SHANNON INFORMATION ENTROPY WITH IMPROVED KRATZER POTENTIAL UNDER THE EFFECTS OF MAGNETIC AND AHARONOV-BOHM FLUX FIELDS

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ABSTRACT

In this research article, the influence of magnetic and Aharonov-Bohm flux fields on Shannon entropy with improved Kratzer potential for Scandium fluoride (ScF) and hydrogen (H_2) molecules are studied analytically and numerically for three low-lying states. The wave function and probability density which controls the chemical and physical properties of atomic and molecular systems have been obtained by solving the Schrodinger wave equation coupled with charged particle Hamiltonian via the Nikiforov-Uvarov functional analysis method. The total normalized wave function was expressed in terms of the hypergeometric function of Jacobi polynomials and then utilized to evaluate the Shannon entropy for two diatomic molecules in position and momentum spaces. The wave function and electronic densities were graphically analyzed. Our numerical results of Shannon entropies sum as applied to ScF and H_2 were verified to obey the Shannon-entropy-based uncertainty relation. Observations from our results also reveal negative values of Shannon entropies in the position coordinates depicting high localization of particles and stability. In Addition, the effects of the external fields on the quantum systems were observed to influence the quantum information-theoretic measure by small decrements in the Shannon entropy values when compared to the case of the absence of the external fields, indicating a further improvement in the localization of particles and system's stability. This work has applications in atomic and molecular dynamic, molecular drug design, nanostructure processes, information technology, amongst others.

KEYWORDS: Shannon entropy; Schrödinger equation; improved Kratzer potential, Aharonov-Bohm.

INTRODUCTION

Shannon information entropy is a global quantum information-theoretic measure which describes the uncertainty and localization of the electronic charge density in both position and momentum coordinates. Nanostructure processes are better understood with the psyche of the electron densities (Shannon, 1948; Sears, 1980; Nalewajski, 2005; Okon, *et al.,* 2018; Olendski, 2021). Since its inception, this information theoretic tool has been beneficial in several fields including atomic ionization properties, molecular drug design, quantum communication, computation and information technology, electronic devices among others (Nalewajski, 2006; Nielson and Chuang, 2001; Gadre and Pathak, 1991; Gassi, 2011). The uncertainty relation of this information entropy is known to be more precise than the Heisenberg uncertainty relation because it does not refer to a particular location in the Hilbert space (Edet and Ikot 2021; Bialynicki-Birula and Mycieski, 1975). Beckner *et al* were the first to develop the Shannon entropy uncertainty in 1975 as (Shannon, 1948; Beckner, 1975; Bialynicki-Birula and Mycieski, 1975; Yahya, *et al.,* 2014; Najafizade, *et al.,* 2016; Isonguyo, *et al.,* 2018, Okon, *et al.,* 2020; Ikot, *et al.,* 2020)

$$Sh_T = Sh_r + Sh_p \geq d(1 + In\pi), \tag{1}$$

where Sh_T is the Shannon entropy sum, Sh_r represent the position coordinate Shannon entropy written as

$$Sh_r = -\int_b^a |\psi(r)|^2 In |\psi(r)|^2 dr, \tag{2}$$

and the momentum coordinate Shannon entropy is expressed as

$$Sh_p = -\int_b^a |\psi(p)|^2 In |\psi(p)|^2 dp.$$

The position space wave function is $\psi(r)$, while the momentum space wave function is represented as $\psi(p)$ and d is the spatial dimension. Lower values of this entropy depict high localization and uncertainty of particles and the more stability of the system studied (Dehesa, *et al.,* 2006; Isonguyo, *et al.,* 2018; Okon, *et al.,* 2020, Olendski, 2021).

Aharonov-Bohm (AB) flux fields as well as magnetic fields are external fields in which any quantum systems subjected to these external fields experience behavioral changes in certain properties caused and controlled by these fields. The existence of Aharonov-Bohm flux is felt when the moving charge particle of a system is affected by an external electromagnetic field when placed in the region where electric and magnetic fields are negligible (Aharonov and Bohm 1959; Hiley 2013).

Recently, a lot of research have been carried out in literature on the influence of magnetic and Aharonov-Bohm flux fields on information theoretic measures with quantum mechanical systems (Olendski, 2019; Olenski, 2021; Edet and Ikot 2021; Edet, *et al.,* 2022*, Okon, et al.,* 2023; Omugbe, *et al.,* 2023). Few articles have extended this study to diatomic molecules, hence our motivation to undergo this research work.

The aim of this study was to obtain the bound state solution of Schrodinger wave equation with improved Kratzer potential in the presence of magnetic and Aharonov-Bohm fields, there after utilize the wave function to obtain the Shannon entropy for the physical model and then apply to Scandium fluoride and hydrogen molecules. Rampho and his co-authors proposed the improved Kratzer potential as (Rampho, *et al.*, 2021).

$$V(r) = -4D_e \left(\frac{a}{r} - \frac{b}{r^2}\right) \times \left(e^{-\frac{(\alpha+\delta)r}{2}} Cosh\left(\frac{\alpha+\delta}{2}\right)r + \bar{c}\right). \tag{3}$$

Where α and δ denotes the screening parameters, $a = r_e$, while $b = r_e^2$ and $\bar{c}$ is the control parameter with the range $\bar{c}$ {0,1}.

This article is organized as follows: In the next Section, the bound state solution of improved Kratzer potential is presented. Section three displays the analytical solution of Shannon entropy under the influence of magnetic and Aharonov-Bohm flux fields. The numerical results of the Shannon entropy under the influence of the external fields as applied to two diatomic molecules are also given in section four. Finally, the discussion and conclusion follow.

