



OPEN Determination of probability density, position and momentum uncertainties, and information theoretic measures using a class of inversely quadratic Yukawa potential

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This study utilizes the Nikiforov-Uvarov method to solve the Schrödinger equation for the class of inversely quadratic Yukawa potential (CIQYP), deriving both the energy equation and the normalized wave function. Shannon entropy and Fisher information in both position and momentum spaces are analyzed for low-energy states using the wave function. The Bialynicki-Birula-Mycielski and Stam-Cramer-Rao inequalities are satisfied for the Shannon and Fisher information entropies, illustrating the complementary uncertainties inherent in position and momentum in quantum mechanics. The study underscores the interplay between position and momentum Fisher entropies, reinforcing the Heisenberg uncertainty principle, which imposes limits on the precise simultaneous measurement of conjugate variables. Eigenvalues of the CIQYP for three diatomic molecules (N_2 , O_2 , and NO) are obtained using their respective data, revealing that the bound state energy spectra of these diatomic molecules increase as both the principal quantum number and angular momentum quantum number rise. Expectation values were numerically determined, and the potential model simplifies to the Kratzer potential under specific boundary conditions, thereby ensuring analytical accuracy. The energy spectra of diatomic molecules such as I_2 and CO are examined, showing that for a fixed principal quantum number, the energy spectrum increases with increasing angular momentum quantum number, in very good agreement with previously obtained results using different analytical methods.

Keywords Stam-Cramer-Rao inequality, Schrödinger equation, Expectation values, Wave function, Information theory

Researchers have recently focused on solving both non-relativistic and relativistic equations using potential models with various analytical methods^{1–5}. The derived energy equation and wave function can be applied to analyze a range of quantum mechanical systems, including the quark-antiquark system^{6,7}, the energy spectra of diatomic molecules (DMs)^{8–10}, and information theory^{11–13}, among others. Additionally, researchers have studied devices that coherently transfer quantum information between topological and conventional materials. In these devices, an electromagnetic field transmits a modulated signal and collects propagation channel data¹⁴. Shannon entropy is a key measure of the uncertainty and randomness associated with electron localization and delocalization¹⁵. It has recently gained prominence in quantum physics due to its crucial role in modern quantum communication systems¹⁶. By quantifying uncertainty in quantum systems, Shannon entropy extends Heisenberg's uncertainty principle and helps describe various physical properties¹⁷. In contrast, Fisher information measures the efficiency of measurement procedures and estimates quantum limits¹⁸.

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Although its theoretical basis was established earlier¹⁹, its significance was not fully recognized until Sear et al.²⁰ highlighted its connection to the kinetic energy of quantum systems. Fisher information focuses on local changes in probability density^{21,22} and plays an important role in fields such as density functional theory²³, statistical estimation²⁴, and related areas^{25–34}. Shannon entropy and Fisher information are key concepts for understanding the uncertainty and precision of a system. Higher Shannon entropy indicates greater uncertainty in a system's position or momentum, with a spread-out probability distribution leading to higher entropy, while a sharply peaked distribution results in lower entropy³⁵. Fisher information, on the other hand, measures the sharpness or smoothness of the probability distribution and is inversely related to uncertainty. High Fisher information suggests that small changes in position lead to significant changes in probability density, implying low uncertainty and greater system stability. This is often associated with higher kinetic energy, indicating a more localized and stable system³⁶. Together, Shannon entropy and Fisher information balance uncertainty and precision in describing physical systems.

Over the past decade, research has focused on Shannon and Fisher information (FI) entropies using potential models^{37,38}. For example, Dong et al.³⁹ extensively studied the Shannon information entropy and standard deviations of a particle in a symmetrical squared tangent potential. They illustrated the probability and entropy densities for position and momentum across different potential ranges and depths. The Bialynicki-Birula Mycielski (BBM) inequality highlights the relationship between the sum of position and momentum entropies. In another study, Song and co-workers⁴⁰ conducted a numerical investigation of Fisher information entropy in a one-dimensional system with a “Landau” potential.

The phase transition behavior of the system was effectively characterized through the development of quantum information entropy (QIE). The results show that position and momentum entropies vary with the mass parameter at the critical point of phase transition, while their total remains consistent across all excited states. Additionally, Gil-Barrera et al.⁴¹ examined quantum information entropy in two sets of hyperbolic single potential wells. Wave functions were used to study the behavior of a moving particle under two hyperbolic potential (HP) wells. Although these hyperbolic potentials have similar shapes, their momentum entropy densities change with their widths, and position entropy density decreases as momentum entropy increases. El-Qahtani et al.⁴² studied the effects of temperature on fidelity, entropy squeezing, quantum Fisher information (QFI), and two interacting superconducting qubits (SCQs). They demonstrated that the model's physical parameters can be tuned to control variations in quantum quantifiers. Additionally, they achieved a trapping phenomenon for Fisher information, which enhanced QFI, preserved the data, and protected it from temperature-induced loss. The dynamic features of quantum Fisher information in relation to the model's physical parameters were explained through the fidelity of superconducting qubits. Additionally, they explored how these physical parameters influenced the variation in superconducting qubits' squeezing entropy. Abdelmonem et al.⁴³ used the J-matrix method to study information entropies and related quantities for the Morse potential in both position and momentum spaces, computing the s-wave entropies of diatomic molecules H₂ and LiH numerically.

Furthermore, Edet et al.⁴⁴ investigated quantum information using a theoretical measurement technique with Yukawa potential (YP) in curved space containing a disclination, calculating Shannon entropy based on the system's eigenfunctions. In their study, Ikot et al.⁴⁵ applied a functional approach to derive solutions for the Schrödinger Equation (SE) involving generalized Hulthen and Yukawa potentials, using the wave function to examine information-theoretical measures in both momentum and position spaces for the ground and first excited states. Ikot et al.⁴⁶ also analyzed Shannon and Fisher information entropies in a generalized hyperbolic potential in both position and momentum spaces by solving the SE using the NUFA method. Numerical calculations were performed to determine Shannon entropy and Fisher information entropy in both spaces. Additionally, researchers have explored modified Schrödinger Eqs^{47–51}.

