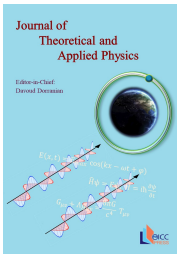

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Quantum mechanical treatment of Shannon entropy measure and energy spectra of selected diatomic molecules with the modified Kratzer plus generalized inverse quadratic Yukawa potential model

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Abstract:
In this research, we have obtained the energy eigenvalues and the corresponding normalized eigenfunction for the linear combination of the modified Kratzer and generalized inverse quadratic Yukawa potential using two different analytical methods: the exact quantization rule and the formula method respectively. The obtained normalized wave function is used to study the Shannon entropy in position and momentum spaces for the ground and first excited states. It was observed that the Shannon entropy in position space decreases as the screening parameter is increased and also increases in momentum space as the screening parameter is increased in such a way that their sum satisfies the Bialynicki-Birula-Mycielski (BBM) inequality that stipulated lower bound state of $S_r + S_p \geq D(1 + \ln \pi)$. Numerical results were generated for some selected diatomic molecules such as N_2, CO, NO, and CH which agreed with other works in the literature. The content of this research finds application in atomic and molecular physics, quantum chemistry, and physics.

Keywords: Bialynicki-Birula-Mycielski inequality; Wave function; Schrödinger equation; Energy spectra; Shannon entropy

1. Introduction

The wave function which is the distribution of particles at any instance in the evolution of a quantum system can only be obtained as the solution of the Schrödinger equation (SE) for a given potential function in quantum physics [1–3]. This wave function contains all the information required for the complete description of the particles at any time [4]. Hence, the attention of most researchers has been drawn to the quest of devising techniques for obtaining this wave function owing to the algebraic problem inherent in the SE, and this is due to the centrifugal barrier posed by the equation [5]. Analytical techniques such as the Nikiforov-Uvarov (NU) method [6], and others [7–9] have been proposed and used to determine the energy equation and wave function [10–14]. It is worth noting here that, if this problem did not exist, the eigenvalue problem would have been given less or no curiosity as it could be obtained through direct algebraic means. However, the development of different techniques and potential models has increased because we seek simpler and better approaches accompanied by generally real complex potentials that produce approximate results closer to experimental outcomes [15, 16]. One such way is the linear combination or superposition of potentials in both relativistic and non-relativistic regimes, this is nonetheless to further constrain the trajectory of the particle

for optimization of the solution and as well provide a wider range of applications [17]. According to the fundamental principle of information theory put forward by Claude Shannon, the global measures of Shannon entropy is crucial to quantum information-theoretic measures [18]. As a result of its numerous applications in physics and chemistry, scientists have actively investigated Shannon and Fisher entropies in various fields in recent years [19, 20]. The theory of communication is one field in which Shannon entropy is applied [21]. The significance of the global measure is to investigate the uncertainty associated with the probability distribution [22]. The position and momentum spaces of the Shannon entropy have an entropic relation derived by Berkner, Bialynicki-Birula, and Mycieslki (BBM) [23] and expressed as $S_r + S_p \geq D(1+\ln\pi)$, where D is the spatial dimension. Given this, many scholars have studied the Shannon and Fisher entropies [19, 20, 24–29], for instance, Edet et al., [30] used a class of Yukawa potential to study the global quantum information-theoretic measurements in the presence of magnetic and Aharanov-Bohm (AB) fields. Also, Edet et al., [31], investigated quantum information by a theoretical measurement approach of an Aharanov-Bohm (AB) ring with Yukawa interaction in curved space with disclination. They obtained the Shannon entropy through the eigenfunctions of the system. Furthermore, Amadi et al. [32] solved the SE with screened Kratzer potential to study the Shannon entropy and Fisher information. Their results show that the sum of the position and momentum entropies satisfies the lower-bound BBM inequality. Additionally, Ayedun et al., [33], investigated the Fisher information and Shannon entropy through the solutions of SE with the Eckart-Hellmann potential using the NU method. Their results showed an increase in the accuracy of the location of the predicted particles occurring in the position and momentum spaces. In recent studies, the Shannon entropy has been done in fractional Schrödinger equation [34–39].
The modified Kratzer potential [40] is used in the description of molecular structures in quantum mechanics in the areas of quantum chemistry, and atomic and molecular physics [41]. It is given as

$$V(r) = D_e\left(\frac{r-r_e}{r}\right)^2 \tag{1}$$

where D_e is the dissociation energy and r_e is the equilibrium inter-molecular distance and r is the inter-molecular distance.
On the other hand, the generalized inverse quadratic Yukawa potential (GIQYP) was first proposed by Ikhdair et al. [42]. Its application cuts across the fields of atomic physics, molecular physics, and the cloud of electronic charges around the nucleus [43]. It is of the form

$$V(r) = -V\left(1-\frac{e^{-\delta r}}{r}\right)^2 \tag{2}$$

where V is the potential coupling strength and δ is the potential range. Combining Eqs. (1) and (2), we obtain the potential under investigation as

$$V(r) = D_0 - \frac{D_1}{r} + \frac{D_2}{r^2} - D_3 - \frac{D_4 e^{-\delta r}}{r} - \frac{D_5 e^{-2\delta r}}{r^2} \tag{3}$$

where $D_0 = D_e$, $D_1 = 2D_e r_e$, $D_2 = D_e r_e^2$, $D_3 = D_5 = V$ and $D_4 = 2V$. These two potentials have received great attention from scholars in recent times and in the past to study selected diatomic molecules [44–46].
Given this, we intend to investigate the Shannon entropy measures and the energy spectra of selected diatomic molecules with the combined potential (modified Kratzer and generalized inverse quadratic Yukawa potential) using the exact quantization rule approach and formula method.
This paper is organized thus; we present a brief review of the Exact quantization rule in section 2, while in section 3, this method is applied to obtain the bound state solutions of the modified Kratzer plus Generalized Inverse Quadratic Yukawa Potential (MKGIQYP). In section 4 the Shannon entropy measure is studied. Section 5 is the results and discussion., and finally, our concluding remarks are captured in section 6.