IMPROVED KRATZER POTENTIAL AND ITS ANALYTICAL SOLUTION

The Schrodinger wave equation under the influence of magnetic and Aharonov-Bohm flux fields is expressed as (Greiner, 2000; Okon, *et al.*, 2022)

$$\left\{\frac{1}{2\mu}\left(i\hbar\nabla - \frac{e}{c}\vec{A}\right) + V(r)\right\}\psi_{nm}(r,\phi) = E_{nm}\,\psi_{nm}(r,\phi) \tag{4}$$

where E_{nm} is the energy eigenvalue, $\psi_{nm}(r,\phi)$ is the wave function, μ represents the reduced mass, *n* denotes the principal quantum number, m represents the magnetic quantum number, *r* is the inter-nuclear separation, $\vec{A}$ is the vector potential, e is the electronic charge and c is the speed of light. On substituting equation (3) into equation (4) leads to equation (5) according to Rampho *et al.* (2021).

$$\left\{\frac{1}{2\mu}\left(i\hbar\nabla - \frac{e}{c}\vec{A}\right) - 4D_e\left(\frac{a}{r} - \frac{b}{r^2}\right) \times \left(e^{-\frac{(\alpha+\delta)r}{2}} Cosh\left(\frac{\alpha+\delta}{2}\right)r + \bar{c}\right)\right\}\psi_{nm}(r,\phi) = E_{nm}\,\psi_{nm}(r,\phi). \tag{5}$$

By using the Nikiforov-Uvarov functional analysis method to solve equation (5) gives the two-dimensional wave function and energy eigenvalue equation for the improved Kratzer potential respectively as (Rampho, *et al.*, 2021)

$$\psi_{nm}(r,\phi) = N_{nm}\, z^{\sqrt{\lambda_{nm}-\theta_1+\theta_2+\gamma}}\,(1-z)^{\frac{1}{2}+\sqrt{\frac{1}{4}-\epsilon_1+\epsilon_2+\epsilon_3+\theta_4+\theta_2+\gamma}}\;\;{}_2F_1(a,b,c;s)$$
$$= N_{nm}\, z^k\,(1-z)^Q P_n^{(2k,\;2Q-1)}(1-2z)\,,\;\; z = e^{-(\alpha+\delta)r} \tag{6}$$

and

$$E_{nm} = -\frac{\hbar^2(\alpha+\delta)^2\lambda_{nm}}{2\mu}, \tag{7}$$

where

$$\lambda_{nm} = \theta_1 - \theta_2 - \gamma + \frac{1}{4}\left(\frac{\theta_1-\theta_2+\theta_3-\gamma+\epsilon_2-\epsilon^2}{\varepsilon}\right)^2,\; \theta_1 = \frac{2\mu\beta_1}{\hbar^2(\alpha+\delta)},\; \theta_2 = \frac{2\mu\beta_2}{\hbar^2},\; \theta_3 = \frac{2\mu\beta_3}{\hbar^2(\alpha+\delta)},\; \theta_4 = \frac{2\mu\beta_{24}}{\hbar^2},$$

$$\epsilon_1 = \frac{2n\eta\bar{B}}{\hbar(\alpha+\delta)},\;\; \epsilon_2 = \frac{\eta^2\,\bar{B}^2}{\hbar^2(\alpha+\delta)^2},\; \epsilon_3 = \frac{\eta\,\bar{B}\,\Phi_{AB}}{\hbar^2(\alpha+\delta)^2},\; \gamma = (m+\varepsilon)^2 - \frac{1}{4},\; \beta_1 = 2D_e a + 2D_e a\bar{c},\; \beta_2 = 2D_e b + 2D_e b\bar{c},$$

$$\beta_3 = 2D_e a,\; \beta_{41} = 2D_e b,\;\; \eta = \frac{hc}{e},\; \phi_0 = \frac{hc}{e},\; \xi = \frac{\Phi_{AB}}{\phi_0},\; \varepsilon = n + \frac{1}{2} + \sqrt{\frac{1}{4} - \epsilon_1 + \epsilon_2 + \epsilon_3 + \theta_4 + \theta_2 + \gamma}\;\;. \tag{8}$$

The probability density $\rho(r,\phi) = |\psi_{nm}(r,\phi)|^2$ is the squared of the wave function. The wave function can be normalized using (Galindo, *et al.*, 1978)

$$\int_0^\infty \int_0^{2\pi} |\psi_{nm}(r,\phi)|^2\, dr\, d\phi = 1\,. \tag{9}$$

On inserting equation (6) into equation (9) leads to

$$-\frac{2\pi N_{nm}^2}{\alpha}\int_0^\infty z^{2k}\,(1-z)^Q\,|P_n^{(2k,\;2Q-1)}(1-2z)|^2\,\frac{1}{z}\,dz = 1, \tag{10}$$

By replacing $t = 1 - 2z$ and the boundary of integration changed from $z \in (1,0)$ to $t \in (-1,1)$, then equation (10) becomes

$$-\frac{2\pi N_{nm}^2}{\alpha}\int_{-1}^1\left(\frac{1-t}{2}\right)^{2Q-1}\left(\frac{1+t}{2}\right)^k\,|P_n^{(2k,\;2Q-1)}(t)|^2\,dt = 1, \tag{11}$$

Implementing the standard integral (Adamowitz, 1965)

$$\int_{-1}^1\left(\frac{1-x}{2}\right)^\beta\left(\frac{1+x}{2}\right)^\gamma\,|P_n^{(\beta,\;\gamma-1)}(x)|^2\,dx = \frac{2^{\beta+\gamma+1}\,\Gamma(\beta+n+1)\,\Gamma(\gamma+n+1)}{n!\,\Gamma(\beta+\gamma+1)\,\Gamma(\beta+\gamma+2n+1)}, \tag{12}$$

The gamma function $\Gamma(y) = \int_0^\infty h^{y-1}e^{-y}\,dy$. Setting $t = x, \beta = 2Q - 1, \gamma = 2k$, therefore, the normalization constant can be written as

$$N_{nm} = \sqrt{\frac{2\pi\,(\alpha+\delta)\,n!\,\Gamma(2k+2Q+1)\,\Gamma(2k+2Q+2n)}{\Gamma(2k+n+1)\,\Gamma(2Q+n+1)}}. \tag{13}$$

Hence, the two-dimensional total wave function is given as

$$\psi_{nm}(r,\phi_r) = \frac{e^{im\phi_r}}{\sqrt{2\pi r}}\,\psi_{nm}(r,\phi) = \frac{e^{im\phi_r}}{\sqrt{2\pi r}}\,z^k\,(1-z)^Q\,P_n^{(2k,\,2Q-1)}(1-2z). \tag{14}$$