Inspired by their methodology, we study Shannon and Fisher information entropies in one dimension and the energy spectra of selected diatomic molecules using the class of inversely quadratic Yukawa potential (CIQYP) proposed by Inyang et al.⁵².

The potential is provided as:

$$V(r_q) = -\frac{d_0}{r_q} - \frac{d_1}{r_q^2} + \frac{d_2 e^{-\delta r_q}}{r_q^2} \quad (1)$$

where δ represents the screening parameter, while d_0 , d_1 , and d_2 are parameters related to potential strength and r_q is the particle distance. The CIQYP could have significant applications in various fields of physics, such as atomic physics, nuclear physics, condensed matter physics, and molecular physics. This study aims to utilize normalized wave functions and energy equation to analyze information-theoretical measures in one dimension, including the expectation values of $\langle r_q \rangle$, $\langle r_q^2 \rangle$, $\langle \hat{p}^2 \rangle$, the energy spectra of selected diatomic molecules, and the uncertainty principle for states with low energy levels. To our knowledge, these results have not been recorded in any previously published literature.

The solutions of the Schrödinger equation with the class of inversely quadratic Yukawa potential

In this research, we use the Nikiforov-Uvarov (NU) method to solve the hypergeometric second-order differential equation. For details, refer to⁵³. The radial Schrödinger equation for a quantum system with reduced mass (μ_a) is given as⁵⁴.

$$\frac{d^2 R_{nl}}{dr_q^2} + \frac{2\mu_a}{\hbar^2} \left(E_{nl} - V(r_q) - \frac{l(l+1)\hbar^2}{2\mu_a r_q^2} \right) R_{nl}(r_q) = 0 \quad (2)$$

To solve the radial Schrödinger equation, we insert Eq. (1) into (2) and obtain

$$\frac{d^2 R_{nl}}{dr_q^2} + \frac{2\mu_a}{\hbar^2} \left(E_{nl} + \frac{d_0}{r_q} + \frac{d_1}{r_q^2} - \frac{d_2 e^{-\delta r_q}}{r_q^2} - \frac{l(l+1)\hbar^2}{2\mu_a r_q^2} \right) R_{nl}(r_q) = 0, \quad (3)$$

The inserted potential model cannot be solved exactly in Eq. (3). To handle the centrifugal barrier, the Greene-Aldrich approximation scheme, $r_q^{-2} \approx \delta^2 (1 - e^{-\delta r_q})^{-2}$; $r_q^{-1} \approx \delta (1 - e^{-\delta r_q})^{-1}$ is used. This method approximates the centrifugal term well for $\delta \ll 1$ ⁵⁵. The change of variable $r_q \rightarrow x_c$ gives us $x_c = e^{-\delta r_q}$ as our new coordinate. With this, we can solve Eq. (3) and get

$$\frac{d^2 R_{nl}(x_c)}{dx_c^2} + \frac{1-x_c}{x_c(1-x_c)} \frac{dR(x_c)}{dx_c} + \frac{1}{[x_c(1-x_c)]^2} [-\varepsilon x_c^2 + (2\varepsilon - \beta_x - \beta_z)x_c - (\varepsilon - \beta_x - \beta_y + \gamma_a)] R(x_c) = 0, \quad (4)$$

where

$$-\varepsilon = \frac{2\mu_a E_{nl}}{\delta^2 \hbar^2}, \beta_x = \frac{2\mu_a d_0}{\delta \hbar^2}, \beta_y = \frac{2\mu_a d_2}{\hbar^2}, \beta_z = \frac{2\mu_a d_1}{\hbar^2}, \gamma_a = l(l+1) \left. \right\}. \quad (5)$$

Comparing Eqs. (4) and (1) of Ref. 53 yields the following polynomials:

$$\begin{aligned} \tilde{\tau}(x_c) &= 1 - x_c; \sigma(x_c) = x_c(1 - x_c); \sigma'(x_c) = 1 - 2x_c, \\ \tilde{\sigma}(x_c) &= -\varepsilon x_c^2 + (2\varepsilon - \beta_x - \beta_z)x_c - (\varepsilon - \beta_x - \beta_y + \gamma_a) \end{aligned} \quad (6)$$

Putting the polynomials in Ref. 53 of Eq. (11) gives the polynomial

$$\pi(x_c) = -\frac{x_c}{2} \pm \sqrt{(\Upsilon_1 - K_s)x_c^2 + (K_s + \Upsilon_2)x_c + \Upsilon_3}, \quad (7)$$

where

$$\Upsilon_1 = \left(\frac{1}{4} + \varepsilon \right), \Upsilon_2 = -(2\varepsilon - \beta_x - \beta_z), \Upsilon_3 = (\varepsilon - \beta_x - \beta_y + \gamma_a) \quad (8)$$

The NU method states that the discriminant of this quadratic equation (QE) is set to zero. The discriminant provides a new QE that can be solved to find the two roots for the constant. Here, we consider the negative square root provided as

$$K_s = -(\Upsilon_2 + 2\Upsilon_3) - 2\sqrt{\Upsilon_3}\sqrt{\Upsilon_3 + \Upsilon_2 + \Upsilon_1}. \quad (9)$$

We then put K_s into $\pi(x_c) = -\frac{x_c}{2} \pm \sqrt{(\Upsilon_1 - K_s)x_c^2 + (K_s + \Upsilon_2)x_c + \Upsilon_3}$, and obtain, $\pi(x_c)$ has the most suitable expression given as

$$\pi(x_c) = -\frac{x_c}{2} - \left[(\sqrt{\Upsilon_3} + \sqrt{\Upsilon_3 + \Upsilon_2 + \Upsilon_1})x_c - \sqrt{\Upsilon_3} \right], \quad (10)$$