2. Review of exact quantization rule approach

The exact quantization rule (EQR) [47] is an improvement of the WKB approximation [48] with the addition of a $N\pi$ term and an integral term (also known as a quantum correction Q_c). The quantum correction term is constant for exactly solvable potentials, independent of the number of nodes in the wave function. The exact quantization rule can be easily generalized to the proper quantization rule [49,50]. The EQR solution for the ground state can be obtained by solving the Riccati equation [51].
The one-dimensional SE is given by [52]

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2\mu}{\hbar^2}[E-V(x)]\psi(x), \tag{4}$$

where $V(x)$ is the piecewise continuous real potential function of x satisfying the following conditions:

$$\begin{aligned} &V(x) < E,\ x_a < x < x_b, \\ &V(x) = E,\ x_a = x \text{ or } x = x_b, \\ &V(x) > E,\ x \in (-\infty, x_a) \text{ or } x \in (x_b, \infty), \end{aligned} \tag{5}$$

where x_a and x_b are two turning points determined by $E - V(x) = 0$.
In the form of a non-linear Ricatti equation (RE), Equation (4) can be written as:

$$\frac{d}{dx}\phi(x) = -\frac{2\mu}{\hbar^2}[E-V(x)]\psi(x) - \phi(x)^2 \tag{6}$$

where $\phi(x) = \psi(x)^{-1}d\psi(x)/dx$ is the logarithmic derivative of the wave function $\psi(x)$; for the SE, $\phi(x)$ represents the phase angle of the wave function. The RE as given by Equation (6) reveals that for $E \geq V(x)$, as the variable increases across the nodes of the wave function $\psi(x)$, the logarithmic derivative decreases to $-\infty$, jumps to $+\infty$, and then, decreases again.
As proposed and studied by Ma and Xu [53], the EQR for the one-dimensional SE is given by

$$\begin{aligned} &\int_{x_a}^{x_b} k_n(x)dx = (n+1)\pi + \int_{x_a}^{x_b}\phi(x)\left[\frac{dk_n(x)}{dx}\right]\left[\frac{d\phi(x)}{dx}\right]^{-1}dx \\ &\text{and } k_n(x) = \sqrt{\frac{2\mu}{\hbar^2}}[E-V_{eff}(x)]^{\frac{1}{2}} \quad E \geq V_{eff}(x), \end{aligned} \tag{7}$$

where again, x_a and x_b are the two turning points obtained by solving the quadratic equation posed by $E - V_{eff}(r) = 0$. The first term $(n+1)$ is the contribution from the nodes of $\phi(x)$ and the second term is the quantum correction Q_c. For all exactly solvable quantum systems, the quantum correction (QC) is independent of the number of nodes of the wave function, so that the ground state quantum correction Q_{c0} can be calculated as

$$Q_{c0} = \int_{x_a}^{x_b} \phi_0(x) \left[\frac{dk_0(x)}{dr}\right] \left[\frac{d\phi_0(r)}{dr}\right]^{-1} dx. \tag{8}$$

The Q_{c0} term is usually evaluated from standard integration tables, but in a case where the resultant integrand is not available in the literature, it can be obtained computationally using any computing package such as Maple, Python, etc. In the generalization of this method to the three-dimensional SE with a central potential, the radial part of the SE becomes

$$\frac{d^2R(r)}{dr^2} = -\frac{2\mu}{\hbar^2}[E - V_{eff}(r)]R(r), \tag{9}$$

where $V_{eff}(r) = V(r) + [\hbar^2 l(l+1)]/2\mu r^2$.
By comparing Equations (4) and (9), the energy eigenvalues of the SE can be calculated by simply matching the conditions of the logarithmic derivatives, where, the logarithmic derivative is defined as $\phi(r) = [dR/dr]/R(r)$. Doing so, we see that from the quantization rule (Equation (7)), the energy eigenvalues of the three-dimensional SE will thus be

$$\begin{aligned} \int_{r_a}^{r_b} k_n(r)dr &= (n+1)\pi + \int_{r_a}^{r_b} \phi(r) \left[\frac{dk(r)}{dr}\right] \left[\frac{d\phi(r)}{dr}\right]^{-1} dr \\ k_n(r) &= \sqrt{\frac{2\mu}{\hbar^2}}[E - V_{eff}(r)]^{\frac{1}{2}} \quad E \geq V_{eff}(r) \end{aligned} \tag{10}$$

where r_a and r_b are the two turning points obtained by solving the quadratic equation posed by $E = V_{eff}(r)$.

3. Application of the exact quantization rule to modified Kratzer and generalized inverse quadratic Yukawa potential

In this section, we use the exact quantization rule technique to calculate the energy equation of the MKGIQYP. The SE with interaction potential $V(r)$ in D-dimensions [54] is given by

$$-\frac{\hbar^2}{2\mu}\nabla_D^2 \psi(r,\Omega_D) + [E - V(r)]\psi(r,\Omega_D) = 0 \tag{11}$$

where D is the dimensionality and $D \geq 2$; $\hbar$ and μ are the reduced Planck constant and mass respectively; ∇_D^2 is the Laplacian in D-dimensions; E is the non-relativistic energy and the wave function is expressed as $\psi(r,\Omega_D) = r^{-(D-1)/2} R_{nl}(r) Y_{lm}(\Omega_D)$ and $Y_{lm}(\Omega_D)$ is the generalized spherical harmonic function. The eigenvalues of the angular momentum operator L_D^2 for this function are $L_D^2 Y_{lm}(\Omega_D) = l(l+D-2)Y_{lm}(\Omega_D)$.
From the foregoing, (see Appendix A) the radial SE with the combined potential can be written as:

$$\begin{aligned} \frac{d^2R_{nl}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\Bigg[E_{nl} - \Bigg(D_0 - \frac{D_1}{r} + \frac{D_2}{r^2} - D_3 - \frac{D_4 e^{-\delta r}}{r} \\ - \frac{D_5 e^{-2\delta r}}{r^2} + \frac{K(K+1)\hbar^2}{2\mu r^2}\Bigg)\Bigg] R_{nl}(r) = 0 \end{aligned} \tag{12}$$

where $K = l + 1/2(D-3)$; n and l are the principal and orbital angular momentum quantum numbers respectively; r is the inter-nuclear distance. To overcome the inverse square term in Eq. (12), the Greene and Aldrich approximation scheme [55] is introduced, thus;

$$\frac{1}{r^2} \approx \frac{\delta^2 e^{2\delta r}}{(e^{\delta r} - 1)^2} \tag{13}$$

Using Equation (13), the SE in Equation (12) becomes

$$\begin{aligned} \frac{d^2R_{nl}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\Bigg[E_{nl} - \Bigg\{ & D_0 - \frac{D_1\delta}{(1-e^{-\delta r})} + \frac{D_2\delta^2}{(1-e^{-\delta r})^2} \\ & -D_3 - \frac{D_4\delta e^{-\delta r}}{(1-e^{-\delta r})} - \frac{D_5\delta^2 e^{-2\delta r}}{(1-e^{-\delta r})^2} \\ & + \frac{K(K+1)\hbar^2\delta^2}{2\mu r^2(1-e^{-\delta r})^2} \Bigg\}\Bigg] \\ & \times R_{nl}(r) = 0. \end{aligned} \tag{14}$$

