$, $\gamma(\vec{p})$] in coordinate space and momentum space. These wave functions and the single particle charge densities are used to compute the numerical values of the Shannon (S) and Fisher (I) information entropies for both the correlated and uncorrelated systems in coordinate space and momentum spaces and furthermore to examine their correlation effects in coordinate and momentum spaces. The uncorrelated and correlated values of Shannon information entropies indicate the reciprocity between the coordinate and momentum spaces such that low values of the Shannon information entropy in coordinate space (S_ρ), are associated with the high values of Shannon information entropy in momentum space (S_γ) . The uncorrelated and correlated values of Shannon information entropies (S) also validate the entropic uncertainty relations Bialynicki-Birula and Mycielski (BBM) inequality which reads as $(S_\rho + S_\gamma) \geq 3(1 + ln\pi)$, as well as another stronger version of the uncertainty relation that is $\left(S_{\rho_c} + S_{\gamma_c}\right) > (S_{\rho_{uc}} + S_{\gamma_{uc}})$. Further, both the products of uncorrelated and correlated values of Fisher information entropies $I_{\rho_{uc}} I_{\gamma u_c}$ and $I_{\rho_c} I_{\gamma_c}$ satisfy the inequality condition $I_{\rho_c} I_{\gamma_c} > I_{\rho_{uc}} I_{\gamma_{uc}}$ in coordinate and momentum spaces. At the same time these products also satisfy the Fisher based uncertainty relation, $I_\rho I_\gamma \geq 36$. The consistency of the results satisfying the uncertainty relations can be checked from the data demonstrated in the Table 1 and Table 2.

KEYWORDS: Correlated and uncorrelated systems; Coordinate and momentum space, Effect of correlation, Single particle charge densities; Shannon information entropy; Fisher information entropy; Uncertainty relation.

1. Introduction: In the independent–electron model the effect of inter-electronic repulsion, globally referred to as correlation is disregarded. The correlation effect can, however, have major influence on measureable quantities in atomic systems. The correlation energy of a many-electron system is defined by the difference between the exact total energy and Hartree-Fock energy. Traditionally, the correlation energy is used as a guide **[1]** for the amount of correlation in a given system. We deal with the effect of correlation for two-electron systems using the 'Hartree and Ingman (1933)' type trial wave function which can be written as

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

where 'c' is the normalization constant of the wave function and α, λ and μ are the variational parameters. When $\lambda = 1$ and $r_{12} = 0$, the wave function takes the form as $\psi(\vec{r}_1, \vec{r}_2, r_{12}) = 0$. The system having explicitly r_{12} dependent term is called 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 $\psi(\vec{r}_1, \vec{r}_2, r_{12}) = ce^{-\alpha(r_1+r_2)}$. Mechanistically, this implies when the inter-electronic separation is very large, the system becomes uncorrelated.

A few years ago, attempts were made by Bhattacharyya *et al* **[2]** to find out the ground-state energy of the two-electron system working with the 'Hartree and Ingman (1933)' 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, α = 1.8395, λ = 0.586 and μ = 0.379. These values of variation parameters led them to the result for the ground-state energy of the two-electron system as −2.8894 atomic unit (a.u.)

which is not far from the exact value of −2.9037 a.u.. Very recently, Tripathy *et al* **[3]** derived an interesting approach to compute the ground-state energies of the helium iso-electronic sequence justifying the claim that correlation can also be accounted for by introducing variational parameters in the Hamiltonian.

In this article we are going to study the effect of correlation of two-electron system as a measure of information entropy. The concept of entropy was introduced in thermodynamics by Clausius (1862) and Boltzmann (1896) and was later applied by Shannon (1948) and Jaynes (1957) to information theory [**4-6**]. Entropy of a system is associated with the disorder and related information. It quantifies the amount of uncertainty involved in the value of a random variable or the outcome of a random process. In hypothetical concept, the system in perfect order has no information. The information contained in the system is proportional to the disorderliness of the system. The information content of a system is typically evaluated by the probability density of the system.

