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Entropic system in the relativistic Klein-Gordon Particle

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Abstract

The solutions of Kratzer potential plus Hellmann potential was obtained under the Klein-Gordon equation via the parametric Nikiforov-Uvarov method. The relativistic energy and its corresponding normalized wave functions were fully calculated. The theoretic quantities in terms of the entropic system under the relativistic Klein-Gordon equation (a spinless particle) for a Kratzer-Hellmann's potential model were studied. The effects of a and b respectively (the parameters in the potential that determine the strength of the potential) on each of the entropy were fully examined. The maximum point of stability of a system under the three entropies was determined at the point of intersection between two formulated expressions plotted against a as one of the parameters in the potential. Finally, the popular Shannon entropy uncertainty relation known as Bialynick-Birula, Mycielski inequality was deduced by generating numerical results.

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1. Introduction

The understanding of correlations in quantum systems is based on the analytic tools provided by the entropic measures. These entropic measures are Shannon entropy, Rényi entropy, and Tsallis entropy. The most outstanding of the entropic measures is the Shannon entropy introduced by Shannon [1]. The Shannon entropy has several applications in various scientific disciplines. In the concept of information, for instance, it presents a discrete source without memory as a functional that quantifies the uncertainty of a random variable at each discrete time. It is the expected amount of information in a given event drawn from a distribution that serves as a measure of uncertainty or variability that is associated with random variables. Shannon entropy has examined entropic uncertainty and has been tested for different potential models. It serves as another form of Heisenberg uncertainty relation. In physics, Shannon entropy has been widely reported under the non-relativistic wave equation over the years for different potential models [2-25]. However, all the reports given in refs. [2-25] dwell under the non-relativistic wave equation leaving out the relativistic wave equation. This motivates the present work. In the present study, the authors want to examine the entropic system under the relativistic Klein-Gordon equation using Kratzer-Hellmann potential. The accuracy of Shannon entropy for any calculation can be checked by the uncertainty relation of Shannon entropy that relates position space and momentum space with the spatial dimension. This is otherwise called Bialynick-Birula, Mycielski (BBM) inequality given as

$$S(\rho) + S(\gamma) = D(1 + \ln \pi), \tag{1}$$

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where

$$S(\rho) = -\frac{-4\pi}{\delta}\int_0^{\text{inf}} \rho(r)\log\rho(r)\,dr,$$
$$S(\gamma) = -\frac{-4\pi}{\delta}\int_0^{\text{inf}} \gamma(p)\log\gamma(p)\,dp, \tag{2}$$

$\rho(r)$ and $\gamma(p)$ are probability densities. D refers to the spatial dimension, and $\ln\pi$ is a constant term. In this work, numerical results will be generated for equation (1) to verify whether the results from the relativistic Klein-Gordon equation will satisfy the BBM inequality. The Kratzer-Hellmann potential comprises of Kratzer potential and Hellmann potential. The physical form of Kratzer-Hellmann potential is

$$V(r) = D_e\left(\frac{r-r_e}{r}\right)^2 - \left(\frac{a-be^{-\delta r}}{r}\right), \tag{3}$$

where D_e is the dissociation energy, r_e is the equilibrium bond length, a and b are the strengths of the Hellmann potential, r is internuclear separation while δ (screening parameter) characterized the range of the Hellmann potential. The two sub-sets of the potential (3) have received attention in the bound states and other areas of sciences. The Hellmann potential is known to be suitable for the study of inner-shell ionization problems. The potential was equally studied for alkali hydride molecules by Varshni and Shukla [26]. Recently, the Hellmann potential was used in ref. [27] as a tensor interaction for the breaking of energy degenerate doublets in the Dirac equation. The Kratzer potential, on the other hand, forms a potential pocket that is useful for vibrational and rotational energy eigenvalues [28]. The combination of these potentials is considered necessary because of their applications.