Utilizing the polynomials and Eq. (10). Hence, we deduce $\tau(x_c)$ and $\tau'(x_c)$ in the following manner:

$$\tau(x_c) = 1 - 2x_c - 2\sqrt{\Upsilon_3}x_c - 2\sqrt{\Upsilon_3 + \Upsilon_2 + \Upsilon_1}x_c + 2\sqrt{\Upsilon_3}, \quad (11)$$

$$\tau'(x_c) = -2 \left[1 + \sqrt{\Upsilon_3} + \sqrt{\Upsilon_3 + \Upsilon_2 + \Upsilon_1} \right]. \quad (12)$$

The expressions for λ_n and λ can be found in Eq. (10) and Eq. (13) of Reference 53.

$$\lambda_n = n^2 + \left[1 + 2\sqrt{\Upsilon_3} + 2\sqrt{\Upsilon_3 + \Upsilon_2 + \Upsilon_1} \right] n, \quad (13)$$

$$\lambda = -\frac{1}{2} - \sqrt{\Upsilon_3} - \sqrt{\Upsilon_3 + \Upsilon_2 + \Upsilon_1} - (\Upsilon_2 + 2\Upsilon_3) - 2\sqrt{\Upsilon_3}\sqrt{\Upsilon_3 + \Upsilon_2 + \Upsilon_1}, \quad (14)$$

Equating Eqs. (13) and (14), and substituting Eq. (5), the energy eigenvalues of the SE for CIQYP are obtained.

$$E_{nl} = \frac{\delta^2 \hbar^2 l(l+1)}{2\mu_a} - d_2 \delta^2 - d_0 \delta - \frac{\delta^2 \hbar^2}{8\mu_a} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu_a d_2}{\hbar^2} - \frac{2\mu_a d_1}{\hbar^2}} \right)^2}{n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2} \right)^2 + \frac{2\mu_a d_2}{\hbar^2} - \frac{2\mu_a d_1}{\hbar^2}}} - \frac{2\mu_a d_0}{\delta \hbar^2} - \frac{4\mu_a d_2}{\hbar^2} + \frac{2\mu_a d_1}{\hbar^2} + l(l+1) \right] \quad (15)$$

The wave function is obtained as

$$R_{nl}(x_c) = N_{nl} x_c \sqrt{\Upsilon_3} (1-x_c)^{\frac{1}{2} + \sqrt{\Upsilon_1 + \Upsilon_2 + \Upsilon_3}} \times P_n^{(2\sqrt{\Upsilon_1}, 2\sqrt{\Upsilon_1 + \Upsilon_2 + \Upsilon_3})} (1-2x_c) \quad (16)$$

Let $S_1 = \sqrt{\Upsilon_3}$
 $S_2 = \sqrt{\Upsilon_1 + \Upsilon_2 + \Upsilon_3}$
 $R_{nl}(x_c) = N_{nl} x_c^{S_1} (1-x_c)^{\frac{1}{2} + S_2} \times P_n^{(2S_1, 2S_2)} (1-2x_c)$
 $x_c = e^{-\delta r_q}$ (17)

The normalization constant condition is:

$$\int_0^\infty R_{nl}(r_q) R_{nl}^*(r_q) dr_q = 1 \quad (18)$$

Utilizing the wave function

$$N_{nl}^2 \int_0^\infty dr_q (e^{-\delta r_q})^{2S_1} (1-e^{-\delta r_q})^{2S_2+1} [P_n^{(2S_1, 2S_2)} (1-2e^{-\delta r_q})]^2 \quad (19)$$

$x_c = e^{-\delta r_q} \in (1, 0)$
 Let $dx_c = -\delta x_c dr_q$

$$dr_q = -\frac{dx_c}{\delta x_c}$$

By changing variable of Eq. (19) We have,

$$\frac{N_{nl}^2}{\delta} \int_0^1 x_c^{2S_1-1} (1-x_c)^{2S_2+1} \times [P_n^{(2S_1, 2S_2)} (1-2x_c)]^2 dx_c \quad (20)$$

The Jacobi function $P_n^{(2S_1, 2S_2)} (1-2x_c)$ given in Refs^{56,57} can be expressed respectively as

$$P_n^{(2S_1, 2S_2)} (1-2x_c) = (-1)^n \Gamma(n+2S_1+1) \Gamma(n+2S_2+1) \times \sum_{j=0}^n \frac{(-1)^j x_c^{n-j} (1-x_c)^j}{j!(n-j)! \Gamma(n+2S_1-j+1)} \times \Gamma(2S_2+j+1) \quad (21)$$

$$P_n^{(2S_1, 2S_2)} (1-2x_c) = \frac{\Gamma(n+2S_2+1)}{\Gamma(n+2S_2+2S_1+1)} \times \sum_{k=0}^n \frac{(-1)^k \Gamma(n+2S_2+2S_1+k+1) x_c^k}{k!(n-k)! \Gamma(2S_1+k+1)} \quad (22)$$

Substituting Eqs. (21) and (22) into Eq. (20) yields

$$(-1)^n \frac{\Gamma[n+2S_1+1]^2 \Gamma(n+2S_2+1)}{\Gamma(2S_1+2S_2+n+1)} \times \sum_{j=0}^n \sum_{k=0}^n \frac{(-j)^{j+k} \Gamma(n+2S_1+2S_2+k+1) \times I_{nl}(j,k)}{j!(n-j)! k!(n-k)! \Gamma(n+2S_1-j-1) \times \Gamma(2S_1+k+1)} \quad (23)$$

where

$$I_{nl}(j, k) = \frac{N_{nl}^2}{\delta} \int_0^1 x_c^{2S_1+n+k-j-1} (1-x_c)^{2S_2+j+1} dx_c \tag{24}$$

Equation 24 can be written in a conventional format as described in references^{56,57}.

$$\int_0^1 x_c^{t-1} (1-x_c)^{-h} dx_c = \frac{{}_2F_1(t, h : t + 1 : 1)}{t} \tag{25}$$

The Hypergeometric function is defined as

$${}_2F_1(t, h : t + 1 : 1) = \frac{\Gamma(t+1)\Gamma(1-h)}{\Gamma(t-h+1)} \tag{26}$$

Using (24) and (25), one obtains

$$I_{nl}(j, k) = \frac{\Gamma(n+2S_1+k-j)(2S_2+j+1)\Gamma(2S_2+j+1)}{(n+2S_1+2S_2+k+1)\Gamma(n+2S_1+2S_2+k+1)} \times \frac{N_{nl}^2}{\delta} \tag{27}$$

Substituting (27) into (23).