The Shannon information entropy [**4**] (*S*) and Fisher information entropy [**5**] (*I*) both are characterized by probability density corresponding to changes in some observable. The coordinate space Shannon information entropy (s_ρ) for a normalized wave function of the N-electron system with $\psi(\vec{r}_1, \vec{r}_2 \ldots\ldots \vec{r}_N)$ is written by

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

where

$$\rho(\vec{r}) = \int |\psi(\vec{r}, \vec{r}_2 \ldots\ldots \vec{r}_N)|^2 d\vec{r}_2 \ldots\ldots d\vec{r}_N. \tag{3}$$

The charge density $\rho(\vec{r})$ is also normalized to unity.

Correspondingly, the momentum-space Shannon information entropy (s_γ) is defined as

$$s_\gamma = -\int \gamma(\vec{p}) ln\, \gamma(\vec{p}) d\vec{p}. \tag{4}$$

Here $\gamma(\vec{p}) = \int |\phi(\vec{p}, \vec{p}_2 \ldots\ldots \vec{p}_N)|^2\, d\vec{p}_2 \ldots\ldots d\vec{p}_N$ is the single particle charge density, where the momentum space wave function $\phi(\vec{p}, \vec{p}_2 \ldots\ldots \vec{p}_N)$ is obtained by the Fourier transform of the coordinate space wave function. The coordinate and momentum space entropies as defined by equations (2) and (4) allowed Bialynicki-Birula and Mycielski **[7]** to introduce another version of the uncertainty relation which for a 3-dimensional system reads as follows:

$$S_\rho + S_\gamma \geq 3(1 + ln\pi). \tag{5}$$

Equation (5) is known as the BBM inequality. Clearly, this inequality indicates the reciprocity between the coordinate and momentum space Shannon information entropies such that high values of S_γ are associated with low values of S_ρ.

For the N-electron atom the coordinate and momentum space Fisher information entropy (I_ρ and I_γ) **[5]** are defined by

$$I_\rho = \int \frac{1}{\rho(\vec{r})} [\vec{\nabla}\rho(\vec{r})]^2 d\vec{r} \tag{6}$$

and

$$I_\gamma = \int \frac{1}{\gamma(\vec{p})} [\vec{\nabla}\gamma(\vec{p})]^2 d\vec{p}. \tag{7}$$

The above mentioned expressions for Fisher information entropies in coordinate and momentum space can also be written in equivalent forms **[8]** as

$$I_\rho = 4\int |\vec{\nabla}\ \psi(\vec{r})|^2 d\vec{r} \tag{8}$$

and

$$I_\gamma = 4\int |\vec{\nabla}\ \emptyset(\vec{p})|^2 d\vec{p}\ . \tag{9}$$

For computational purposes it will be profitable to work with equations (8) and (9). The disorder aspect of Fisher information entropy has been studied in some length by Frieden **[9]**. The uncertainty properties are clearly delineated by the Stam inequalities **[10].** The product $I_\rho I_\gamma$ has been conjectured to exhibit a nontrivial lower bound **[11]** such that for three-dimensional systems it reads as:

$$I_\rho I_\gamma \geq 36. \tag{10}$$

Equation (10) is sometimes called a Fisher-based uncertainty relation. Information entropies of two-electron systems can be expressed in closed analytic form for separable approximation of the wave function. However, the explicitly r_{12}dependent non-separable two-particle correlated wave function can be dealt with by following an alternative approach as contained in the ref. **[12]**.

The aim of our present work is to derive an analytical model to quantify the correlation in two-electron systems described by wave function containing explicitly r_{12}dependent term. We shall use our model to compute the uncorrelated and correlated Shannon and Fisher information entropies both in the coordinate and momentum spaces. In applicative context it will, therefore, be quite interesting to examine how Shannon (*S*) and Fisher (*I*) information entropies respond to important physical effects like the electron-electron correlation which plays an important role in the physics of many-electron systems.

Section-2 have 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. The graphical representations of the wave functions and the single particle charge densities as a function of *r* in the coordinate space and as a function of *p* in the momentum space are shown respectively. Later the response of the effect of the correlation on the single particle charge densities [$\rho(\vec{r})$, $\gamma(\vec{p})$] as a function of *r* in the coordinate space and as a function of *p* in the momentum-space are also shown graphically.