In order to obtain the two-dimensional wave function in momentum space, the Fourier transform of the position wave function is calculated as

$$\psi_{nm}(p,\phi_p) = \frac{1}{\sqrt[3]{2\pi}}\int_0^\infty\int_0^{2\pi}\frac{\psi_{nm}(r,\phi_r)}{\sqrt{r}}\,e^{i[m\phi_r - pr\cos(\phi_r-\phi_p)]}\,r\,dr\,d\phi_r, \tag{15}$$

the angular part can be simplified in terms of the Bessel function as (Olendski, 2021; Omugbe, *et al.*, 2023)

$$\int_0^{2\pi} e^{i[m\phi_r - pr\cos(\phi_r-\phi_p)]}\,r\,dr\,d\phi_r = (-1)^m\,2\pi\,J_{|m|}(pr)e^{im\phi_r}, \tag{16}$$

where

$$J_{|m|}(pr) \approx \sqrt{\frac{2}{\pi pr}}\,\cos\!\left(pr - \frac{|m|\pi}{2} - \frac{\pi}{4}\right), \tag{17}$$

Equation (17) is the asymptotic series of the Bessel function and $J_{|m|}(pr)$ is the Bessel function of order m (Omugbe, *et al.*, 2023).

Figure 1: Position space wave function plot in the ground state for IKP

Figure 2: Position space wave function plot in the first excited state for IKP

Figure 3: Position space wave function plot in the second excited state for IKP
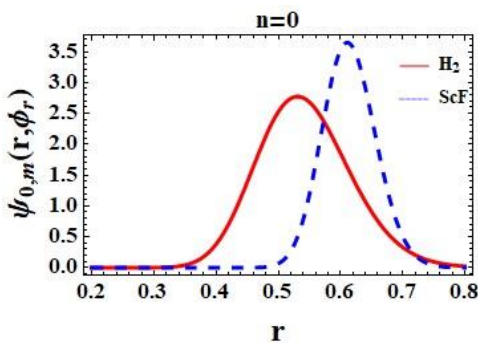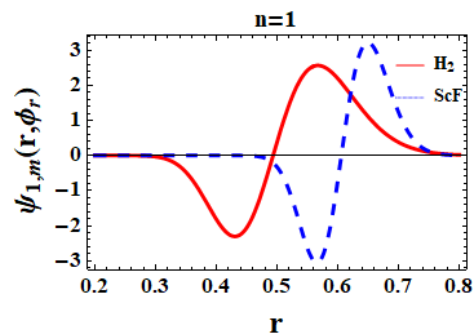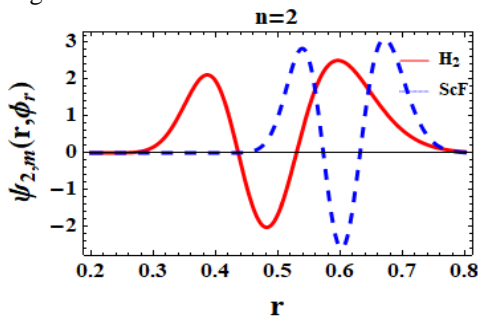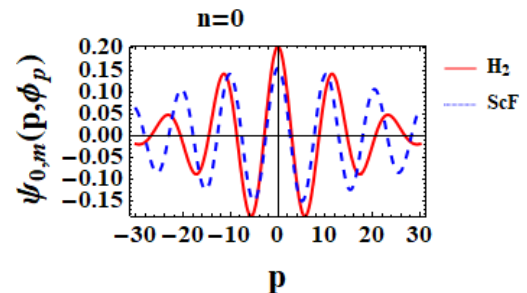

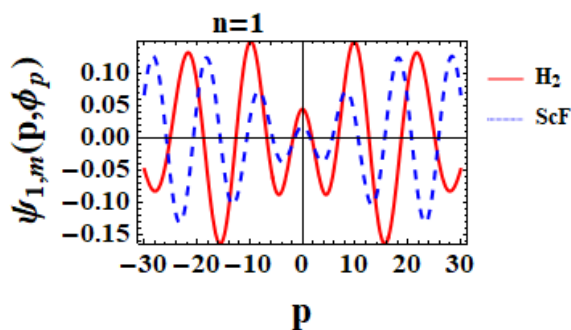Figure 4: Momentum space wave function plot in the ground state for IKP

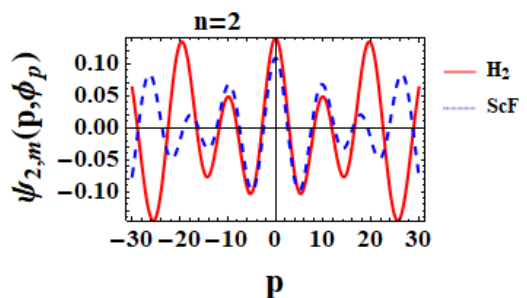Figure 5: Momentum space wave function plot in the first excited state for IKP

Figure 6: Momentum space wave function plot in the second excited state for IKP.

SHANNON ENTROPY WITH IMPROVED KRATZER POTENTIAL UNDER THE EFFECTS OF MAGNETIC AND AHARONOV-BOHM FLUX FIELDS

The Shannon entropy is obtained by utilizing the wave function in equation (15). In position and momentum, the Shannon entropies are analytically solved respectively as

$$Sh_r = \int_0^\infty \int_0^{2\pi} |\psi_{nm}(r,\phi_r)|^2 \ln |\psi_{nm}(r,\phi_r)|^2 \, r \, dr \, d\phi \quad , \tag{18}$$

and

$$Sh_p = \int_0^\infty \int_0^{2\pi} |\psi_{nm}(p,\phi_p)|^2 \ln |\psi_{nm}(p,\phi_p)|^2 \, p \, dp \, d\phi \quad , \tag{19}$$

Further analytical solution of Shannon entropy in two-dimension is complex and difficult, especially in momentum coordinate because of the Fourier transform calculations. Therefore, we have obtained the results numerically with Mathematica 9.0 software and the spectroscopic parameters in Table 1.