The normalization constant is obtained as

$$N_{nl} = \frac{1}{\sqrt{L_{nl}}} \tag{28}$$

where

$$L_{nl} = \frac{(\Gamma(2S_1+n+1))^2 \Gamma(n+2S_2+1)}{\delta \Gamma(n+2S_1+2S_2+1)} (-1)^n \times \sum_{j=0}^n \sum_{k=0}^n \frac{(-1)^{j+k} \Gamma(n+2S_1+k-j)(2S_2+j+1)}{j!(n-j)!k!(n-k)! \Gamma(n+2S_1-j+1) \Gamma(2S_1+k+1)} \times (2S_1+2S_2+n+k+1) \tag{29}$$

The Fourier transform is used to derive the momentum WF in one dimension.

$$R_{nl}(p) = \frac{1}{\sqrt{2\pi}} \int_0^\infty R_{nl}(r_q) e^{-ipr_q} dr_q \tag{30}$$

Using the explicit notation for the Jacobi function (22), Eq. (30) reduces to

$$R_{nl}(p) = \frac{N_{nl}}{\sqrt{2\pi}} \frac{\Gamma(2S_1+n+1)}{\Gamma(2S_1+2S_2+n+1)} \times \sum_{k=0}^n \frac{(-1)^k \Gamma(n+2S_1+2S_2+k+1)}{k!(n-k)! \Gamma(2S_1+k+1)} \times \int_0^\infty (e^{-\delta r_q})^{2S_1+k} (1-e^{-\delta r_q})^{2S_2+\frac{1}{2}} e^{-ipr_q} dr_q \tag{31}$$

The Mathematica 13 software yields the value of $R_{nl}(p)$ as

$$R_{nl}(p) = \frac{N_{nl}}{\sqrt{2\pi}} \times \frac{\Gamma(n+2S_1+1) \Gamma(S_2+\frac{3}{2}) \Gamma(S_1+\frac{ip}{\delta})}{\phi_a \Gamma(2S_1+1) n! \Gamma(S_1+S_2+\frac{3}{2}+\frac{ip}{\delta})} \times P F_q \left[\left(-n, n+2S_1+2S_2+1, S_1+\frac{ip}{\delta} \right), \left(2S_1+1, S_1+S_2+\frac{3}{2}+\frac{ip}{\delta} \right), 1 \right] \tag{32}$$

Mathematica 13 allows users to input equations and expressions in symbolic form. It performs symbolic manipulation, numerical computation, and optimization using Wolfram Language programming.

Expectation values of position (r_q), position square (r_q^2), and momentum square (\hat{p}^2) of r_q , r_q^2 and \hat{p}^2 for the CIQYP and the Heisenberg Uncertainty principle

Expectation value for position

The expression provides the expectation value (EV) of position (r_q) as follows⁵⁸.

$$\langle r_q \rangle_n = \int_0^{\infty} R_{nl} r_q R_{nl} dr_q \quad (33)$$

Expectation value for position square

The expression provides the expectation value of position square (r_q^2) as follows⁵⁸.

$$\langle r_q^2 \rangle_n = \int_0^{\infty} R_{nl} r_q^2 R_{nl} dr_q \quad (34)$$

Expectation value of momentum square

Similarly, the expectation value of momentum square (\hat{p}^2) is represented as⁵⁸.

$$\langle \hat{p}^2 \rangle_n = \int_0^{\infty} R_{nl} \hat{p}^2 R_{nl} dr_q = - \int_0^{\infty} R_{nl}(r) \hbar^2 \frac{d^2}{dr_q^2} R_{nl}^*(r) dr_q \quad (35)$$

The one-dimensional average momentum value $\langle p^2 \rangle$ can also be calculated using integral relationships.

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} R_{nl}(p) p^2 R_{nl}^*(p) dp \quad (36)$$

It is essential to confirm that Eqs. (35) and (36) are equal and in one dimension the expectation value would be zero as a result of symmetry.

Heisenberg Uncertainty

When assessing ground state uncertainty, the uncertainties of position and momentum are evaluated in the following manner:

Uncertainty in position
Applying the relation⁵⁸;

$$\Delta r_q = \sqrt{\langle r_q^2 \rangle - \langle r_q \rangle^2} \quad (37)$$

Uncertainty in momentum
Applying the relation⁵⁸;

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \quad (38)$$

Using the Wolfram Mathematica 13 software program, the expectation values for r_q , r_q^2 , \hat{p}^2 will be determined, along with the associated uncertainties.

The Shannon entropy

Shannon entropy measures the degree of randomness and unpredictability in a particle's spatial location through a logarithmic function. Reference⁵⁹ contains the Shannon entropy calculated in both position and momentum spaces.

$$S_{r_q} = - \int_0^{\infty} \rho(r_q) \ln \rho(r_q) dr_q \quad (39)$$

and

$$S_p = - \int_0^{\infty} \rho(p) \ln \rho(p) dp \quad (40)$$

where S_{r_q} represents the Shannon entropy in position space, while S_p represents the Shannon entropy in momentum space.