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.

We have also shown, on one hand that the sum of correlated Shannon entropies in coordinate and momentum space are greater than that of the sum of the uncorrelated Shannon entropies in coordinate and momentum space [$S_{\rho_c} + S_{\gamma_c} > S_{\rho_{uc}} + S_{\gamma_{uc}}$]. Each of the sums also satisfies the BBM inequality $S_\rho + S_\gamma \geq 3(1 + ln\pi)$. In case of Fisher information entropies, it has been examined 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 $\left[I_{\rho_{uc}} I_{\gamma_{uc}}\right]$. Both the products [$I_{\rho_c} I_{\gamma_c}$ and $I_{\rho_c} I_{\gamma_c}$] also satisfy the Fisher based uncertainty relation $I_\rho I_\gamma \geq 36$.

Finally, Section-4 has been devoted for summarizing the present work. The inferences which we have drawn from this work have also been discussed in this section.

2. Single particle wave function and Single particle charge density of two electron systems: We have chosen to work with the 'Hartree and Ingman (1933)' type correlated trial wave function **[13]** written as

$$\psi(\vec{r}_1, \vec{r}_2, r_{12}) = ce^{-\alpha(r_1+r_2)} \chi(r_{12}) \tag{11}$$

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

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

Here α, λ and μ are adjustable parameters of the trial wave function.

Now integrating the wave function in (11) over $d\vec{r}_2$ we have,

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

$$= ce^{-\alpha r_1} I_1 - c\lambda e^{-\alpha r_1} I_2 \tag{13}$$

where $I_1 = \int e^{-\alpha r_2}\, d\vec{r}_2 = \frac{8\pi}{\alpha^3}$. (13a)

and $I_2 = \int e^{-\alpha r_2}\, e^{-\mu r_{12}} d\vec{r}_2 = \frac{4\pi\left(-\frac{8(e^{-r\alpha}-e^{-r\mu})\alpha\mu}{(-\alpha^2+\mu^2)^3} + \frac{2e^{-r\mu} r\alpha}{(-\alpha^2+\mu^2)^2} + \frac{2e^{-r\alpha} r\mu}{(-\alpha^2+\mu^2)^2}\right)}{r}$, (13b)

here 'c' is the normalization constant.

Finally, the complete coordinate space wave function $\psi(\vec{r})$ can be written as follows

$$\psi(\vec{r}) = \psi_1(\vec{r}) + \psi_2(\vec{r}) = ce^{-\alpha r_1} I_1 - c\lambda e^{-\alpha r_1} I_2$$

$$= \frac{8e^{-r\alpha} c\pi}{\alpha^3} + \frac{4\pi c\lambda e^{-r\alpha}\left(\frac{8(e^{-r\alpha}-e^{-r\mu})\alpha\mu}{(-\alpha^2+\mu^2)^3} - \frac{2e^{-r\mu} r\alpha}{(-\alpha^2+\mu^2)^2} - \frac{2e^{-r\alpha} r\mu}{(-\alpha^2+\mu^2)^2}\right)}{r} \tag{14}$$

where $\psi_1(\vec{r}) = \frac{8e^{-r\alpha} c\pi}{\alpha^3}$, (15a)

and $\psi_2(\vec{r}) = \left[\frac{4\pi c\lambda e^{-r\alpha}\left(\frac{8(e^{-r\alpha}-e^{-r\mu})\alpha\mu}{(-\alpha^2+\mu^2)^3} - \frac{2e^{-r\mu} r\alpha}{(-\alpha^2+\mu^2)^2} - \frac{2e^{-r\alpha} r\mu}{(-\alpha^2+\mu^2)^2}\right)}{r}\right]$. (15b)

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

$$\psi_{uc}(\vec{r}) = \psi_1(\vec{r}) = \frac{8e^{-r\alpha} c\pi}{\alpha^3}, \tag{16a}$$

with normalization constant $c = 0.348606$,

and

$$\psi_c(\vec{r}) = \psi(\vec{r}) = \left[\frac{8e^{-r\alpha} c\pi}{\alpha^3} + \frac{4\pi c\lambda e^{-r\alpha}\left(\frac{8(e^{-r\alpha}-e^{-r\mu})\alpha\mu}{(-\alpha^2+\mu^2)^3} - \frac{2e^{-r\mu} r\alpha}{(-\alpha^2+\mu^2)^2} - \frac{2e^{-r\alpha} r\mu}{(-\alpha^2+\mu^2)^2}\right)}{r}\right] \tag{16b}$$

with normalization constant $c = 0.503149$.