NUMERICAL RESULTS

Table 1: Spectroscopic parameter and reduced masses for selected molecules (Okon, *et al.,* 2018)

Molecules	D_e (eV)	r_e (A^0)	$\alpha\left(\frac{1}{A0}\right)$	μ(amu)
H_2	4.7446	0.7416	1.9426	0.50391
ScF	5.85	1.794	1.46102	13.35894

Table 2: Numerical results of Shannon entropy for Improved Kratzer potential for Hydrogen molecule in the absence of Magnetic and Aharonov-Bohm flux fields and singular effects of Aharonov-Bohm flux fields for the ground state ($Sh_{T=}Sh_r + Sh_p \geq d(1 + ln\pi) \geq 4.28946, m = 0, n = 0$).

$\bar{c}$	$Sh_r(\xi=\vec{B}=0)$	$Sh_p(\xi=\vec{B}=0)$	$Sh_T(\xi=2,\vec{B}=0)$	$Sh_r(\xi=2,\vec{B}=0)$	$Sh_p(\xi=2,\vec{B}=0)$	$Sh_T(\xi=2\ \vec{B}=0)$
0	-0.351271	124.030	123.679	-0.350073	125.538	125.188
0.1	-0.347290	134.233	133.886	-0.346164	135.722	135.376
0.2	-0.343702	144.192	143.848	-0.342664	145.320	145.320
0.3	-0.340474	153.918	153.578	-0.339479	155.371	155.031
0.4	-0.337570	163.422	163.085	-0.336632	164.856	164.519
0.5	-0.334955	172.714	172.379	-0.334070	174.130	173.795
0.6	-0.332599	181.803	181.471	-0.331761	183.201	182.869
0.7	-0.330470	190.701	190.370	-0.329677	191.751	191.751
0.8	-0.328546	199.414	199.086	-0.327792	200.450	200.450
0.9	-0.326802	207.954	207.627	-0.326085	208.975	208.975
1.0	-0.325220	216.327	216.002	-0.324536	217.333	217.333

Table 3: Numerical results of Shannon entropy for Improved Kratzer potential for Hydrogen molecule in the combine effects of Magnetic and Aharonov-Bohm flux fields, and singular effect of magnetic field for the ground state ($Sh_{T=}Sh_r + Sh_p \geq d(1 + ln\pi) \geq 4.28946, m = 0, n = 0$)

$\bar{c}$	$Sh_r(\xi = \vec{B} = 2)$	$Sh_P(\xi = \vec{B} = 2)$	$Sh_T(\xi = \vec{B} = 2)$	$Sh_r(\xi = 0, \vec{B} = 2)$	$Sh_P(\xi = 0, \vec{B} = 2)$	$Sh_r(\xi = 0, \vec{B} = 2)$
0	-0.453210	191.085	190.631	-0.534513	76.1806	75.6461
0.1	-0.449855	197.412	196.962	-0.528456	83.3115	82.7830
0.2	-0.446654	203.691	203.245	-0.522161	90.4203	89.8982
0.3	-0.443596	209.923	209.479	-0.515834	97.5012	96.9854
0.4	-0.440674	216.108	215.667	-0.509600	104.549	104.039
0.5	-0.437880	222.245	221.807	-0.503533	111.560	111.056
0.6	-0.435207	228.336	163.455	-0.497676	118.531	118.033
0.7	-0.432649	234.382	233.949	-0.492054	125.459	124.966
0.8	-0.430199	240.381	239.951	-0.486674	132.341	131.855
0.9	-0.427850	246.336	245.908	-0.481540	139.178	138.696
1.0	-0.425598	252.247	251.821	-0.476647	145.966	145.489

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Table 4: Numerical results of Shannon entropy for Improved Kratzer potential for Hydrogen molecule in the absence of Magnetic and Aharonov-Bohm flux fields and singular effects of Aharonov-Bohm flux fields for the first excited state ($Sh_T = Sh_r + Sh_p \geq d(1 + ln\pi) \geq 4.28946, m = 0, n = 1$).

$\bar{c}$	$Sh_r(\xi = \vec{B} = 0)$	$Sh_P(\xi = \vec{B} = 0)$	$Sh_T(\xi = \vec{B} = 0)$	$Sh_r(\xi = 2, \vec{B} = 0)$	$Sh_P(\xi = 2, \vec{B} = 0)$	$Sh_r(\xi = 2, \vec{B} = 0)$
0	-0.317743	374.076	373.759	-0.316831	378.237	377.920
0.1	-0.314779	402.263	401.949	-0.313912	406.371	406.057
0.2	-0.312064	429.769	429.457	-0.311242	433.823	433.512
0.3	-0.309589	456.626	456.317	-0.308809	460.627	460.318
0.4	-0.307335	482.866	482.558	-0.306595	486.815	486.508
0.5	-0.305285	508.519	508.213	-0.304582	512.417	512.112
0.6	-0.303419	533.614	557.311	-0.302750	537.463	537.160
0.7	-0.301720	558.180	557.879	-0.301082	561.981	561.679
0.8	-0.300170	582.243	581.943	-0.299562	585.996	585.697
0.9	-0.298757	605.528	605.528	-0.298175	609.534	609.236
1.0	-0.297465	628.955	628.658	-0.296909	632.618	632.321

Table 5: Numerical results of Shannon entropy for Improved Kratzer potential for Hydrogen molecule in the combine effects of Magnetic and Aharonov-Bohm flux fields, and singular effect of magnetic field for the first excited state ($Sh_T = Sh_r + Sh_p \geq d(1 + ln\pi) \geq 4.28946, m = 0, n = 1$)