Position and momentum space probability densities (PD) are, $\rho(r_q) = |\psi(r_q)|^2$ and $\rho(p) = |R(p)|^2$ respectively. The BBM suggested Shannon entropic uncertainty relation has $S_T = S_{r_q} + S_p \geq D[1 + (\ln\pi)]$, where D is the spatial dimension⁶⁰. All quantum states normalized wave function in momentum space is calculated using the Fourier transform⁶¹.

$$R(p) = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} \psi(r_q) e^{-ipr_q} dr_q \quad (41)$$

The Fisher information

In position and momentum spaces, Fisher information focuses on local probability.

distribution changes. Density functional is essential for studying Fisher information⁶². As stated in reference⁶³,

$$I_{r_q} = \int \frac{|\rho'(r_q)|^2}{\rho(r_q)} dr_q = 4 \int |\psi'(r_q)|^2 dr_q = 4\langle p^2 \rangle - 2(2l+1)|m\rangle\langle r_q^{-2} \rangle \quad (42)$$

$$I_p = \int \frac{|\rho'(p)|^2}{\rho(p)} dp = 4 \int |\psi'(p)|^2 dp = 4\langle r_q^2 \rangle - 2(2l+1)|m\rangle\langle p^{-2} \rangle \quad (43)$$

We use Mathematica 13 software to solve Eqs. (42) and (43) because they are difficult to solve analytically due to the integral's complex form.

Application to diatomic molecules

Diatomic molecules, consisting of just two atoms bonded together, are fundamental building blocks in physics and chemistry. They are essential to everything in our world, from the materials we use to the air we breathe. Recent studies by authors^{64–68} have explored these molecules in greater detail. Our adopted potential can be used to investigate diatomic molecules through setting $d_0 = 2D_e r_e$, $d_1 = -D_e r_e^2$, $d_2 = 0$ of Eq. (1), we have the Kratzer potential⁶⁹ and the energy equation is given as Eq. (44), when $\delta = 0$. The Kratzer potential has become increasingly significant in atomic and molecular physics, as well as in vibrational and rotational spectroscopy⁷⁰. Its importance in molecular physics is substantial and widely recognized.

$$E_{nl} = -\frac{2\mu_\alpha}{\hbar^2} D_e^2 r_e^2 \left[n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 + \frac{2\mu_\alpha D_e r_e^2}{\hbar^2}} \right]^{-2} \quad (44)$$

Results and discussion

The NU method is used to determine the Schrödinger equation eigenstates with the CIQYP in closed form. For any principal quantum number (PQN), the wave function is normalized using the normalization condition and orthogonal functions, such as Jacobi and hypergeometric functions. The one-dimensional Fourier transform is applied to obtain the momentum space wave function. We then analyze Shannon and Fisher information entropies in both position and momentum spaces, along with the expectation values of $\langle r_q \rangle$, $\langle r_q^2 \rangle$, $\langle p^2 \rangle$, and uncertainty relations to assess the localization of a quantum mechanical system.

Tables 1 and 2 demonstrate that as the screening parameter (α) increases, the Shannon entropy in momentum space decreases for the ground and first excited states, while the Shannon entropy in position space increases. This adjustment ensures that the sum meets the BBM inequality, which requires that the lower bound of Shannon entropy be greater than or equal to $(1 + \ln(\pi))$. Shannon entropy measures the overall uncertainty or disorder in a system, reflecting how spread out its possible states are. As the screening parameter increases for the ground and first excited states, Fisher information in position space increases, while Fisher entropies in momentum space decrease, thereby satisfying the inequality relations $I_{r_q} I_p \geq 4$. Fisher information is related to the kinetic energy of a system, where higher Fisher information typically indicates higher kinetic energy. This suggests that the system is more localized and less uncertain, contributing to greater stability. Conversely, lower Fisher information implies a more diffuse state, potentially leading to lower stability. By exploring the interplay between position and momentum Fisher entropies, this study sheds light on a fundamental aspect of the Heisenberg uncertainty principle, which emphasizes the inherent limitations in simultaneously measuring certain conjugate variables (such as position and momentum) with absolute precision. Fisher information measures the sensitivity or precision of a system, indicating how much information can be extracted from small changes. Both entropies are crucial for balancing uncertainty and precision in describing physical systems. Numerical calculations for various expectation values at the ground and first excited states are presented in Table 2, showing a more concentrated distribution for smaller values of the screening parameter. The product of the uncertainties in position and momentum for these states validates the Heisenberg uncertainty relation (HUR)^{71–75}. The HUR asserts that as uncertainty in position increases, uncertainty in momentum decreases, and vice versa. Our results confirm this behavior. The potential model was simplified to the Kratzer potential using specific boundary conditions, ensuring the mathematical precision of our analytical calculations. Spectroscopic

$n_{=0}$	δ	S_{r_q}	S_p	$S_T \geq 2.14473$
	0.01	-0.285132	2.491861	2.206729
	0.02	0.0755000	2.132443	2.887443
	0.03	0.2892130	1.917739	2.206952
	0.04	0.4444960	1.762474	2.206970
	0.05	0.5671890	1.639808	2.206997
	0.06	0.6254311	1.576345	2.201776
	0.07	0.7342100	1.467320	2.201530
	0.10	0.9704820	1.368850	2.273670
$n=1$	0.01	0.1894810	2.695827	2.885308
	0.02	0.5524940	2.332825	2.885319
	0.03	0.7703690	2.114981	2.885350
	0.04	0.9285480	1.956865	2.885413
	0.05	1.0539950	1.831525	2.885520
	0.06	1.2541010	1.732647	2.986748
	0.07	1.3152080	1.693356	3.008564
	0.10	1.4728750	1.414263	2.887138

Table 1. The ground and first excited states of the Shannon entropy values for CIQYP.