2. Parametric Nikiforov-Uvarov method (PNUM)

This PNUM is a straight forward method that uses transformation of variable. The PNUM is short and accurate for solving bound state problems. According to Tezcan and Sever [29], the reference or standard equation for the PNUM is

$$\left(\frac{d^2}{ds^2} + \frac{c_1-c_2}{s(1-c_3s)}\frac{d}{ds} + \frac{-\xi_1s^2+\xi_2s-\xi_3}{s^2(1-c_3s)^2}\right)\psi(s) = 0. \tag{4}$$

According to ref. [29], the eigenvalues and eigenfunction respectively can be obtained using [29, 30]

$$nc_2 - (2n+1)\,c_5 + c_7 + 2c_3c_8 + n\,(n-1)\,c_3$$
$$+ (2n+1)\,\sqrt{c_9} + \left(2\sqrt{c_9} + c_3\,(2n+1)\right)\sqrt{c_8} = 0, \tag{5}$$

$$\psi_{n,\ell}(s) = N_{n,\ell}s^{c_{12}}\,(1-c_3s)^{-c_{12}-\frac{c_{13}}{c_3}} \times P_n^{\left(c_{10}-1,\,\frac{c_{11}}{c_3}-c_{10}-1\right)}(1-2c_3s), \tag{6}$$

The parameters in equations (5) and (6) are deduced as follows

$$c_4 = \frac{1-c_1}{2}, c_5 = \frac{c_2-2c_3}{2}, c_6 = c_5^2+\xi_1, c_7 = 2c_4c_5-\xi_2,,$$
$$c_9 = c_3\,(c_7+c_3c_8)+c_6, c_{10} = c_1+2c_4+2\sqrt{c_8}, c_8 = c_4^2+\xi_3$$
$$c_{11} = c_2-2c_5+2\left(\sqrt{c_9}+c_3\sqrt{c_8}\right), c_{12} = c_4+\sqrt{c_8},$$
$$c_{13} = c_5-\left(\sqrt{c_9}+c_3\sqrt{c_8}\right) \tag{7}$$

2.1. The Klein-Gordon equation (KGE) with Kratzer-Hellmann potential

The KGE is use to describe spinless particles in the domain of relativistic wave equation [31, 32, 33, 34, 35, 36, 37, 38]. The Klein-Gordon equation for space-time scalar potential $S(r)$ and the time component of the Lorentz four-vector potential $V(r)$ arising from minimal coupling, in the relativistic unit ($\hbar = c = 1$), reads

$$\left[\hat{p}^2 + (M+S(r))^2 - (E-V(r))^2\right]R(r) = 0, \tag{8}$$

where $\hat{p}$ is the momentum operator, M is the particle's mass, E is the relativistic energy and $R(r)$ is the wave function. The KGE above has a potential $2V$ in which the nonrelativistic limit cannot give the solutions of the Schrödinger equation. A critical investigation was done by Alhaidari et al. [39] who proved that $S = \pm V$. This is the nonrelativistic limit for the potential $2V$. Thus, in the relativistic limit, the interacting potential becomes V instead of $2V$. Therefore, to obtain a solution of the Klein- Gordon equation for any arbitrary $\ell-$state whose energy equation in the nonrelativistic limit equals the solution of the Schrödinger equation, equation (8) becomes [39, 40, 41, 42, 43, 44, 45]

$$\left[\hat{p}^2 - M^2 + E^2 - V(r)(M+E) - \frac{\ell(\ell+1)}{r^2}\right]R(r) = 0, \tag{9}$$

The solutions of the Klein-Gordon equation above and some diatomic molecular potential models have been obtained for different molecules [46, 47, 48, 49, 50], and the results compared with experimental values. To get rid of the inverse squared term in equation (9), we need to adopt a suitable approximation scheme. In this work, we adopt the following approximation that is valid for $\delta \ll 1$,

$$\frac{1}{r^2} \approx \frac{\delta^2}{(1-e^{-\delta r})^2}. \tag{10}$$

Plugging equations (3) and (10) into equation (9) and making a simple transformation of the form $y = e^{-\delta r}$, equation (9) turns to be