$\bar{c}$	$Sh_r(\xi = \vec{B} = 2)$	$Sh_P(\xi = \vec{B} = 2)$	$Sh_T(\xi = \vec{B} = 2)$	$Sh_r(\xi = 0, \vec{B} = 2)$	$Sh_P(\xi = 0, \vec{B} = 2)$	$Sh_r(\xi = 0, \vec{B} = 2)$
0	-0.400769	560.747	560.347	-0.456237	241.137	240.681
0.1	-0.398244	578.303	578.905	-0.452640	261.066	260.614
0.2	-0.395824	595.724	595.329	-0.448730	280.911	280.463
0.3	-0.393503	613.013	612.619	-0.444671	300.659	300.214
0.4	-0.391276	630.169	629.778	-0.440571	320.299	319.858
0.5	-0.389140	647.194	646.805	-0.436500	339.821	339.385
0.6	-0.387088	664.090	663.703	-0.432503	359.220	358.788
0.7	-0.385119	680.858	680.473	-0.428610	378.490	378.062
0.8	-0.383226	597.500	697.500	-0.424839	397.626	397.201
0.9	-0.381407	714.017	713.635	-0.421200	416.625	416.204
1.0	-0.379658	730.410	730.031	-0.417698	435.485	435.067

Table 6: Numerical results of Shannon entropy for Improved Kratzer potential for Hydrogen molecule in the absence of Magnetic and Aharonov-Bohm flux fields and singular effects of Aharonov-Bohm flux fields for the second excited state ($Sh_T = Sh_r + Sh_p \geq d(1 + ln\pi) \geq 4.28946, m = 0, n = 2$).

$\bar{c}$	$Sh_r(\xi = \vec{B} = 0)$	$Sh_p(\xi = \vec{B} = 0)$	$Sh_T(\xi = \vec{B} = 0)$	$Sh_r(\xi = 2, \vec{B} = 0)$	$Sh_P(\xi = 2, \vec{B} = 0)$	$Sh_T(\xi = 2, \vec{B} = 0)$
0	-0.311374	689.133	688.822	-0.310538	696.104	695.793
0.1	-0.308459	736.326	736.018	-0.307664	743.197	742.890
0.2	-0.305787	782.329	782.023	-0.305032	789.103	788.798
0.3	-0.303343	827.206	826.902	-0.302627	833.885	833.582
0.4	-0.301110	871.018	870.717	-0.300430	877.606	877.305
0.5	-0.299070	913.824	913.525	-0.298423	920.322	920.024
0.6	-0.297203	955.678	955.380	-0.296587	962.088	961.792
0.7	-0.295494	996.629	996.333	-0.294907	1002.96	1002.66
0.8	-0.293928	1036.72	1036.43	-0.293366	1042.97	1042.68
0.9	-0.292490	1076.01	1075.72	-0.291952	1082.18	1081.88
1.0	-0.291168	1114.52	1114.23	-0.290654	1120.61	1120.32

Table 7: Numerical results of Shannon entropy for Improved Kratzer potential for Hydrogen molecule in the combine effects of Magnetic and Aharonov-Bohm flux fields, and singular effect of magnetic field for the first excited state ($Sh_{T=}Sh_r + Sh_p \geq d(1 + ln\pi) \geq 4.28946, m = 0, n = 2$)

$\bar{c}$	$Sh_r(\xi=\vec{B}=2)$	$Sh_p(\xi=\vec{B}=2)$	$Sh_T(\xi=\vec{B}=2)$	$Sh_r(\xi=0,\vec{B}=2)$	$Sh_P(\xi=0,\vec{B}=2)$	$Sh_T(\xi=0,\vec{B}=2)$
0	-0.381474	1001.06	1000.68	-0.431402	463.414	462.983
0.1	-0.379208	1030.43	1030.05	-0.427976	497.229	496.801
0.2	-0.377032	1059.55	1059.17	-0.424371	530.842	530.418
0.3	-0.374942	1088.44	1088.07	-0.420693	564.239	563.818
0.4	-0.372934	1117.11	1116.73	-0.417014	597.407	596.990
0.5	-0.371004	1145.54	1145.17	-0.413381	630.338	629.925
0.6	-0.369148	1173.76	1173.39	-0.409827	663.024	662.614
0.7	-0.367363	1201.75	1201.38	-0.406369	695.460	695.054
0.8	-0.365646	1229.52	1229.16	-0.403021	727.239	727.239
0.9	-0.363993	1257.08	1256.72	-0.399789	759.568	759.168
1.0	-0.362402	1284.43	1284.07	-0.396676	791.235	790.839

Table 8: Numerical results of Shannon entropy for Improved Kratzer potential for Scandium fluoride molecule in the absence of Magnetic and Aharonov-Bohm flux fields and singular effects of Aharonov-Bohm flux fields for the ground state ($Sh_{T=}Sh_r + Sh_p \geq d(1 + ln\pi) \geq 4.28946, m = 0, n = 0$).

$\bar{c}$	$Sh_r(\xi=\vec{B}=0)$	$Sh_p(\xi=\vec{B}=0)$	$Sh_T(\xi=\vec{B}=0)$	$Sh_r(\xi=2,\vec{B}=0)$	$Sh_P(\xi=2,\vec{B}=0)$	$Sh_T(\xi=2,\vec{B}=0)$
0	-0.856790	497.446	496.589	-0.856646	497.644	496.787
0.1	-0.834444	544.223	543.388	-0.834315	544.418	543.584
0.2	-0.815220	589.932	589.117	-0.815103	590.126	589.310
0.3	-0.798530	634.608	633.810	-0.798424	634.800	634.001
0.4	-0.783930	678.290	677.506	-0.783828	678.479	677.696
0.5	-0.771054	721.018	720.246	-0.770965	721.205	720.434
0.6	-0.759640	762.831	762.072	-0.759558	763.016	762.257
0.7	-0.749461	803.771	803.022	-0.749385	803.954	803.205
0.8	-0.740338	843.876	843.136	-0.740266	844.057	843.317
0.9	-0.732123	883.184	882.452	-0.732056	883.363	882.631
1.0	-0.724695	921.730	921.006	-0.724632	921.907	921.182

Table 9: Numerical results of Shannon entropy for Improved Kratzer potential for Scandium fluoride molecule in the combine effects of Magnetic and Aharonov-Bohm flux fields, and singular effect of magnetic field for the ground state ($Sh_{T=}Sh_r + Sh_p \geq d(1 + ln\pi) \geq 4.28946, m = 0, n = 0$)