$n=0$	δ	I_{r_b}	I_p	$I_{r_b} I_p \geq 4$	$\langle r_b^2 \rangle$	r_q	$\langle p^2 \rangle$	$\Delta p \Delta r_q \geq 0.50$
	0.01	34.71861	0.120755	4.192445	0.421263	0.621311	8.679500	0.553021
	0.02	16.91987	0.247887	4.194215	0.864441	0.890019	4.229689	0.553024
	0.03	11.01348	0.380673	4.192534	1.328041	1.103154	2.753094	0.553033
	0.04	8.072889	0.519415	4.193179	1.811529	1.288400	2.018198	0.553051
	0.05	6.317723	0.664826	4.200186	2.314971	1.456455	1.579153	0.553082
	0.06	5.533879	0.765438	4.235839	2.456363	1.623410	1.324510	0.553145
	0.07	4.765202	0.887462	4.317681	3.564321	1.834215	1.108945	0.553189
	0.10	2.422903	1.849996	4.482361	5.172624	2.176789	0.705726	0.553566
$n=1$	0.01	54.83589	0.141302	7.748420	1.123415	0.999211	13.93149	1.319596
	0.02	26.96296	0.269361	7.262769	2.321883	1.436505	6.740463	1.319584
	0.03	17.43840	0.417279	7.276678	3.589722	1.786148	4.359600	1.319550
	0.04	12.71918	0.570792	7.260006	4.924980	2.092132	3.177295	1.319483
	0.05	9.799187	0.732765	7.180501	6.328248	2.371530	2.472297	1.319367
	0.06	7.787354	0.877995	7.022514	7.432567	2.598345	2.109845	1.319235
	0.07	6.008098	0.932146	6.899746	9.875432	2.754327	1.845624	1.317986
	0.10	3.278714	1.864930	6.114572	14.58355	3.600116	1.069679	1.317489

Table 2. Expectation values of $\langle r_q \rangle$, $\langle r_q^2 \rangle$, $\langle p^2 \rangle$, Fisher Information entropy, and the uncertainty relation for the ground and first excited states for the CIQYP.

Molecules	D_e (eV)	r_e (Å)	μ (amu)
CO	10.84514471	1.1282	6.860586000
I ₂	1.581791863	2.6620	63.45223502

Table 3. Spectroscopic parameters of the selected diatomic molecules⁷⁶.

data for these molecules, sourced from reference⁷⁶, are presented in Table 3. The calculations were performed using the conversions outlined by $1 \text{ amu} = 931.494028 \text{ MeV}/c^2$ and $\hbar = 1973.29 \text{ eV} \text{ \AA}^{77}$. The selection of these diatomic molecules was based on extensive applications and studies conducted by various researchers. We calculate the energy eigenvalues using Eq. (44) and the parameters given in Table 3 for CO and I₂ diatomic molecules. The energy eigenvalues are presented in Table 4 for different n and l quantum numbers and are in good agreement with results obtained previously using different analytical methods^{76,78}. It was observed that for constant n and varying l , the energy increases. This implies that, for a quantum system such as an atom, increasing the orbital angular momentum quantum number (l) at a constant principal quantum number (n)

n	l	I ₂	I ₂ ⁷⁶	CO	CO ⁷⁶
0	0	-1.5790825	-1.579082577	-10.794315	-10.79431532
1	0	-1.5736871	-1.573687151	-10.693839	-10.69383992
	1	-1.5736779	-1.573677925	-10.693371	-10.69337123
2	0	-1.5683193	-1.568319330	-10.594760	-10.59476089
	1	-1.5683101	-1.568310152	-10.594298	-10.59429869
	2	-1.5682917	-1.568291796	-10.593374	-10.59337441
3	0	-1.5629789	-1.562978927	-10.497052	-10.49705246
	1	-1.5629697	-1.562969796	-10.496596	-10.49659664
	2	-1.5629515	-1.562951533	-10.495685	-10.49568512
	3	-1.5629241	-1.562924140	-10.494318	-10.49431814
4	0	-1.5576657	-1.557665755	-10.400689	-10.40068947
	1	-1.5576566	-1.557656670	-10.400239	-10.40023992
	2	-1.5576385	-1.557638501	-10.399340	-10.39934092
	3	-1.5576112	-1.557611248	-10.397992	-10.39799272
	4	-1.5575749	-1.557574911	-10.396195	-10.39619567
5	0	-1.5523796	-1.552379630	-10.305647	-10.30564735
	1	-1.5523705	-1.552370591	-10.305203	-10.30520394
	2	-1.5523525	-1.552352514	-10.304317	-10.30431723
	3	-1.5523253	-1.552325399	-10.302987	-10.30298747
	4	-1.5522892	-1.552289247	-10.301214	-10.30121499
	5	-1.5522440	-1.552244060	-10.299000	-10.29900024

Table 4. Comparison of the bound state Energy (in eV) for the various n and l quantum numbers for a few diatomic molecules at constant n .

Molecule	$\alpha \left(\frac{\text{Å}}{\text{Å}} \right)^{-1}$	μ (amu)
N ₂	2.69860	7.0033500000
O ₂	1.295515	7.9974575040
NO	2.75340	7.4684410000

Table 5. Spectroscopic parameters of the molecules used in this work⁸¹.