The term in curly brackets in Equation (14) is the effective potential $V_{eff}(r)$, containing the combined potential and the centrifugal barrier. That is,

$$\begin{aligned} V_{eff}(r) = D_0 - \frac{D_1\delta}{(1-e^{-\delta r})} + \frac{D_2\delta^2}{(1-e^{-\delta r})^2} \\ -D_3 - \frac{D_4\delta e^{-\delta r}}{(1-e^{-\delta r})} - \frac{D_5\delta^2 e^{-2\delta r}}{(1-e^{-\delta r})^2} \\ + \frac{K(K+1)\hbar^2\delta^2}{2\mu r^2(1-e^{-\delta r})^2} \end{aligned} \tag{15}$$

Using the coordinate transformation, $x = 1/(e^{\delta r} - 1)$, we will have $e^{\delta r} = (1+x)/x$, so that

$$\begin{aligned} V_{eff}(x) = & D_0 - D_1\delta(1+x) + D_2\delta^2(1+x)^2 - D_3 \\ & -D_4\delta x - D_5\delta^2 x^2 + \frac{K(K+1)\hbar^2\delta^2}{2\mu}(1+x)^2. \end{aligned} \tag{16}$$

From Eq. (16), we obtain

$$\begin{aligned} V_{eff}(x) = & \big(D_0 - D_1\delta + D_2\delta^2 - D_3 + \frac{K(K+1)\hbar^2\delta^2}{2\mu}\big) \\ & + \big(-D_1\delta + 2D_2\delta^2 - D_4\delta + \frac{2K(K+1)\hbar^2\delta^2}{2\mu}\big)x \\ & + \big(D_2\delta^2 - D_5\delta^2 + \frac{K(K+1)\hbar^2\delta^2}{2\mu}\big)x^2 \end{aligned} \tag{17}$$

The two turning points x_a and x_b which are determined by solving $V(x) = E_{nl}$ quadratically are given as

$$x_a = -\frac{G}{2C} - \frac{\sqrt{G^2 - 4C(H - E_{nl})}}{2C}, \tag{18}$$

$$x_b = -\frac{G}{2C} + \frac{\sqrt{G^2 - 4C(H - E_{nl})}}{2C}, \tag{19}$$

where

$$\begin{cases} H = & D_0 - D_1\delta + D_2\delta^2 - D_3 + \frac{K(K+1)\hbar^2\delta^2}{2\mu}, \\ G = & -D_1\delta + 2D_2\delta^2 - D_4\delta + \frac{2K(K+1)\hbar^2\delta^2}{2\mu}, \\ C = & D_2\delta^2 - D_5\delta^2 + \frac{K(K+1)\hbar^2\delta^2}{2\mu}. \end{cases} \tag{20}$$

The momentum between the two turning points x_a and x_b is

$$k(x) = \sqrt{\frac{2\mu}{\hbar^2}}[E_{nl} - V_{eff}(x)]^{\frac{1}{2}} \tag{21}$$

By substituting Equation (20) into Equation (17) and making use of the two properties of turning points, that is, $x_a + x_b = -G/C$ and $x_a x_b = (H - E_{nl})/C$, we obtain

$$k(x) = \sqrt{\frac{2\mu C}{\hbar^2}}[(-1)(x_a - x)(x - x_b)]^{\frac{1}{2}} \tag{22}$$

In terms of the variable τ, the non-linear Ricatti equation for the ground state becomes

$$-\delta x(1+x)\frac{d}{dx}\phi_0(x) + \phi_0^2(x) + \frac{2\mu}{\hbar^2}[E_{0l} - V_{eff}(x)]\phi_0(x) = 0. \tag{23}$$

From its monotonic property, the logarithmic derivative of $\phi_0(x)$ for the ground state has one node and no pole, therefore, we assume a trial solution of the form $\phi_0(x) = A + Bx$. Upon substituting this into Equation (23), and evaluating, we obtain the following expression:

$$A^2 + (2AB - \delta B)x + (B^2 - \delta B)x^2 = \frac{2\mu}{\hbar^2}[H - E_{0l} + Gx - Cx^2] \tag{24}$$

Comparing the LHS and RHS of Equation (24), gives

$$\begin{cases} A^2 = & \frac{2\mu}{\hbar^2}(H - E_{0l}) \\ B = & \frac{\delta}{2} \pm \frac{1}{2}\sqrt{\delta^2 + \frac{8\mu C}{\hbar^2}}. \end{cases} \tag{25}$$

The above problem is physically solvable for only B since here, the logarithmic derivative of $\phi_0(x)$ will decrease exponentially as physically required.

From the foregoing, the integral of the momentum $k(r)$ (i.e. LHS of Eq. (10)) for $n = 0$ is evaluated as follows:

$$\begin{aligned} \int_{r_a}^{r_b} k_0(r)dr &= -\int_{x_a}^{x_b} k(x)\frac{dx}{\delta x(1+x)} \\ &= -\frac{1}{\delta}\sqrt{\frac{2\mu C}{\hbar^2}}\int_{x_a}^{x_b}\frac{\sqrt{(-1)(x-x_a)(x-x_b)}}{x(1+x)}dx \\ &= -\frac{\pi}{\delta}\sqrt{\frac{2\mu C}{\hbar^2}}\left[\sqrt{(x_a+1)(x_b+1)} - 1 - \sqrt{x_a x_b}\right] \\ &= -\frac{\pi}{\delta}\sqrt{\frac{2\mu C}{\hbar^2}}\left[\sqrt{\frac{H - E_{n\ell} - G + C}{C}} - 1 - \sqrt{\frac{H - E_{nl}}{C}}\right] \end{aligned} \tag{26}$$

and the ground state quantum correction Q_{c0}(which can be generalized to any value of n), is evaluated as