$\bar{c}$	$Sh_r(\xi=\vec{B}=2)$	$Sh_p(\xi=\vec{B}=2)$	$Sh_T(\xi=\vec{B}=2)$	$Sh_r(\xi=0,\vec{B}=2)$	$Sh_P(\xi=0,\vec{B}=2)$	$Sh_T(\xi=0,\vec{B}=2)$
0	-0.866334	511.537	510.670	-0.880964	484.421	483.540
0.1	-0.844702	557.038	556.194	-0.857344	530.483	529.626
0.2	-0.825943	601.566	600.740	-0.836967	575.559	574.722
0.3	-0.809541	645.148	644.339	-0.819231	619.674	618.855
0.4	-0.795096	687.818	687.023	-0.803674	662.858	662.055
0.5	-0.782292	729.608	728.825	-0.789935	705.145	704.355
0.6	-0.770877	770.553	769.782	-0.777725	746.567	745.790
0.7	-0.760648	809.927	809.927	-0.766815	787.161	786.394
0.8	-0.751438	849.295	849.295	-0.757018	826.959	826.202
0.9	-0.743110	887.917	887.917	-0.748180	865.994	865.246
1.0	-0.735551	926.561	925.826	-0.740176	904.300	903.560

Table 10: Numerical results of Shannon entropy for Improved Kratzer potential for Scandium fluoride molecule in the absence of Magnetic and Aharonov-Bohm flux fields and singular effects of Aharonov-Bohm flux fields for the first excited state ($Sh_{T=}Sh_r + Sh_p \geq d(1 + ln\pi) \geq 4.28946, m = 0, n = 1$).

$\bar{c}$	$Sh_r(\xi=\vec{B}=0)$	$Sh_p(\xi=\vec{B}=0)$	$Sh_T(\xi=\vec{B}=0)$	$Sh_r(\xi=2,\vec{B}=0)$	$Sh_P(\xi=2,\vec{B}=0)$	$Sh_T(\xi=2,\vec{B}=0)$
0	-0.751167	1404.33	1403.58	-0.751051	1404.88	1404.13
0.1	-0.733601	1534.79	1534.06	-0.733497	1535.34	1534.61
0.2	-0.718403	1662.31	1661.60	-0.718308	1662.85	1662.14
0.3	-0.705148	1786.99	1786.28	-0.705061	1787.52	1786.82
0.4	-0.693505	1908.92	1908.23	-0.693426	1909.45	1908.76
0.5	-0.683214	2028.22	2027.54	-0.683141	2028.75	2028.06
0.6	-0.674066	2145.00	2144.33	-0.673998	2145.52	2144.84
0.7	-0.665891	2259.37	2258.70	-0.665828	2259.88	2259.21
0.8	-0.658553	2371.43	2370.77	-0.658493	2371.93	2371.27
0.9	-0.651931	2481.28	2480.63	-0.651872	2481.78	2481.13
1.0	-0.645950	2589.03	2588.39	-0.645897	2589.53	2588.88

Table 11: Numerical results of Shannon entropy for Improved Kratzer potential for Scandium fluoride molecule in the combine effects of Magnetic and Aharonov-Bohm flux fields, and singular effect of magnetic field for the first excited state ($Sh_{T=}Sh_r + Sh_p \geq d(1 + ln\pi) \geq 4.28946, m = 0, n = 1$)

$\bar{c}$	$Sh_r(\xi=\vec{B}=2)$	$Sh_p(\xi=\vec{B}=2)$	$Sh_T(\xi=\vec{B}=2)$	$Sh_r(\xi=0,\vec{B}=2)$	$Sh_P(\xi=0,\vec{B}=2)$	$Sh_T(\xi=0,\vec{B}=2)$
0	-0.759836	1443.66	1442.90	-0.771318	1368.04	1367.27
0.1	-0.742797	1570.58	1569.84	-0.752792	1496.50	1495.75
0.2	-0.727940	1694.82	1694.09	-0.736702	1622.65	1621.52
0.3	-0.714894	1816.46	1815.75	-0.722629	1745.36	1744.64
0.4	-0.703362	1935.58	1934.88	-0.710235	1865.90	1865.19
0.5	-0.693111	2052.28	2051.59	-0.699253	1983.96	1983.27
0.6	-0.683950	2166.64	2165.96	-0.689467	2099.65	2098.96
0.7	-0.675723	2278.77	2278.10	-0.680703	2213.04	2212.36
0.8	-0.668305	2388.75	2388.08	-0.672819	2324.24	2323.56
0.9	-0.661588	2496.68	2496.02	-0.665696	2433.33	2432.66
1.0	-0.655486	2602.63	2601.97	-0.659237	2540.40	2539.74

Table 12: Numerical results of Shannon entropy for Improved Kratzer potential for Scandium fluoride molecule in the absence of Magnetic and Aharonov-Bohm flux fields and singular effects of Aharonov-Bohm flux fields for the second excited state ($Sh_{T=}Sh_r + Sh_p \geq d(1 + ln\pi) \geq 4.28946, m = 0, n = 2$).

$\bar{c}$	$Sh_r(\xi=\vec{B}=0)$	$Sh_p(\xi=\vec{B}=0)$	$Sh_T(\xi=\vec{B}=0)$	$Sh_r(\xi=2,\vec{B}=0)$	$Sh_P(\xi=2,\vec{B}=0)$	$Sh_T(\xi=2,\vec{B}=0)$
0	-0.696781	2387.04	2386.35	-0.696679	2387.96	2387.96
0.1	-0.681555	2604.21	2603.53	-0.681463	2605.12	2605.12
0.2	-0.668332	2816.43	2815.76	-0.668284	2817.33	2817.33
0.3	-0.656765	3023.87	3023.21	-0.656688	3024.76	3024.76
0.4	-0.646579	3226.71	3226.06	-0.646508	3227.59	3227.59
0.5	-0.637557	3425.14	3424.50	-0.637491	3426.01	3426.01
0.6	-0.629552	3619.35	3618.72	-0.629461	3620.21	182.484
0.7	-0.622331	3809.53	3808.91	-0.622274	3810.38	178.513
0.8	-0.615868	3995.85	3995.24	-0.615815	3996.69	174.963
0.9	-0.610036	4178.50	4177.89	-0.609986	4179.33	171.846
1.0	-0.604754	4357.63	4357.02	-0.604707	4358.45	169.172