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 **[14]** have been used,

$$\int e^{-\gamma\xi} e^{+i\vec{\mu}.\vec{\xi}}\, d\vec{\xi} = \frac{8\pi\gamma}{(\gamma^2+\mu^2)^2} \tag{17}$$

$$\int \frac{1}{\xi} e^{-\gamma\xi} e^{+i\vec{\mu}.\vec{\xi}}\, d\vec{\xi} = \frac{4\pi}{(\gamma^2+\mu^2)}. \tag{18}$$

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:

$$\phi(\vec{p}) = \phi_1(\vec{p}) + \phi_2(\vec{p}) = \frac{64\pi^2\tilde{c}}{(2\pi)^{3/2}\alpha^2(\alpha^2+p^2)^2} + \frac{128\pi^2\tilde{c}\lambda\alpha\mu}{(2\pi)^{3/2}(-\alpha^2+\mu^2)^3}\left[\frac{1}{(4\alpha^2+p^2)} - \frac{1}{\{(\alpha+\mu)^2+p^2\}}\right] - \frac{64\pi^2\tilde{c}\lambda\alpha(\alpha+\mu)}{(2\pi)^{3/2}(-\alpha^2+\mu^2)^2\{(\alpha+\mu)^2+p^2\}^2} - \frac{128\pi^2\tilde{c}\lambda\alpha\mu}{(2\pi)^{3/2}(-\alpha^2+\mu^2)^2(4\alpha^2+p^2)^2}. \tag{19}$$

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

$$\phi_{uc}(\vec{p}) = \phi_1(\vec{p}) = \frac{64\pi^2\tilde{c}}{(2\pi)^{3/2}\alpha^2(\alpha^2+p^2)^2} \tag{20a}$$

with the normalization constant $\tilde{c} = 0.348606$, and

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

(20b)

with the normalization constant $\tilde{c} = 0.503149$.

To study the correlation effects the coordinate space wave functions have to be plotted as a function of r. Since they are exponentially decaying functions they have to be multiplied by scaling factor r to make them viable for studying their variation with r.

In the following expressions $\psi_{uc}(\vec{r})$ represents the uncorrelated and $\psi_c(\vec{r})$ represents the correlated wave functions.

$$r\,\psi_{uc}(\vec{r}) = r\,\psi_1(\vec{r}) = r\frac{8e^{-r\alpha}c\pi}{\alpha^3}, \tag{21a}$$

c is the normalization constant.

and

$$r\,\psi_c(\vec{r}) = r\,\psi(\vec{r}) = r\left[\frac{8e^{-r\alpha}c\pi}{\alpha^3} + \frac{4\pi c\lambda e^{-r\alpha}\left(\frac{8(e^{-r\alpha}-e^{-r\mu})\alpha\mu}{(-\alpha^2+\mu^2)^3} - \frac{2e^{-r\mu}r\alpha}{(-\alpha^2+\mu^2)^2} - \frac{2e^{-r\alpha}r\mu}{(-\alpha^2+\mu^2)^2}\right)}{r}\right], \tag{21b}$$

c is the normalization constant.

In the following figure we have plotted $r\,\psi_{uc}(r)\ Vs.r$ and $r\,\psi_c(r)\ Vs.r$.