$$\begin{aligned} Q_{c0} &= \int_{r_a}^{r_b}\phi_0(r)\left[\frac{dk_0(r)}{dr}\right]\left[\frac{d\phi_0(r)}{dr}\right]^{-1}dr \\ &= -\int_{x_a}^{x_b}\frac{\phi_0(x)}{\delta x(1+x)}\left[\frac{dk_0(x)}{dx}\right]\left[\frac{d\phi_0(x)}{dx}\right]^{-1}dx \\ &= \frac{1}{\delta}\sqrt{\frac{2\mu C}{\hbar^2}}\int_{x_a}^{x_b}\frac{(x - \frac{x_a+x_b}{2})(x + \frac{A}{B})}{x(1+x)\sqrt{(-1)(x-x_a)(x-x_b)}}dx \\ &= \frac{\pi}{\delta}\sqrt{\frac{2\mu C}{\hbar^2}}\left[\frac{(\frac{A}{B} - 1)(1 + \frac{x_a+x_b}{2})}{\sqrt{(x_a+1)(x_b+1)}} - \frac{\frac{A}{B}(\frac{x_a+x_b}{2})}{\sqrt{x_a x_b}} + 1\right] \\ &= \frac{\pi}{\delta}\sqrt{\frac{2\mu C}{\hbar^2}}\left[\frac{1}{B}\frac{\sqrt{2\mu C}}{\hbar} + 1\right] \\ &= \pi\left(\frac{B}{\delta} - 1 + \frac{1}{\delta}\frac{\sqrt{2\mu C}}{\hbar}\right) \end{aligned} \tag{27}$$

Noting that for all exactly solvable quantum systems, the quantum correction Q_c is independent of the number of nodes n of the wave function, we can put Equation (26) and Equation (27), in Equation (10). Doing so, Equation (10) becomes

$$\begin{aligned} -\frac{\pi}{\delta}\sqrt{\frac{2\mu C}{\hbar^2}}\left[\sqrt{\frac{H - E_{nl} - G + C}{C}} - \sqrt{\frac{H - E_{nl}}{C}} - 1\right] \\ = (n+1)\pi + \pi\left(\frac{B}{\delta} - 1 + \frac{1}{\delta}\frac{\sqrt{2\mu C}}{\hbar}\right) \end{aligned} \tag{28}$$

From the above expression, the energy spectra $E_{nl}$is thus given explicitly as

$$\begin{aligned} E_{nl} = D_0 - D_1\delta + D_2\delta^2 - D_3 + \frac{K(K+1)\hbar^2\delta^2}{2\mu} - \frac{\hbar^2}{8\mu} \\ \left[\frac{\frac{2\mu}{\hbar^2}(D_1\delta - D_2\delta^2 + D_4\delta - D_5\delta^2 - \frac{K(K+1)\hbar^2\delta^2}{2\mu})}{(B + \alpha n)} - (B + \alpha n)\right]^2 \end{aligned} \tag{29}$$

where

$$B = \frac{\alpha}{2} + \sqrt{\frac{\delta^2}{4} + \frac{2\mu C}{\hbar^2}} \tag{30}$$

It is worth noting that one of the major setbacks of the exact quantization rule is that the wave function of a quantum system cannot be explicitly obtained within its framework. In this wise, we apply the techniques used in the formula method developed by authors in ref. [56] (see Appendix C), to obtain the wave function of the potential under study. From this method, we deduced from Equation (14) the following parameters:

$$k_4 = \sqrt{\varepsilon - \sigma_1}, \tag{31}$$

$$k_5 = G, \tag{32}$$

Thus, in terms of Jacobi polynomials, the resulting wave function for the MKGIQYP for $s = e^{-\delta r}$ is given as

$$\begin{aligned} R(s) = & N_{nl}e^{\sqrt{\varepsilon - \sigma_1}}(1-s)^G \ {}_2F_1(-n, n + 2(\sqrt{\varepsilon - \sigma_1} + G); \\ & 2\sqrt{\varepsilon - \sigma_1} + 1, s), \end{aligned} \tag{33}$$

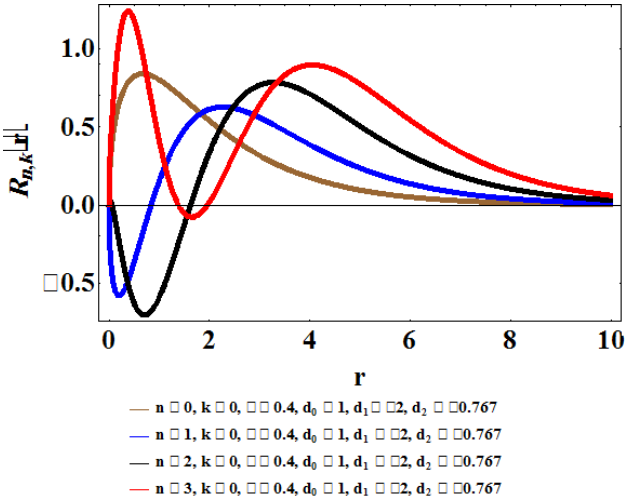

Figure 1. The wave function of the modified Kratzer plus Generalized Inverse Quadratic Yukawa Potential as a function of the position for various principal quantum number at $k = 0$.

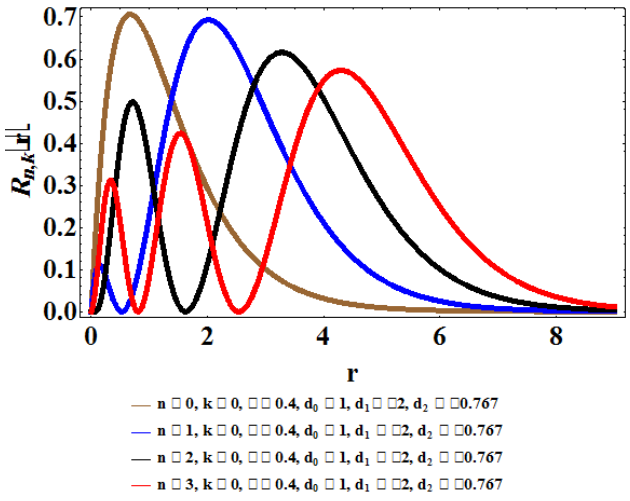

Figure 2. The probability density of the modified Kratzer plus Generalized Inverse Quadratic Yukawa Potential as a function of the position for various principal quantum number at $k = 0$.

where

$$G = \frac{1}{2} + \sqrt{\frac{1}{4} + 4\varepsilon - \sigma_4 - \sigma_2}, \qquad \sigma_1 = \frac{2\mu D_1}{\hbar^2},$$
$$\sigma_2 = -\frac{2\mu D_1}{\hbar^2} + K(K+1), \qquad \sigma_3 = \frac{2\mu D_4}{\hbar^2},$$
$$\varepsilon = -\frac{2\mu}{\hbar^2}(E_{nl} - D_0 + D_3), \qquad \sigma_4 = \frac{2\mu D_5}{\hbar^2}$$