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Table 13: Numerical results of Shannon entropy for Improved Kratzer potential for Scandium fluoride molecule in the combine effects of Magnetic and Aharonov-Bohm flux fields, and singular effect of magnetic field for the second excited state ($Sh_{T=}Sh_r + Sh_p \geq d(1 + ln\pi) \geq 4.28946, m = 0, n = 2$)

$\bar{c}$	$Sh_r(\xi=\vec{B}=2)$	$Sh_p(\xi=\vec{B}=2)$	$Sh_T(\xi=\vec{B}=2)$	$Sh_r(\xi=0,\vec{B}=2)$	$Sh_P(\xi=0,\vec{B}=2)$	$Sh_T(\xi=0,\vec{B}=2)$
0	-0.704821	2452.45	2451.75	-0.714769	2326.55	2325.83
0.1	-0.690041	2663.73	2663.04	-0.698729	2540.42	2539.72
0.2	-0.677109	2870.49	2869.81	-0.684751	2749.72	2749.04
0.3	-0.665719	3072.87	3072.21	-0.672485	2954.57	2953.90
0.4	-0.655627	3271.03	3270.38	-0.661654	3155.12	3154.46
0.5	-0.646638	3465.14	3464.49	-0.652034	3351.51	3350.86
0.6	-0.638590	3655.63	3654.70	-0.643446	3543.92	3543.27
0.7	-0.631353	3841.79	3841.16	-0.635743	3732.49	3731.85
0.8	-0.624818	4024.66	4024.04	-0.628803	3917.39	3916.76
0.9	-0.618896	4204.10	4203.48	-0.622526	4098.78	4098.15
1.0	-0.613511	4380.25	4379.64	-0.616829	4276.79	4276.17

DISCUSSION

In this work, we have investigated the Shannon entropy with improved Kratzer potential (IKP) model under the influence of external fields and applied to scandium fluoride molecule as well as hydrogen molecule for three low-lying quantum states using equations (6), (14), (18), (19) and the spectroscopic parameters in Table 1. The following conversions factors were used for our computations: 1amu = 931.494028 $MeV/_{c^2}$ and $\hbar$c = 1973.29eVA^0.

In Figures 2-6, the variation of the wave function in position and momentum coordinates are demonstrated for the ground, first excited and second excited states for scandium fluoride as well as hydrogen molecules. Characteristics features of the wave function for both molecules indicate that higher quantum states exhibit more oscillations and peaks which is similar to an ideal condition for experimental and theoretical description of wave functions.

The numerical values of Shannon entropy Sh_r , Sh_p and their sum Sh_T for three low-lying quantum states with the potential control parameter $\bar{c}$ have been displayed in Tables 2-13 for hydrogen and scandium fluoride molecules in the absence ($\xi=\vec{B}=0$), combined ($\xi=\vec{B}=2$) and singular ($\xi=0, \vec{B}=2$ or $\xi=2, \vec{B}=0$) influence of magnetic ($\vec{B}$) and Aharonov-Bohm flux fields (ξ). Negative values of the position Shannon entropy were observed for IKP as applied to both molecules. Observations from our results show lower values of position Shannon entropies for singular presence of magnetic field as well as in the combined effects of both magnetic and AB flux fields when compared to the Shannon entropy values in the absence of the two fields. A reverse situation occurs for the singular influence of AB fields for H$_2$ and ScF. In the case of momentum Shannon entropies, greater values were observed for a singular influence of AB field as well as in the combined presence of both magnetic and AB fields, while lower values were discovered for singular effect of magnetic field when compared with values in the absence of both external fields for the two molecules.

In Tables 2-13, Our results obey the Shannon entropy uuncertainty relation $Sh_T = Sh_r + Sh_p \geq d(1+In\pi)$ for the two molecules. In all, the external fields are seen to influence the Shannon entropy as such enhances the localization of particle and stability of the system we considered.

CONCLUSION

We have studied the effects of magnetic and Aharonov-Bohm flux field on Shannon entropy with improved Kratzer potential model in position and momentum spaces for scandium fluoride and hydrogen molecules. The wave function of IKP was obtained by solving the bound state solution of the two-dimensional Schrodinger wave equation using Nikiforov-Uvarov functional analysis method. The probability density was obtained by squaring the wave function and then used to calculate the Shannon information entropy for the ground state, first excited state and second excited states for two diatomic molecules analytically and numerically. Observations from our results reveals negative values for the Shannon entropy in position space which physically indicate high localization of the particles in the system. Also, our numerical values show that the Shannon entropy uncertainty relation is obeyed. Moreover, the Shannon entropy values are influenced by the external fields which in turn boost the localization of particle and stability of the system studied which can find applications in the dynamics of atomic and molecular systems subjected to external fields, nanostructure processes in information technology amongst others.

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APPENDICES
Nikiforov-Uvarov-Functional Analysis Method

The Nikiforov-Uvarov Functional Analysis (NUFA) method is a combination of the concepts of Nikiforov-Uvarov (NU) method and the functional analysis method developed by Ikot and his co- authors (Ikot, *et al.,* 2021; Nikiforov and Uvarov 1988; Okon, *et al.,* 2020). NU is applied to solve a second-order differential equation of the form

$$\frac{d^2\psi(s)}{ds^2} + \frac{\tilde{\tau}(s)}{\sigma(s)}\frac{d\psi(s)}{ds} + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0 \tag{1}$$

where $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials at most second degree and $\tilde{\tau}(s)$ is a first-degree polynomial. (Tezcan and Sever, 2009) latter introduced the parametric form of NU method in the form

$$\frac{d^2\psi(s)}{ds^2} + \frac{\alpha_1 - \alpha_2 s}{s(1-\alpha_3 s)}\frac{d^2\psi(s)}{ds^2} + \frac{1}{s^2(1-\alpha_3 s)^2}\left[-U_1 s^2 + U_2 s - U_3\right]\psi(s) = 0 \tag{2}$$

where α_i and $\xi_i (i = 1, 2, 3)$ are all parameters. It can be observed in equation (2) that the differential equation has two singularities all $s \to 0$ and $s \to \frac{1}{\alpha_3}$ thus we take wave function in the form.