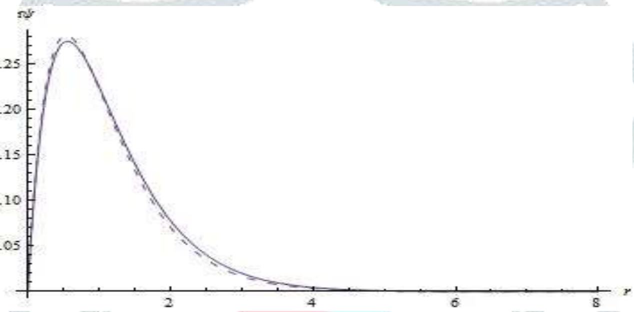

Figure A: $r\,\psi(r)$ Vs. r graph

The dashed and solid lines in Figure A represent the uncorrelated and correlated wave functions in coordinate space respectively. In Figure A, it is observed that near the origin and at infinity both the systems tend to merge together. As r increases we find that $r\,\psi_c(\vec{r}) > r\,\psi_{uc}(\vec{r})$. Thus the uncorrelated system tends to decay faster than the correlated system.

Similarly the wave functions in momentum space have to be multiplied by scaling factor p to make them viable for studying the variations of uncorrelated and correlated wave functions with p. The expressions of uncorrelated and correlated wave functions are rewritten as follows:

$$p\,\phi_{uc}(\vec{p}) = p\,\phi_1(\vec{p}) = p\frac{64\pi^2\,\tilde{c}}{(2\pi)^{3/2}\alpha^2(\alpha^2+p^2)^2}, \tag{22a}$$

where $\tilde{c}$ is the normalization constant,

and

$$p\,\phi_c(\vec{p}) = p\,\phi(\vec{p}) = p\,\frac{64\pi^2\tilde{c}}{(2\pi)^{3/2}\alpha^2(\alpha^2+p^2)^2} + p\left[\frac{128\pi^2\tilde{c}\lambda\alpha\mu}{(2\pi)^{3/2}(-\alpha^2+\mu^2)^3}\left\{\frac{1}{(4\alpha^2+p^2)} - \frac{1}{(\alpha+\mu)^2+p^2}\right\} - \frac{64\pi^2\tilde{c}\lambda\alpha(\alpha+\mu)}{(2\pi)^{3/2}(-\alpha^2+\mu^2)^2\{(\alpha+\mu)^2+p^2\}^2} - \frac{128\pi^2\,\tilde{c}\,\lambda\alpha\mu}{(2\pi)^{3/2}(-\alpha^2+\mu^2)^2(4\alpha^2+p^2)^2}\right], \tag{22b}$$

where $\tilde{c}$ is the normalization constant.

In the following figure we have plotted $p\,\phi_{uc}(p)\ Vs.\ p$ and $p\,\phi_c(p)\ Vs.\ p$.

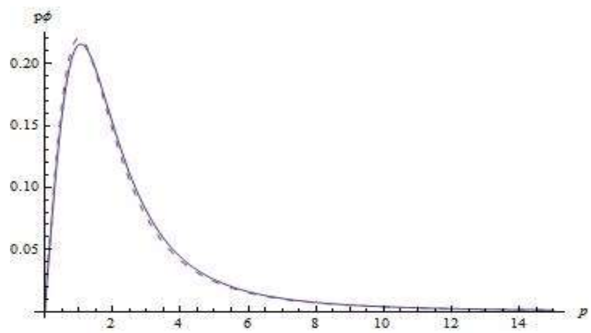

Figure B: $p\,\phi(p)\ Vs.\ p$ graph.

The dashed and solid lines in Figure B represent the uncorrelated and correlated wave functions in momentum space respectively.

In Figure B, it is observed that near the origin and at the infinity both curves tend to merge. After reaching a peak both the curves start decaying exponentially. But in momentum space the trend is opposite to the coordinate space and the correlated system is seen decaying faster.

The uncorrelated and correlated single-particle charge densities in coordinate space are written as follows:

$$\rho_{uc} = |\psi_{uc}(\vec{r})|^2 = 4\pi|\psi_1(r)|^2\, r^2 \quad (23a)$$

and

$$\rho_c = |\psi_c(\vec{r})|^2 = 4\pi|\psi(r)|^2\, r^2 \quad (23b)$$

In the following figure we have plotted the coordinate space charge densities $\rho_{uc}(r)\ Vs. r$ and $\rho_c(r)\ Vs. r$.