leads to higher bound state energy. Higher l values correspond to higher centrifugal barriers, which reduce the effective potential well depth experienced by the particle. As a result, the particle is less tightly bound, leading to higher energy states. In Table 5, we numerically present the eigenvalues of the CIQYP for three diatomic molecules (N₂, O₂, and NO) using the energy equation given in Eq. (15). This was done by inputting the model parameters for each molecule⁷⁹, as shown in Table 6. The results indicate that the bound state energy spectra of these diatomic molecules increase as the various quantum numbers n and l increase. Figure 1a,b display the behavior of the wave function and probability density in position space for various principal quantum numbers, with angular momenta equal to 1 and 2. Figure 1a shows that as the principal quantum number increases, the wave function exhibits a corresponding increase. Figure 1b illustrates how the wave function changes with different potential parameters to meet the BBM conditions. The wave functions display multiple sinusoidal curves representing various quantum states, which intertwine with each other while all other parameters remain constant. The BBM inequality implies a trade-off between the uncertainties in different properties of a system, such as position and momentum. It sets a lower bound on these uncertainties, meaning that as one property becomes more precisely known, the uncertainty in the other increases, and reflecting inherent limitations in the system's precision. Figure 2a, b depict the graphs of the probability density function for $l=1$ and $l=2$. The probability density plots show normal distribution curves with multiple peaks, each representing a distinct quantum state. Figure 2a indicates higher accuracy in predicting particle localization and greater stability in the quantum system. Figure 2(b) displays a probability density with comparable patterns, suggesting that the probability densities for these entropies are concentrated in specific regions. Under ideal conditions, the peak of the probability density plot is expected to rise with an increase in the quantum state, and the wave function typically becomes more complex, with more nodes or oscillations. The plot of the momentum space probability density for $n=0$ with different potential parameters as a function of p is depicted in Fig. 3. The probability density plot follows a spectrally Gaussian distribution, exhibiting quantized curves with varying peaks depending on the optimization parameter. Sinusoidal wave functions representing different quantum states highlight position and momentum uncertainty, consistent with the Heisenberg Uncertainty Principle. Increased uncertainty raises Shannon entropy, while reduced clarity in quantum states lowers Fisher information, demonstrating the trade-off

n		N_2	O_2	NO
0	0	-2.932142	-1.535081	-2.987606
1	0	-2.882584	-1.508025	-2.938646
	1	-2.880808	-1.507290	-2.936923
2	0	-2.839697	-1.483071	-2.896155
	1	-2.838125	-1.482391	-2.894625
	2	-2.834998	-1.481037	-2.891582
3	0	-2.803121	-1.460106	-2.859798
	1	-2.801742	-1.459479	-2.858451
	2	-2.799003	-1.458230	-2.855772
	3	-2.794939	-1.456367	-2.851796
4	0	-2.772524	-1.439024	-2.829262
	1	-2.771330	-1.438448	-2.828089
	2	-2.768958	-1.437299	-2.825758
	3	-2.765443	-1.435586	-2.822300
	4	-2.760837	-1.433321	-2.817763
5	0	-2.747603	-1.419728	-2.804259
	1	-2.746584	-1.419199	-2.803252
	2	-2.744562	-1.418146	-2.801251
	3	-2.741570	-1.416576	-2.798289
	4	-2.737656	-1.414500	-2.794408
	5	-2.732885	-1.411936	-2.789668

Table 6. Energy spectra (in eV) of the class of inversely quadratic potential for

between uncertainty and information in the system. The characteristics of the position and momentum densities align with previous research on one-dimensional systems with various potential functions, as documented in the literature^{80,81}.

Conclusions

In this research, we solve the Schrödinger equation with the CIQYP using the NU technique. With the derived energy equation and normalized wave function, we examine the expectation values of $\langle r_q \rangle$, $\langle r_q^{-2} \rangle$, $\langle p^{-2} \rangle$, as well as the Shannon entropy and Fisher information for position and momentum spaces. The information theory measures, including Shannon entropy and Fisher information, provide an alternate uncertainty relation. A physical system must satisfy the BBM and Stam-Cramer-Rao (SCR) inequalities to be considered physically stable. Our results, as shown in the tables, satisfy the BBM and SCR inequalities, and we theoretically prove that the Heisenberg uncertainty principle is also satisfied. The eigenvalues of the CIQYP for three diatomic molecules (N_2 , O_2 , and NO) are numerically presented, showing that the bound state energy spectra of these diatomic molecules increase as various quantum numbers increase. Additionally, our potential model was simplified to the Kratzer potential through the application of specific boundary conditions, ensuring the mathematical precision of our analytical calculations. The energy eigenvalues obtained for the CO and I_2 diatomic molecules are in excellent agreement with previously obtained results using different analytical methods.