$$\left[\frac{d^2}{dy^2} + \frac{1-y}{y-y^2}\frac{d}{dy} + \frac{Ay^2+By+C}{y^2(1-y)^2}\right]R_{n,\ell}(y) = 0, \tag{11}$$

$$A = \frac{\Upsilon + b\delta\beta}{\delta^2} \tag{12}$$

$$B = \frac{2\Upsilon - (b+a+2D_er_e)\delta\beta}{\delta^2}, \tag{13}$$

$$C = \frac{E^2 - M^2 + \beta\vartheta - \ell(\ell+1)\delta^2}{\delta^2}, \tag{14}$$

$$\beta = M+E, \tag{15}$$

$$\vartheta = 2D_er_e\delta - D_e + a\delta - D_er_e^2\delta^2, \tag{16}$$

$$\Upsilon = M^2 - E^2 + D_e\beta. \tag{17}$$

Comparing equation (11) with equation (4), equation 7 numerically becomes

$$c_1 = c_2 = c_3 = 1, c_4 = 0, c_5 = -\frac{1}{2}, c_6 = \frac{1}{4} - A, c_7 = -B,$$
$$c_8 = -C, c_9 = \frac{1}{4} - A - B - C, c_{10} = 1 + 2\sqrt{-C},$$
$$c_{11} = 2\left(1 + \sqrt{-C}\right) + \sqrt{1 - 4(A+B+C)}, c_{12} = \sqrt{-C},$$
$$c_{13} = -\frac{1}{2} - \frac{1}{2}\sqrt{1 - 4(A+B+C)} - \sqrt{-C} \quad (18)$$

Substituting c_1 to c_9 in equation (18) into equation (5), we have energy equation for the Kratzer-Hellmann potential as

$$\frac{\Upsilon - \beta(\vartheta + D_e) + \ell(\ell+1)\delta^2}{\delta^2} = \left[\frac{(\vartheta - D_e - b\delta)\beta - n(n+1) - \frac{1}{2} - 2\ell(\ell+1) - \left(n + \frac{1}{2}\right)\sqrt{1 - 4(A+B+C)}}{1 + 2n + \sqrt{1 - 4(A+B+C)}}\right]^2. \quad (19)$$

The energy equation obtained for Kratzer-Hellmann potential in equation (19) above has subset energy equations for Kratzer potential, Yukawa potential, and Coulomb potential. However, the wave function for the Kratzer-Hellmann potential is obtained by substituting $c_{10}$to c_{13}in Eq. 18 into Eq. 6 to have

$$R(s) = N s^{\eta}(1-s)^{\frac{1}{2}+\frac{\lambda}{2}} P_n^{(}2\eta, \lambda)(1-2s), \quad (20)$$

where

$$\eta = \sqrt{\frac{\Upsilon - 2D_e r_e \delta\beta - a\delta\beta}{\delta^2} + \beta D_e r_e^2 + \ell(\ell+1)}, \quad (21)$$

$$\lambda = \sqrt{(1 + 2\ell) + 4\beta D_e r_e^2}. \quad (22)$$

and N is a normalization factor which can easily be calculated using normalization condition. Using

$$\int_0^{\infty} |R(r)|^2 \, dr = 1, \quad (23)$$

the normalization factor can easily be obtained. Consider the transformation $y = e^{-\delta r}$ and another transformation of the form $x = 2y - 1$, with a relation of the form $1 - x = 1 - \left(\frac{1-x}{2}\right)$, when invoked on equation (23), using an appropriate integral, we have the normalization factor as

$$N_{n,\ell}^2 = -\frac{n! 2\delta\eta\Gamma(2\eta + \lambda + n + 1)}{\Gamma(2\eta+1)\Gamma(\lambda + n + 2)}. \quad (24)$$

2.2. *Kratzer-Hellmann potential and entropies*

The three entropies mentioned in the introduction will be calculated here using equation (20).