And from the definition of Jacobi polynomials [57]

$$P_n^{(\theta,\varphi)}(x) = \frac{\Gamma(n+\theta+1)}{n!\Gamma(\theta+1)}\ {}_2F_1\big(-n, \theta+\varphi+n+1, \theta+1; \frac{1-x}{2}\big) \tag{34}$$

$$R(s) = N_{nl} e^{\sqrt{\varepsilon-\sigma_1}}(1-s)^G P_n^{(2\sqrt{\varepsilon-\sigma_1}, 2G-1)}(1-2s), \tag{35}$$

where N_{nl} is the normalization constant and it is obtained as follows;

$$\int_0^\infty |R_{nl}(r)|^2 dr = 1 \tag{36}$$

$$-\int_1^0 |R_{nl}(s)|^2 \frac{ds}{\delta s} = 1 \tag{37}$$

Changing the variable as $y = 1-2s$, and then, $(1-y)/2 = s$ and $(1+y)/2 = 1-s$, Eq. (37) becomes

$$\frac{N^2}{2\delta}\int_{-1}^{1}\left(\frac{1-y}{2}\right)^{2A-1}\left(\frac{1+y}{2}\right)^{2G}[P_n^{2A,2G-1}(y)]^2 dy = 1$$
$$\text{and} A = \sqrt{\varepsilon-\sigma_1} \tag{38}$$

noting that

$$\frac{N^2}{2\delta}\int_{-1}^{1}\left(\frac{1-y}{2}\right)^{a}\left(\frac{1+y}{2}\right)^{b}[P_n^{(a,b)}(y)]^2 dy = \frac{2\Gamma(a+n+1)\Gamma(b+n+1)}{n!a\Gamma(a+b+n+1)} \tag{39}$$

Hence, our normalization constant becomes

$$N = \sqrt{\frac{2\delta n!(2A-1)\Gamma(2A+2G+n)}{2\Gamma(2A+n)\Gamma(2G+n+1)}} \tag{40}$$

The total wave function is then given as

$$R(s) = N = \sqrt{\frac{2\delta n!(2A-1)\Gamma(2A+2G+n)}{2\Gamma(2A+n)\Gamma(2G+n+1)}}\, e^{\sqrt{\varepsilon-\sigma_1}} \times (1-s)^G P_n^{2\sqrt{\varepsilon-\sigma_1}, 2G-1}(1-2s). \tag{41}$$

4. Shannon entropy

The physics of various systems have been aided by quantum information entropy (QIT) [58, 59]. This is because it

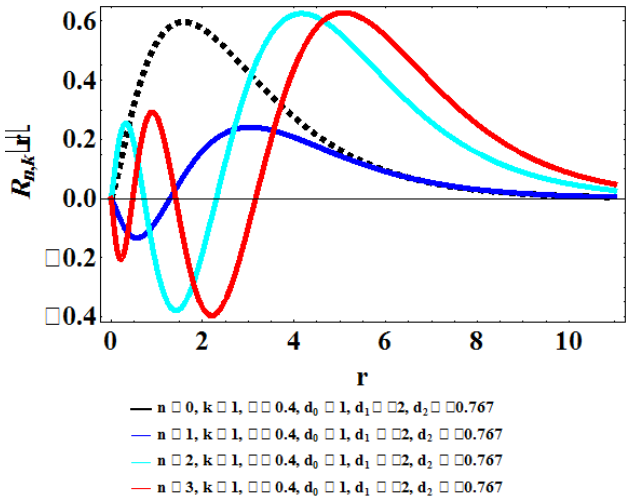

Figure 3. The wave function of the modified Kratzer plus Generalized Inverse Quadratic Yukawa Potential as function of the position for various principal quantum number at $k = 1$.

Table 1. Numerical values of Shannon entropy for modified Kratzer plus Generalized Inverse Quadratic Yukawa Potential.

n	δ	S_r	S_p	S_T
0	0.1	9.17887	-1.66212	7.51675
	0.2	6.16495	1.06183	7.22678
	0.3	4.56399	2.50622	7.07021
	0.4	3.52719	3.45174	6.97893
	0.5	2.78809	4.13361	6.92171
	0.6	2.22580	4.65795	6.88375
	0.7	1.77660	5.08082	6.85742
	0.8	1.40392	5.43452	6.83844
	0.9	1.08551	5.73881	6.82432
1	0.1	8.97945	-0.647543	8.331907
	0.2	6.31299	1.633411	7.946401
	0.3	4.91064	2.811482	7.722122
	0.4	3.99154	3.592791	7.584331
	0.5	3.31959	4.174671	7.494261
	0.6	2.79324	4.639091	7.432331
	0.7	2.36095	5.027031	7.387981
	0.8	1.99359	5.361471	7.355061
	0.9	1.67348	5.656411	7.329891

contains crucial information about the physical system. Studies of a trigonometrically symmetric Rosen-Morse potential [60], a profile of the solitonic mass [61], and a hyperbolic-single potential well [62] are some examples of applications of quantum entropy.

Shannon entropy is one of the quantum entropies used to analyze the information contained in quantum systems. To characterize the most effective method of information transmission between a source and a receiver, Shannon's entropy was developed [18]. Studies on the thermodynamics of an ensemble of particles led to mathematical formulations with a similar profile, which helped establish the Shannon entropy notion in physics. Because Shannon information and Boltzmann entropy are similar, Shannon's entropy can be used to assess uncertainty in non-Hermitian particle systems, and to interpret information in quantum systems [63]. Shannon formalism also made it possible to investigate fermionic particles [64], issues with effective mass distribution [65, 66], and mechanical-quantum models with double-well potential [67]. The degree of uncertainty in a probability distribution connected to an information source can be determined by interpreting the Shannon entropy of a quantum-mechanical system [67, 68]. The statistical experience of the stationary quantum system is what the Born interpretation of quantum physics [69] leads us to understand.

$$\rho(\mathbf{r})dr = |\psi(\mathbf{r},t)|^2 dr \equiv |\psi(\mathbf{r})|^2 dr. \tag{42}$$

In this case, $\rho(\mathbf{r})$ is the probability of finding the particle in the state $\psi(\mathbf{r},t)$ between $\mathbf{r}$ and $\mathbf{r}+d\mathbf{r}$ [69]. Furthermore, $|\psi(\mathbf{r},t)|^2$ is the probability density of the quantum-mechanical system. Now let's examine Shannon's entropy