$$\Psi_n(s) = s^\lambda (1-\alpha_3 s)^\nu f(s) \tag{3}$$

Substituting equation (3) into equation (2) leads to the following equation,

$$s(1-\alpha_3 s)\frac{d^2 f(s)}{ds^2} + \left[\alpha_1 + 2\lambda - (2\lambda\alpha_3 + 2\nu\alpha_3 + \alpha_2)s\right]\frac{df(s)}{ds}$$

$$-\alpha_3\left(\lambda + \nu + \frac{1}{2}\left(\frac{\alpha_2}{\alpha_3} - 1\right) + \sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{U_1}{\alpha_3^2}}\right)\left(\lambda + \nu + \frac{1}{2}\left(\frac{\alpha_2}{\alpha_3} - 1\right) - \sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{U_1}{\alpha_3^2}}\right)f(s)$$

$$+\left[\frac{\lambda(\lambda-1) + \alpha_1\lambda - U_3}{s} + \frac{\nu(\nu-1)\alpha_3 + \alpha_2\nu - \alpha_1\alpha_3\nu - \frac{U_1}{\alpha_3} + U_2 - U_3\alpha_3}{(1-\alpha_3 s)}\right]f(s) = 0 \tag{4}$$

Equation (4) can be reduced to a Gauss hypergeometric equation if and only if the following functions vanished

$$\lambda(\lambda-1) + \alpha_1\lambda - U_3 = 0 \tag{5}$$

$$\upsilon(\upsilon-1)\alpha_3 + \alpha_2\upsilon - \alpha_1\alpha_3\upsilon - \frac{U_1}{\alpha_3} + U_2 - U_3\alpha_3 = 0. \tag{6}$$

Thus equation (4) now becomes

$$s(1-\alpha_3 s)\frac{d^2 f(s)}{ds^2}\left[\alpha_1 + 2\lambda - (2\lambda\alpha_3 + 2\nu\alpha_3 + \alpha_2)s\right]\frac{df(s)}{ds}$$

$$-\alpha_3\left(\lambda + \nu + \frac{1}{2}\left(\frac{\alpha_2}{\alpha_3} - 1\right) + \sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{U_1}{\alpha_3^2}}\right)\left(\lambda + \nu + \frac{1}{2}\left(\frac{\alpha_2}{\alpha_3} - 1\right) - \sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{U_1}{\alpha_3^2}}\right)f(s) = 0 \tag{7}$$

Solving equations (5) and (6) completely give,

$$\lambda = \frac{1}{2}\left((1-\alpha_1) \pm \sqrt{(1-\alpha_1)^2 + 4U_3}\right) \tag{8}$$

$$\upsilon = \frac{1}{2\alpha_3}\left((\alpha_3 + \alpha_1\alpha_3) \pm \sqrt{(\alpha_3 + \alpha_1\alpha_3)^2 + 4\left(\frac{U_1}{\alpha_3} + \alpha_3 U_3 - U_2\right)}\right) \tag{9}$$

Equation (7) is the hypergeometric equation type of the form

$$x(1-x)\frac{d^2 f(s)}{ds^2} + \left[c - (a+b+1)x\right]\frac{df(x)}{dx} - \left[ab\right]f(x) = 0 \tag{10}$$

where a, b and c are given as follows:

$$a = \sqrt{\alpha_3}\left(\lambda + v + \frac{1}{2}\left(\frac{\alpha_2}{\alpha_3} - 1\right) + \sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{U_1}{U_3^2}}\right) \tag{11}$$

$$b = \sqrt{\alpha_3}\left(\lambda + v + \frac{1}{2}\left(\frac{\alpha_2}{\alpha_3} - 1\right) - \sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{U_1}{\alpha_3^2}}\right) \tag{12}$$

$$c = \alpha_1 + 2\lambda \tag{13}$$

Setting either a or b equal to a negative integer –n, the hypergeometric function f(s) turns to a polynomial of degree n. Hence, the hypergeometric function f(s) approaches finite in the following quantum condition, i.e., $a = -n$ where $n = 0, 1, 2, 3 .... n_{max}$ or $b = -n$.

On using the quantum condition,

$$\sqrt{\alpha_3}\left(\lambda + \upsilon + \frac{1}{2}\left(\frac{\alpha_2}{\alpha_3} - 1\right) + \sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{U_1}{\alpha_3^2}}\right) = -n \tag{14}$$

$$\lambda + \upsilon + \frac{1}{2}\left(\frac{\alpha_2}{\alpha_3} - 1\right) + \frac{n}{\sqrt{\alpha_3}} = -\sqrt{\frac{1}{4}\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 + \frac{U_1}{\alpha_3^2}} \tag{15}$$

Squaring both sides of equation (15) and rearranging, we obtain the equation for the NUFA method as

$$\lambda^2 + 2\lambda\left(\upsilon + \frac{1}{2}\left(\frac{\alpha_2}{\alpha_3} - 1\right) + \frac{n}{\sqrt{\alpha_3}}\right) + \left(\upsilon + \frac{1}{2}\left(\frac{\alpha_2}{\alpha_3} - 1\right) + \frac{n}{\sqrt{\alpha_3}}\right)^2 - \frac{1}{4}\left(\frac{\alpha_2}{\alpha_3} - 1\right)^2 - \frac{U_1}{\alpha_3^2} = 0 \tag{16}$$

By substituting equations (8) and (9) into equation (3), we obtain the corresponding wave equation for the NUFA method as

$$\Psi_n(s) = N_n S^{\frac{(1-\alpha_1) + \sqrt{(\alpha_1 - 1)^2 + 4U_3}}{2}} (1-\alpha_3)^{\frac{(\alpha_3 + \alpha_1\alpha_3 - \alpha_2) + \sqrt{(\alpha_3 + \alpha_1\alpha_3 - \alpha_2)^2 + 4\left(\frac{U_1}{\alpha_3^2} + \alpha_3 U_3 - U_2\right)}}{2\alpha_2}} \, {}_2F_1(a,b,c;s) \tag{17}$$