2.2.1. *Shannon entropy*

To obtain Shannon entropy, we plug equation (20) into equation (2). For $S(\rho)$, we define a transformation of the form $s = 1 - y$, and using the appropriate integral given in the appendix, we have

$$S(\rho) = \frac{8\pi\eta(n!)\Gamma(2\eta+1)\Gamma(\lambda+n+3)\Gamma(2\eta+\lambda+n+1)}{\Gamma(2\eta+n)\Gamma(\lambda+n+2)\Gamma(2\eta+\lambda+n+3)} \times \log\left[(0.99)^{2\eta}(0.01)^{1+\lambda}\frac{\Gamma(2\eta+n+1)}{\Gamma(2\eta+1)}\right]. \quad (25)$$

To obtain $S(\gamma)$, we define $x = -1 + 2y$ and then, using integral and formula in the appendix, we have

$$S(\gamma) = -\frac{4\pi\Gamma(2\eta+n+1)\Gamma(2\eta+\lambda+n+1)}{\Gamma(2\eta+n)\Gamma(2\eta+\lambda+n+2)} \times \log\left[(0.99)^{2\eta}(0.01)^{1+\lambda} \times \frac{[\Gamma(2\eta+n+1)]^2}{n!\,[\Gamma(2\eta+1)]^2}\right]. \quad (26)$$

2.2.2. *Rényi entropy*

Rényi entropy is a generalization of Shannon entropy and is defined as [51]

$$R_q(\rho) = \frac{1}{1-q}\log 4\pi \int_0^{\infty} \rho(r)^q \, dr. \quad (27)$$

The q is called Tsallis index. Following the procedures used to obtain Shannon entropy for position space, we have $R_q(\rho)$ as

$$R_q(\rho) = -\frac{2.5314\delta^{q-1}}{1-q} \times \left[\frac{2\eta(n!)\Gamma(2\eta+1)\Gamma(\lambda+n+3)\Gamma(2\eta+\lambda+n+1)}{\Gamma(2\eta+n)\Gamma(\lambda+n+2)\Gamma(2\eta+\lambda+n+3)}\right]^q. \quad (28)$$

For the momentum space, we follow step by step as in the Shannon entropy for momentum space to have $R_q(\gamma)$ as

$$R_q(\gamma) = -\frac{1.2657\delta^{q-1}}{(1-q)} \left[\frac{2\Gamma(2\eta+n+1)\Gamma(2\eta+\lambda+n+1)}{\Gamma(2\eta+1)\Gamma(2\eta+\lambda+n+2)}\right]^q. \quad (29)$$

2.2.3. *Tsallis entropy*

The Tsallis entropy was introduced by Tsallis [52]. The concept acts as a basis for generalizing the statistical mechanics. This Tsallis entropy is defined as

$$T_q(\rho) = \frac{1}{q-1}\left(1 - 4\pi\int_0^{\infty} \rho(r)^q \, dr\right), \quad q \neq 1. \quad (30)$$

The Tsallis entropy reduces to the usual Boltzmann-Gibbs entropy as the Tsallis index q approaches one. With the wave function in equation (20) and following previous procedures, we have Tsallis entropy for position space as

$$T_q(\rho) = \frac{1}{q-1} + \frac{4\pi\delta^{q-1}}{q-1} \left(\frac{2\eta\Gamma(2\eta+1)\Gamma(\lambda+n+3)\Gamma(2\eta+\lambda+n+1)(n!)}{\Gamma(2\eta+n)\Gamma(\lambda+n+2)\Gamma(2\eta+\lambda+n+3)}\right)^q \quad (31)$$

Following the procedures to obtain momentum space of Shannon entropy, the Tsallis entropy for momentum space is obtained as

$$T_q(\gamma) = \frac{1}{q-1} \times \left[1 + 2\pi\delta^{q-1}\left(\frac{2\Gamma(2\eta+n+1)\Gamma(2\eta+\lambda+n+1)}{\Gamma(2\eta+1)\Gamma(2\eta+\lambda+n+2)}\right)^q\right]. \quad (32)$$