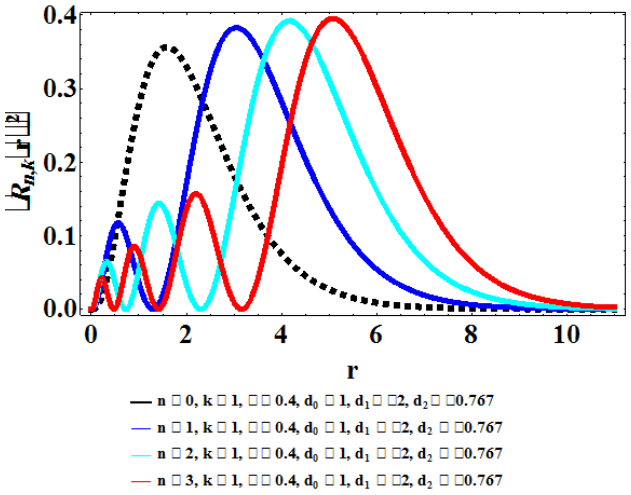

Figure 4. The plot of the position entropy density as a function of the position for various principal quantum number.

in relation to quantum physics. We define Shannon's entropy as, keeping in mind that the probability density has the form of Eq. (42).

$$S = -\sum_i \rho_i \ln \rho_i, \tag{43}$$

Hence, Shannon entropy for a probability density of a continuous system in position space has the following form:

$$S_r = -\int_{-\infty}^{\infty} |\psi(r)|^2 \ln(|\psi(r)|^2) dr. \tag{44}$$

In momentum space, Shannon entropy is

$$S_p = -\int_{-\infty}^{\infty} |\psi(p)|^2 \ln(|\psi(p)|^2) dp. \tag{45}$$

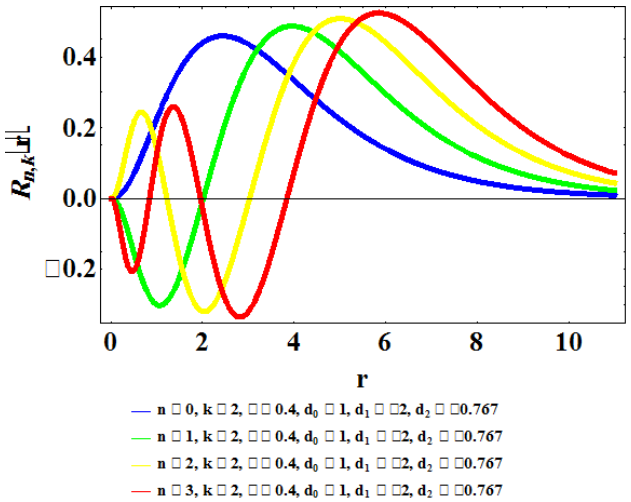

Figure 5. The wave function of the modified Kratzer plus Generalized Inverse Quadratic Yukawa Potential as a function of the position for various principal quantum number at $k = 2$.

Table 2. Energy eigenvalues (eV) of the modified Kratzer plus generalized inverse quadratic Yukawa potential for N_2, CO, NO and CH diatomic molecules.

n	l	N_2	CO	NO	CH
0	0	0.142352681	0.079536704	0.014314254	-0.015022938
1	0	0.231091461	0.161726684	0.077928111	0.087074134
	1	0.231298580	0.161924070	0.078093559	0.088113175
2	0	0.318667994	0.242811630	0.140618894	0.183536394
	1	0.318872465	0.243006426	0.140781998	0.184520073
	2	0.319076937	0.243201199	0.140945119	0.185503039
3	0	0.405102462	0.322811236	0.202404332	0.274770012
	1	0.405304331	0.323003481	0.202565139	0.275702240
	2	0.405506198	0.323195709	0.202725961	0.276633802
	3	0.405708049	0.323387955	0.202886761	0.277564692
4	0	0.490414609	0.401744741	0.263301746	0.361145198
	1	0.490613911	0.401934494	0.263460301	0.362029544
	2	0.490813220	0.402124225	0.263618873	0.362913262
	3	0.491012513	0.402313965	0.263777424	0.363796353
	4	0.491211784	0.402503688	0.263935964	0.364678821
5	0	0.574623738	0.479630988	0.323328038	0.442999946
	1	0.574820524	0.479818282	0.323484388	0.443839670
	2	0.575017318	0.480005559	0.323640739	0.444678804
	3	0.575214097	0.480192846	0.323797087	0.445517353
	4	0.575410853	0.480380105	0.323953415	0.446355317
	5	0.575607626	0.480567359	0.324109740	0.447192694

Also, the wave function in reciprocal space $\psi(k)$ is given by the Fourier transform,

$$\psi(k) = \frac{1}{\sqrt{2}} \int_{-\infty}^{\infty} \psi(r) e^{-irk} dr. \tag{46}$$

A comparable function to the Heisenberg uncertainty measures is played by the entropic quantities in Eqs. (44) and (45) [63, 64]. In order to relate the entropic uncertainties, Beckner [70] and Bialynicki-Birula and Myciuelski (BBM) [23] found an entropic uncertainty relation.
The uncertainty BBM is

$$S_r + S_p \geq D(1 + \ln \pi), \tag{47}$$

where D is the dimension of effective spatial coordinates. In this instance, the outcomes must adhere to the relationship

$$S_r + S_p \geq 2.14473. \tag{48}$$

5. Results and discussion

We use Eqs. (44) and (45) to calculate the Shannon entropy in position space and momentum space respectively. The numerical results of Shannon's entropy for the ground and first energy levels are shown in Table 1. As can be observed in Table1, Shannon entropy in position space decreases as the screening parameter is increased and also

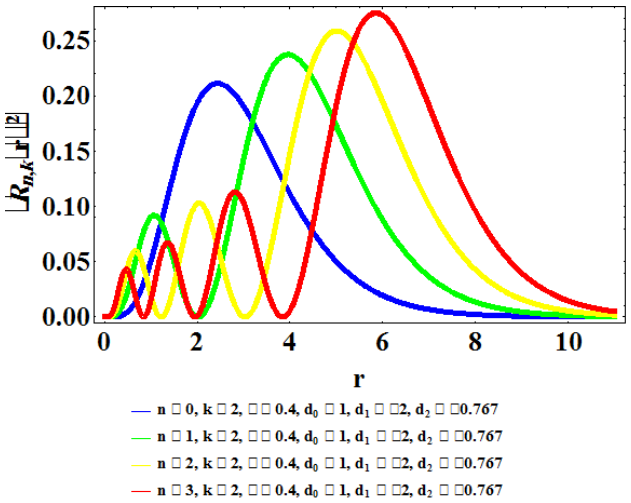

Figure 6. The probability density of the modified Kratzer plus Generalized Inverse Quadratic Yukawa Potential as a function of the position for various principal quantum number at $k = 2$.