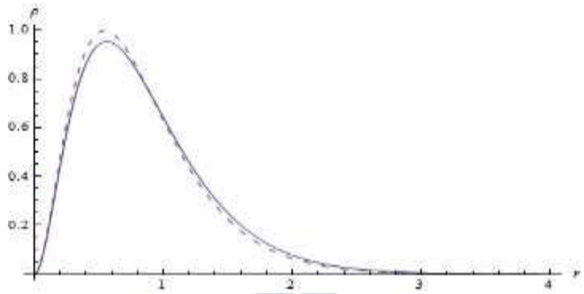

Figure C: $\rho(r)\ Vs. r$ graph.

The dashed and solid lines in Figure C represent the uncorrelated and correlated single particle charge densities in coordinate space respectively.

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

$$\gamma_{uc} = |\phi_{uc}(\vec{p})|^2 = 4\pi|\phi_1(p)|^2\, p^2 \quad (24a)$$

and

$$\gamma_c = |\phi_c(\vec{p})|^2 = 4\pi|\phi(p)|^2\, p^2 \quad (24b)$$

In the following figure we have plotted the uncorrelated and correlated single particle charge densities **[** γ_{uc}, γ_c **]** as a function of p.

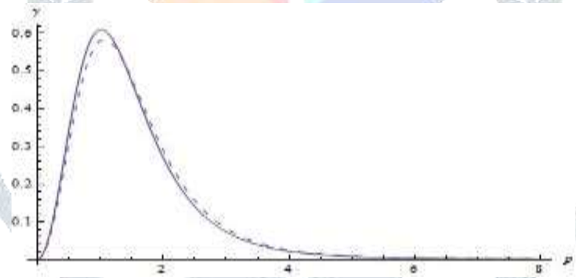

Figure D: $\gamma(p)\ Vs. p$ graph

The dashed and solid lines in Figure D represent the uncorrelated and correlated single- particle charge densities in momentum space respectively.

In Fig. C we have studied the variation of coordinate space charge density as a function of r. The values of ρ_c are less than those of ρ_{uc} for $r \le 1$ but for $r \ge 1$ we observe the opposite. To visualize the role of correlation in modifying the uncorrelated momentum space charge density, we have plotted in Fig.D [γ_{uc}, γ_c] as a function of p. The uncorrelated charge density [γ_{uc}] for small p values (i.e. $p < 1.40$) is less than that of the correlated charge density [γ_c] . However, for large values of p (i.e. $p > 1.40$), the values of the uncorrelated charge density [γ_{uc}] are greater than that of the correlated charge density [γ_c].

3. Shannon's and Fisher's coordinate and momentum space information entropies: In this section we present the results for the Shannon information entropy (S) and Fisher information entropy (I) 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 (2) and (4) respectively. Similarly the uncorrelated Fisher Information entropies in coordinate space [$I_{\rho_{uc}}$] and momentum space [$I_{\gamma_{uc}}$] are computed using the expressions (8) and (9) 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 (2) and (4) respectively.

Similarly we have also done for the correlated Fisher Information entropies in coordinate space $[I_{\rho_c}]$ and momentum space $[I_{\gamma_c}]$ respectively.

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 1 respectively as follows:

Table 1: Shannon information entropies for correlated and uncorrelated 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	2.31621	2.4421	5	4.13402	4.02442	6.45023	6.46656
2	6	2.31625	2.4422	6	4.19282	4.07732	6.50907	6.51952
3	7	2.31625	2.4422	7	4.21952	4.10149	6.53577	6.54369
4	8	2.31625	2.4422	8	4.2327	4.11348	6.54895	6.55568
5	9	2.31625	2.4422	9	4.23967	4.11984	6.55592	6.56204
6	10	2.31625	2.4422	10	4.24359	4.12343	6.55984	6.56563
7	100	2.31625	2.4422	100	4.25034	4.12964	6.56659	6.57184
8	500	2.31625	2.4422	500	4.25034	4.12965	6.56659	6.57185
9	1000	2.31625	2.4422	1000	4.25034	4.12965	6.56659	6.57185
10	2000	2.31625	2.4422	2000	4.25034	4.12965	6.56659	6.57185
11	5000	2.31625	2.4422	5000	4.25034	4.12965	6.56659	6.57185
12	10000	2.31625	2.4422	10000	4.25034	4.12965	6.56659	6.57185
13	20000	2.31625	2.4422	20000	4.25034	4.12965	6.56659	6.57185
14	30000	2.31625	2.4422	30000	4.25034	4.12965	6.56659	6.57185
15	50000	2.31625	2.4422	50000	4.25034	4.12965	6.56659	6.57185
16	100000	2.31625	2.4422	100000	4.25034	4.12965	6.56659	6.57185
17	1000000	2.31625	2.4422	1000000	4.25034	4.12965	6.56659	6.57185
18	5000000	2.31625	2.4422	5000000	4.25034	4.12965	6.56659	6.57185
19	400000000	2.31625	2.4422	400000000	4.25034	4.12964	6.56659	6.57184
20	Infinity	2.31625	2.4422	Infinity	4.25034	4.12965	6.56659	6.57185

From Table: 1, it is observed that correlation augments the Shannon entropies in coordinate space and diminishes it in momentum space. 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 2 respectively as follows:

Table 2: Fisher information entropies for correlated and uncorrelated 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	12.5876	5	3.53904	3.862	47.900906	48.613311
2	6	13.535	12.5876	6	3.54388	3.862	47.966415	48.613311
3	7	13.535	12.5876	7	3.5454	3.86753	47.986989	48.682920
4	8	13.535	12.5876	8	3.54595	3.86799	47.994433	48.688710
5	9	13.535	12.5876	9	3.54616	3.86817	47.997275	48.690976
6	10	13.535	12.5876	10	3.54626	3.86824	47.998629	48.691857
7	100	13.535	12.5876	100	3.54635	3.82173	47.999847	48.106408
8	500	13.535	12.5876	500	3.54635	3.8682	47.999847	48.691354
9	1000	13.535	12.5876	1000	3.54635	3.8682	47.999847	48.691354
10	2000	13.535	12.5876	2000	3.54635	3.86819	47.999847	48.691228
11	5000	13.535	12.5876	5000	3.54635	3.86817	47.999847	48.690976
12	10000	13.535	12.5876	10000	3.54635	3.86813	47.999847	48.690473
13	20000	13.535	12.5876	20000	3.54635	3.86806	47.999847	48.689592
14	30000	13.535	12.5876	30000	3.54635	3.86798	47.999847	48.688585
15	50000	13.535	12.5876	50000	3.54635	3.86783	47.999847	48.686696
16	100000	13.535	12.5876	100000	3.54635	3.86746	47.999847	48.682039

17	1000000	13.535	12.5876	1000000	3.54635	3.86075	47.999847	48.597576
18	5000000	13.535	12.5876	5000000	3.54635	3.83092	47.999847	48.222088
19	400000000	13.535	12.5876	400000000	3.54635	3.8688	47.999847	48.698906
20	Infinity	13.535	12.5876	Infinity	3.54635	3.86921	47.999847	48.704067

From Table: 2 it is observed that correlation diminishes the Fisher entropies in coordinate space and augment it in momentum space. We have also verified from Table: 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 $I_\rho I_\gamma \geq 36$.

4. Concluding remarks: It is widely believed that there are distinct advantages in viewing problems of physics within the framework of analytical models, since it helps in readily expressing and evaluating the physical effects. In atomic and molecular physics it is very difficult to represent realistic systems by analytically solvable model. The difficulties arise due to the presence of interaction terms. 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, 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 1 and Table 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 1 the uncertainty relation $S_\rho + S_\gamma \geq 3(1 + ln\pi)$ 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 2 that $I_{\rho_c} I_{\gamma_c} > I_{\rho_{uc}} I_{\gamma_{uc}}$ and $I_\rho I_\gamma \geq 36$. Since our calculated values of information entropies satisfy their respective uncertainty relationships, it validates our results obtained. 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. This is because information entropy indirectly measures the disorderliness or the information content of the system. Hence we have established the entropic measurement as a tool for studying dynamics of evolution of a two-electron system. It 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.

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