3. Results and Discussion

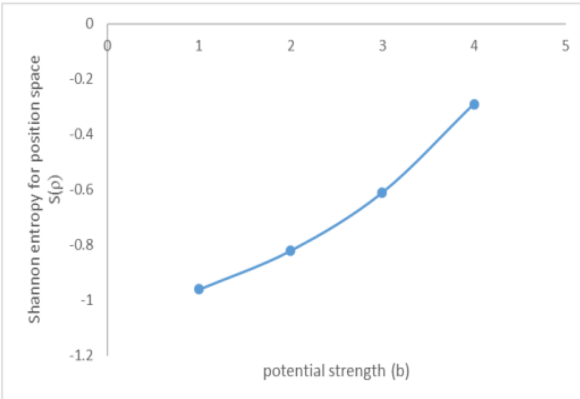

Figure 1. $S(\rho)$ against b

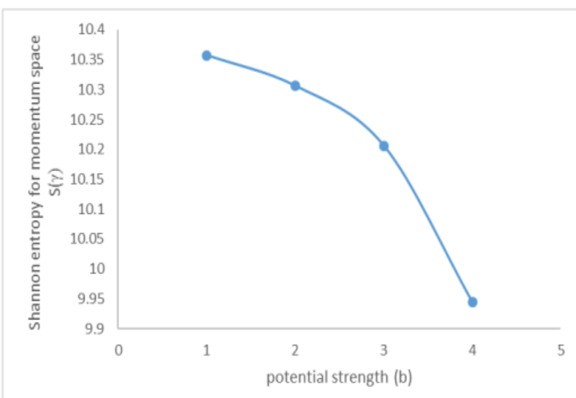

Figure 2. $S(\gamma)$ against b

In Figure 1, we plotted $S(\rho)$ against one of the potential strength at the first excited state with $\ell = 1$, $r_e = 0.1$, $a = 1$, $\delta = 0.25$, $D_e = 2.5$ and $M = 2D_e$. There is less concentration of electron density and so, less concentration of the wave function which makes the system unstable as the potential strength increases. In Figure 2, $S(\gamma)$ is plotted against the potential strength (b) at the first excited state with $\ell = 1$, $r_e = 0.1$, $a = 1$, $\delta = 0.25$, $D_e = 2.5$ and $M = 2D_e$. There is a more concentration of the spreading of electron density which leads to more concentration of the wave function as the potential strength goes up. Thus, there is stability of the system as b goes up. In Figures 3 and 4, we examined the variation of the product of Rényi and Tsallis entropies respectively against the potential strength (a) at the first excited state with $\ell = 1$, $r_e = 0.1$, $b = 2$, $\delta = 0.25$, $D_e = 2.5$ and $M = 2D_e$ and In both cases, there is an inverse variation between the product of the entropy and the potential strength. The point of intersection for the entropies (Shannon, Rényi and Tsallis) is determined by plotting $S = R_T/S_T$; $T = (R_T/T_T) - 0.0a$ against a potential

Table 1. Shannon entropy relation with $n = \ell = 1$, $r_e = 0.1$, $b = 2$, $\delta = 0.25$, $D_e = 2.5$ and $M = 2D_e$.

a	$S(\rho)$	$S(\gamma)$	$S_T = S(\rho) + S(\gamma)$
1	-1.561445865	10.47908433	8.917638464
2	-0.884937778	10.33123825	9.446300475
3	-0.568858951	10.18281361	9.613954654
4	-0.396386446	10.05310205	9.656715603
5	-0.254891378	9.898107966	9.643216588

Table 2. Renyi entropy relation with $n = \ell = 1$, $r_e = 0.1$, $q = b = 2$, $\delta = 0.25$, $D_e = 2.5$ and $M = 2D_e$.

a	$R(\rho)$	$R(\gamma)$	$R_T = R(\rho) + R(\gamma)$
1	0.4291810608	2.803088803	3.232269864
2	0.3386588921	2.886297376	3.224956268
3	0.2792173453	2.936768150	3.215985495
4	0.2373724018	2.970645793	3.208018195
5	0.1937069142	3.004709576	3.198416490

Table 3. Tsallis entropy relation with $n = \ell = 1$, $r_e = 0.1$, $q = b = 2$, $\delta = 0.25$, $D_e = 2.5$ and $M = 2D_e$.