Table 3. Energy eigenvalues (eV) of the modified Kratzer potential for NO and CH diatomic molecules.

n	l	NO	NO [45]	NO [46]	CH	CH [45]	CH [46]
0	0	0.041123182	0.041123195	0.041118000	0.083229281	0.083224184	0.083214000
1	0	0.122325847	0.122325849	0.122311000	0.241166826	0.241151503	0.241123000
	1	0.122532363	0.122738863	0.122724000	0.242796715	0.244409838	0.244381000
2	0	0.202298811	0.202298791	0.202274000	0.389616956	0.389591425	0.389547000
	1	0.202502208	0.202705567	0.202681000	0.391149930	0.392656024	0.392611000
	2	0.202705589	0.203518990	0.203494000	0.392681567	0.398769202	0.398722000
3	0	0.281066784	0.281066733	0.281033000	0.529324618	0.529288943	0.529229000
	1	0.281267123	0.281467399	0.281434000	0.530768211	0.532174862	0.532115000
	2	0.281467447	0.282268597	0.282235000	0.532210564	0.537931848	0.537870000
	3	0.281667764	0.283470085	0.283436000	0.533651675	0.546530346	0.546467000
4	0	0.358653849	0.358653765	0.358611000	0.660963052	0.660917327	0.660844000
	1	0.358851193	0.359048434	0.359006000	0.662324079	0.663638196	0.663565000
	2	0.359048521	0.359837651	0.359795000	0.663683954	0.669066127	0.668992000
	3	0.359245841	0.361021173	0.360997800	0.665042676	0.677173658	0.677098000
	4	0.359443146	0.362598630	0.362555000	0.666400248	0.687920044	0.687842000
5	0	0.435083496	0.435083367	0.435032000	0.785141917	0.785086272	0.785001000
	1	0.435277902	0.435472163	0.435421000	0.786426557	0.787654439	0.787569000
	2	0.435472295	0.436249637	0.436198000	0.787710125	0.792777921	0.792692000
	3	0.435666677	0.437415549	0.437364000	0.788992619	0.800431163	0.800343000
	4	0.435861048	0.438969538	0.438917000	0.790274044	0.810576230	0.810487000
	5	0.436055409	0.440911128	0.440858000	0.791554398	0.823163305	0.823071000

the Shannon entropy in momentum space increases as the screening parameter is increased in such a way that their sum satisfies BBM inequality that stipulated lower bound state of $S_r + S_p \geq D(1+\ln\pi)$ is verified for the MKGIQYP. Using Eq. (29) and the spectroscopic parameters of the selected molecules [45]. The following conversions; $\hbar C = 1973.269$ eV$\mathring{A}$ and 1amu $= 931.5 \times 10^6$ eV$(\mathring{A})^{-1}$ are used for all computations [71–75]. In Table 2, we generate the energy eigenvalues for the modified Kratzer plus generalized inverse quadratic Yukawa potential for four select diatomic molecules (N_2, CO, NO, and CH) to investigate the nature of the potential on bound state problems. It is observed that the energy spectrum increases as the state n, l increase for any bound state system. Table 3, further establishes the reliability of the exact quantization rule approach in bound state problems by comparing our results with those in literature for the modified Kratzer potential for different n, l states. It is seen from Table 3 that the exact quantization rule approach is exact with other techniques which agrees with the numerical computation.
The behavior of the wave function and probability density of the position is plotted for various principal quantum numbers at angular momentum k equal to 0,1 and 2 are shown in Figures 1 to 6. Figure 1 displays the wave function of the combined potential as a function of the position r. We observed an increase with the increase in the principal quantum number while other parameters are kept constant and the wave function showcases intertwining multiple sinusoidal curves representing the different quantum states. The same was observed in Figure 2 being the plot of the probability density with the position and shows a normal distribution curve with multiple peaks, each depicting a different quantum state. This physically means that the lower the Shannon entropies, the higher the accuracy in predicting the localization of the particles and the more stable is this quantum system. Figures 3 and 4 illustrate the plots of the wave function and probability density function when $k = 2$. As can be seen in Figure 3, the wave function increases with various potential parameters to satisfy the BBM conditions. In Figure 4, the probability density shows similar trends. However, this indicates that the probability densities for these entropies are highly localized. In Figures 5 and 6, we depict the variations of the wave function and probability density as a function of the position space. As shown in Figure 5, the wave function plot is higher when the principal quantum number is increased to 3. The same is also noticed in Figure 6 and it agreed excellently with the theoretical and experimental descriptions of probability density. It is expected that in an ideal condition, the peak of the probability density plot should increase as the quantum state increases.

6. Conclusion

The exact quantization rule approach and the formula method were used to obtain the energy eigenvalues and the corresponding normalized eigenfunction for the linear combination of the modified Kratzer plus Generalized Inverse Quadratic Yukawa Potential. In the ground and first excited states, the Shannon entropy values were calculated. For a prospective model to be physically stable in quantum theoretic information, it must follow the BBM relation $S_r + S_p \geq D(1+\ln\pi)$, which has been attained in our findings for our suggested model, as shown in Table 1. The numerical results in Table 1 reveal that when one entropy increases, the other decreases in a way that keeps their sum above the necessary lower bound values. Numerical results were generated for some selected diatomic molecules such as N_2, CO, NO, and CH which agreed with other works in the literature. Figures (1-6) show the plots of the wave function and probability density as functions of position for various values of n and k. Our research is easily adaptable to various soluble quantum systems.

Conflict of interest statement:
The authors declare that they have no conflict of interest.