a	$T_2(\rho)$	$T_2(\gamma)$	$T_T = T_2(\rho) + T_2(\gamma)$
1	0.077255921	8.181988939	8.259244860
2	0.048103385	8.674956863	8.723060249
3	0.032699075	8.980995892	9.013694967
4	0.023632579	9.189394955	9.213027534
5	0.015737688	9.401349043	9.417086731

Table 4. Shannon entropy $S(\rho)$ for Kratzer, Coulomb and Yukawa potentials at different excited states.

n	Kratzer	Coulomb	Yukawa
0	-0.614945865	-0.36740543	-0.373228924
1	-0.489475768	-0.32198215	-0.330603267
2	-0.323785845	-0.19261467	-0.206643987
3	-0.191326241	-0.11715545	-0.130089665

Table 5. Shannon entropy $S(\gamma)$ for Kratzer, Coulomb and Yukawa potentials at different excited states.

n	Kratzer	Coulomb	Yukawa
0	5.670453776	4.870762243	4.873986446
1	4.879443281	4.163817555	4.192208735
2	3.991974378	3.519430921	3.530045080
3	3.268931407	2.980665799	3.001043671

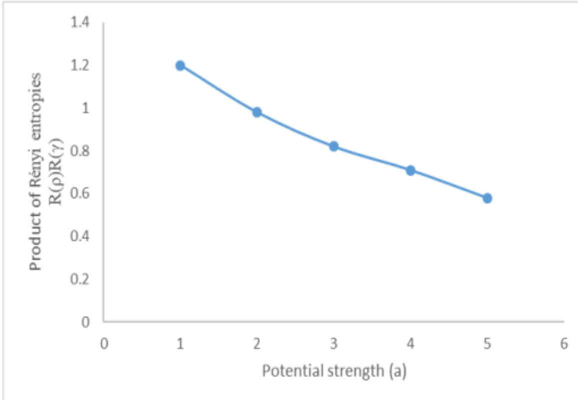

Figure 3. $R(\rho)R(\gamma)$ against a

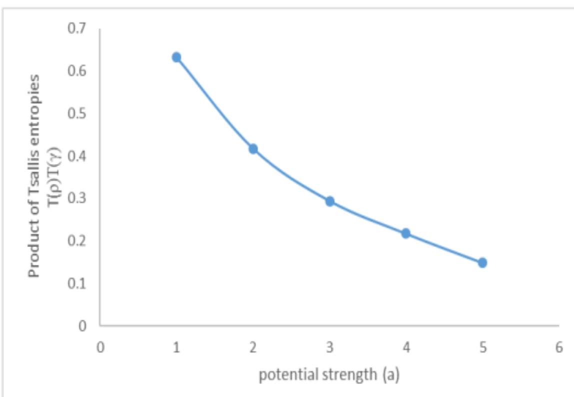

Figure 4. $T(\rho)T(\gamma)$ against a

strength as shown in Figure 5.

Table 1 presented the numerical results for Shannon entropy. The results were numerically verified and confirmed the Bialynick-Birula, Mycielski (BBM) inequality that gives a standard relation $S(\rho) + S(\gamma) \geq D(1 + \log \pi)$. For $D = 1$, $D(1 + \log \pi) = 1.497206180$. However, the lower bound from Table 1 is 8.917638464. This verifies the accuracy of the present work. In Tables 2 and 3, we numerically presented the Rényi entropy and Tsallis entropy respectively for position space and momentum space. In both entropies, the position space and momentum space varies inversely with one another. In Tables 4 and 5, results of $S(\rho)$ against $S(\gamma)$ for the subset potentials were given. The results of these subset potentials are similar to the results of the mother potential. The result for Kratzer potential was obtained by putting $a = b = 0$. The result for Coulomb potential was obtained by putting $b = D_e = 0$. The result for Yukawa potential was obtained by putting $a = D_e = 0$. The results in Tables 1, 2, 3, 4 and 5 showed that a diffused density distribution $\gamma(p)$ in momentum space is associated with a localized density distribution $\rho(r)$ in the position space or configuration space. The physical meaning is that a decrease in the position space corresponds to an increase in the momentum space and