APPENDIX A
Some useful standard integrals used to evaluate the integrals in Equation (7) are given below.

$$\int_{\tau_a}^{\tau_b} \frac{d\tau}{\sqrt{(\tau-\tau_a)(\tau_b-\tau)}} = \pi \tag{49a}$$

$$\int_{\tau_a}^{\tau_b} \frac{\tau d\tau}{\sqrt{(\tau-\tau_a)(\tau_b-\tau)}} = \frac{\pi}{2}(\tau_a+\tau_b) \tag{49b}$$

$$\int_{\tau_a}^{\tau_b} \frac{d\tau}{\tau\sqrt{(\tau-\tau_a)(\tau_b-\tau)}} = \frac{\pi}{\sqrt{\tau_a\tau_b}} \tag{49c}$$

APPENDIX B
In Cartesian coordinates, the 1D Schrödinger wave equation with a central potential as given in Equation (4) is

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2\mu}{\hbar^2}[E-V(x)]\psi(x), \tag{50a}$$

and in 3D it is given by

$$\nabla^2\psi(r) + \frac{2\mu}{\hbar^2}[E-V(r)]\psi(r) = 0, \tag{50b}$$

where $\nabla^2(r)$ is the Laplacian operator Cartesian coordinates.
To transform the one-dimensional Schrödinger equation into a three-dimensional one to accommodate the logarithmic derivative, the Laplacian, $\nabla^2$and the three-dimensional Schrödinger equation must be expressed in spherical polar coordinates. In spherical coordinates ∇^2 is given as

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial r}(\sin\theta\frac{\partial}{\partial r}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}. \tag{50c}$$

The three-dimensional form of the Schrödinger equation in spherical coordinates is written in the form $\psi(r,\theta,\varphi)$ and it is variable separable, i.e. it can be separated into its component as

$$\psi(r,\theta,\varphi) = \chi(r)\Theta(\theta)\phi(\varphi) \tag{50d}$$

Substituting Equations (5 and 6) into Equation (4) yields

$$\begin{aligned}\frac{\Theta(\theta)\phi(\varphi)}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial\chi(r)}{\partial r}) + \frac{\chi(r)\phi(\varphi)}{r^2\sin\theta}\\ \frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta}) + \frac{\chi(r)\Theta(\theta)}{r^2\sin^2\theta}\frac{\partial^2\phi(\varphi)}{\partial\varphi^2}\\ + \frac{2\mu}{\hbar^2}[E-V(r)]\chi(r)\Theta(\theta)\phi(\varphi) = 0\end{aligned} \tag{50e}$$

Dividing Eq. (50e) by $\psi(r,\theta,\varphi) = \chi(r)\Theta(\theta)\phi(\varphi)$ and multiplying through by $r^2\sin^2\theta$ yields

$$\begin{aligned}\frac{\sin^2\theta}{\chi(r)}\frac{\partial}{\partial r}(r^2\frac{\partial\chi(r)}{\partial r}) + \frac{\sin\theta}{\Theta(\theta)}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta})\\ + \frac{2\mu r^2\sin^2\theta}{\hbar^2}[E-V(r)] = -\frac{1}{\phi(\varphi)}\frac{\partial^2\phi(\varphi)}{\partial\varphi^2}\end{aligned} \tag{50f}$$

The RHS and the LHS of equation (50f) are both independent and so they are equal to the same constant m_l^2, say. That is

$$\frac{1}{\phi(\varphi)}\frac{\partial^2\phi(\varphi)}{\partial\varphi^2} = -m_l^2 \tag{50g}$$

where m_l is the magnetic quantum number.
Substituting Equation (50g) into Equation (50f) and dividing through by gives

$$\begin{aligned}\frac{1}{\chi(r)}\frac{\partial}{\partial r}(r^2\frac{\partial\chi(r)}{\partial r}) + \frac{2\mu r^2}{\hbar^2}[E-V(r)]\\ + \frac{1}{\sin\theta}\frac{1}{\Theta(\theta)}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta} - \frac{m_l^2}{\sin^\theta})\end{aligned} \tag{50h}$$

The radial and angular parts of equation (50h) are linearly independent and therefore are equal to a constant, $l(l+1)$ say. That is,

$$\frac{1}{\chi(r)}\frac{\partial}{\partial r}(r^2\frac{\partial\chi(r)}{\partial r}) + \frac{2\mu r^2}{\hbar^2}[E-V(r)] = l(l+1) \tag{50i}$$

and

$$\frac{1}{\sin\theta}\frac{1}{\Theta(\theta)}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\Theta(\theta)}{\partial\theta}) - \frac{m_l^2}{\sin^2\theta} = -l(l+1) \tag{50j}$$

Equation (50i) is the radial part of the Schrödinger equation (which is the equation of interest). Solving and re-writing it as an ordinary differential equation yield

$$\begin{aligned}r^2\frac{d^2\chi(r)}{dr^2} + 2r\frac{d\chi(r)}{dr} + \frac{2\mu r^2}{\hbar^2}[E-V(r) - \frac{\hbar^2}{2\mu r^2}l(l+1)]\\ \chi(r) = 0.\end{aligned} \tag{50k}$$

Multiplying Equation (50k) by r^2 yields

$$\begin{aligned}\frac{d^2\chi(r)}{dr^2} + \frac{2}{r}\frac{d\chi(r)}{dr} + \frac{2\mu}{\hbar^2}[E-V(r) - \frac{\hbar^2}{2\mu r^2}l(l+1)]\\ \chi(r) = 0\end{aligned} \tag{50l}$$

To solve the above equation, we make use of a trial wave function that obeys the cusp condition (or Kato's theorem). One such function is of the form:
$\chi(r) = r^{-1}R(r)$

$$\frac{d}{dr}\chi(r) = -r^{-2}R(r) + r^{-1}\frac{d}{dr}R(r),$$
$$\frac{d^2}{dr^2}\chi(r) = 2r^{-3}R(r) - r^{-2}\frac{d}{dr}R(r) + r^{-1}\frac{d^2}{dr^2}R(r) - r^{-2}R(r) \quad (50m)$$

Substituting equation (50m) into equation (50l) and simplifying gives

$$\frac{d^2R(r)}{dr^2} = -\frac{2\mu}{\hbar^2}[E - V_{eff}(r)]R(r), \quad (50n)$$

as given in Equation (9) of the article.

Appendix C

The second-order differential equation can be written in the form

$$\acute{\psi}(s) + \frac{(k_1 - k_2 s)}{s(1-k_3 s)}\acute{\psi}(s) + \frac{(As^2 + Bs + C)}{s^2(1-k_3 s)^2}\psi(s) = 0 \quad (51a)$$

The wave function of the differential equation above can be determined from the formula

$$\psi(s) = N_n s^{k_4}(1-k_3 s)^{k_5}\ {}_2F_1(-n, n + 2(k_4+k_5) + \frac{k_2}{k_3} - 1; 2k_4 + k_1, k_3 s) \quad (51b)$$

where the parameters are defined as

$$k_4 = \frac{(1-k_1) + \sqrt{(1-k_1)^2 - 4C}}{2} \quad (51c)$$

and

$$k_5 = \frac{1}{2} + \frac{k_1}{2} - \frac{k_2}{2k_3} + \sqrt{\left[\frac{1}{2} + \frac{k_1}{2} - \frac{k_2}{2k_3}\right]^2 - \left[\frac{A}{k_3^2} + \frac{B}{k_3} + C\right]} \quad (51d)$$

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