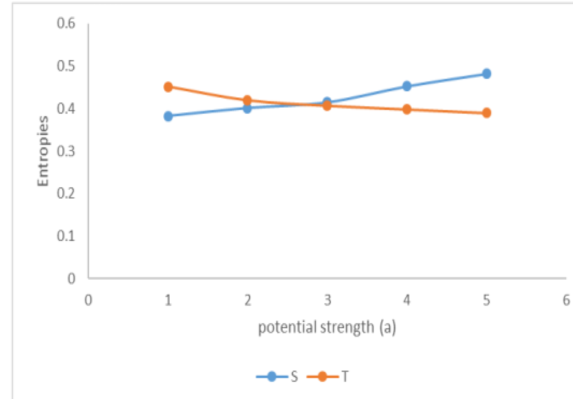

Figure 5. Entropies ($S = R_T/S_T + 0.03a$; $T = R_T/T_T + 0.05$) against the potential strength a

vice visa.

4. Conclusions

We calculated the Shannon information, Rényi information and Tsallis information for position and momentum entropies of a relativistic Klein-Gordon equation. In the first excited state i.e. the Shannon uncertainty yields the minimum value of 8.917638464 which maintains the normal condition for the entropic uncertainty relation with respect to BBM inequality. The $S(\rho)$, $S(\gamma)$, $R(\rho)$, $R(\gamma)$, $T(\rho)$ and $T(\gamma)$ plotted against the potential strengths determined the concentration of the electron and wave density. The results obtained for the relativistic Klein-Gordon equation were found to obey BBM inequality. The results for both the Rényi entropy and Tsallis entropy followed the pattern of the results of the Shannon entropy.

Appendix

$$\int_0^1 y^{\alpha}(1-y)^{\beta}{}_2F_1(-n, n+2(\alpha+\beta); 2\alpha+1; y)^2 dz = \frac{n!\Gamma(\alpha+1)^2\Gamma(\beta+n+2)}{\beta\Gamma(\alpha+n+1)\Gamma(\alpha+\beta+n+2)}$$

$$\int_{-1}^{1}\left(\frac{1-x}{2}\right)^{\eta}\left(\frac{1+x}{2}\right)^{\nu}\times\left[P_n^{(\eta,\nu)}(x)\right]^2 dx = \frac{2\Gamma(\eta+n+1)\Gamma(\nu+n+1)}{n!\eta\Gamma(\eta+\nu+2n+1)\Gamma(\eta+\nu+n+1)}$$

$$\int_{-1}^{1}\left(\frac{1-x}{2}\right)^{s}\left(\frac{1+x}{2}\right)^{\nu}\times\left[P_n^{(s,\nu)}(x)\right]^2 dx = \frac{2\Gamma(s+n+1)\Gamma(\nu+n+1)}{n!s\Gamma(s+\nu+2n+1)\Gamma(s+\nu+n+1)}$$

$$P_n^{(a,b)}(1-2x) = \frac{\Gamma)a+n+1}{n!\Gamma(a+1)}\,{}_2F_1(-n, n+a+b+1; a+1; x)$$

$${}_2F_1(a,b;c;y) = \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)}\sum_{n=0}^{\infty}\frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)}\frac{y^n}{n!}$$

$$\int_{-1}^{1}(1-s)^{a-1}(1+s)^b\left[P_n^{(a,b)}(s)\right]^2 ds$$

$$= \frac{\Gamma(a+n+1)\Gamma(b+n+1)}{n!a\Gamma(a+b+n+1)}$$

$${}_2F_1\left(-n, n+v+u+1; v+1; \tfrac{1-x}{2}\right) = \frac{\Gamma(n+v+1)}{\Gamma(v+1)}$$

$$P_n^{(v,u)}(x) = {}_2F_1\left(-n, n+v+u+1; v+1; \frac{1-x}{2}\right).$$

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