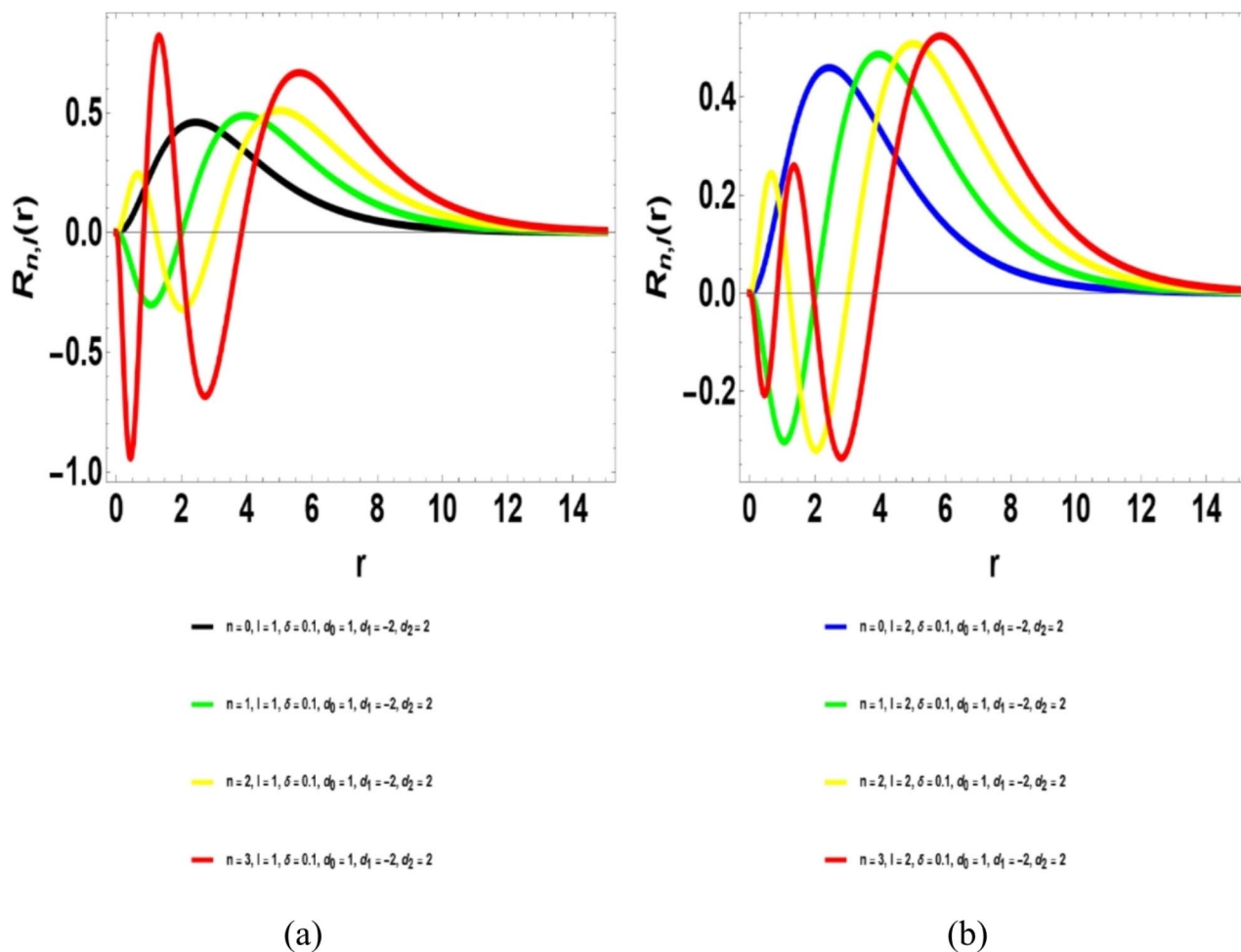


Fig. 1. (a, b): The class of inversely quadratic Yukawa potential wave function as a function of position for various principal quantum numbers at $l=1$ and $l=2$.

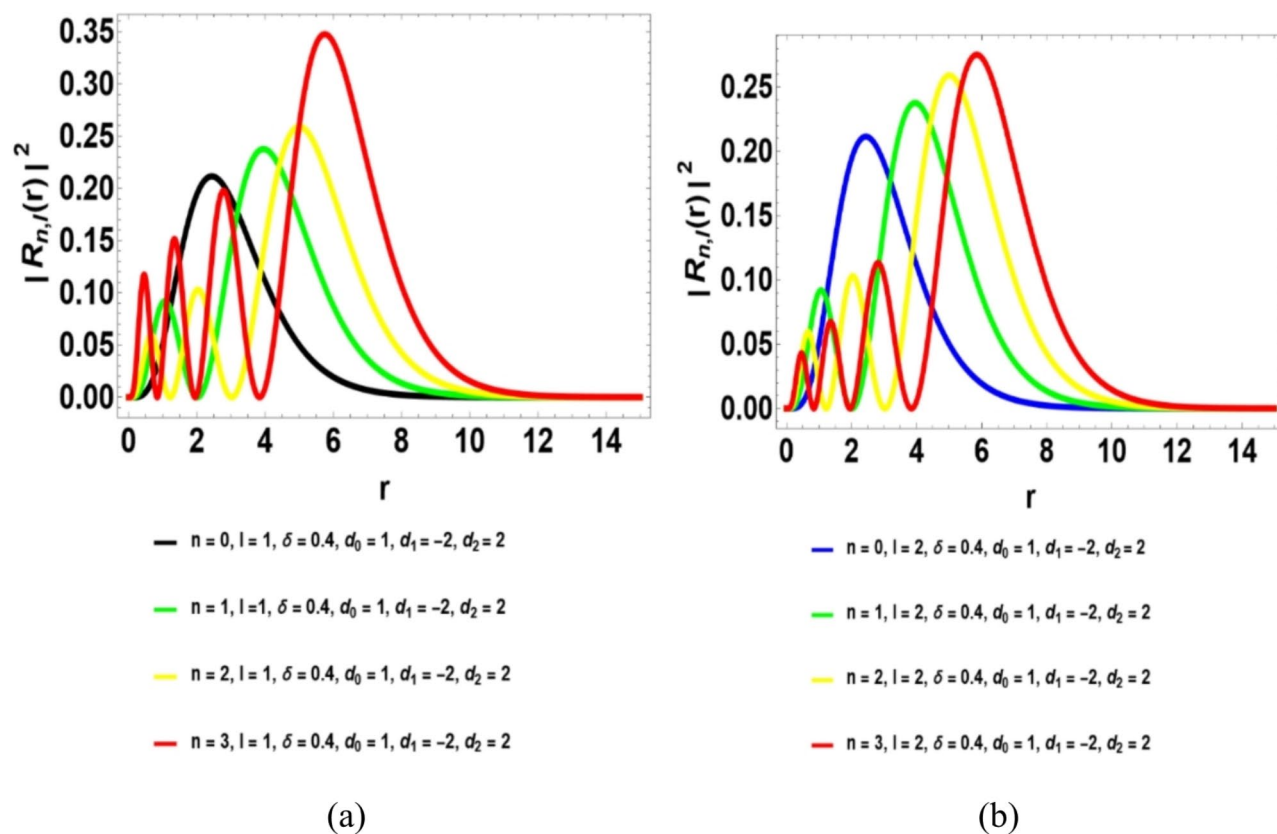


Fig. 2. (a, b): The probability density of the class of inversely quadratic Yukawa potential at $l = 1$ and $l = 2$ as a function of position for various principal quantum numbers.

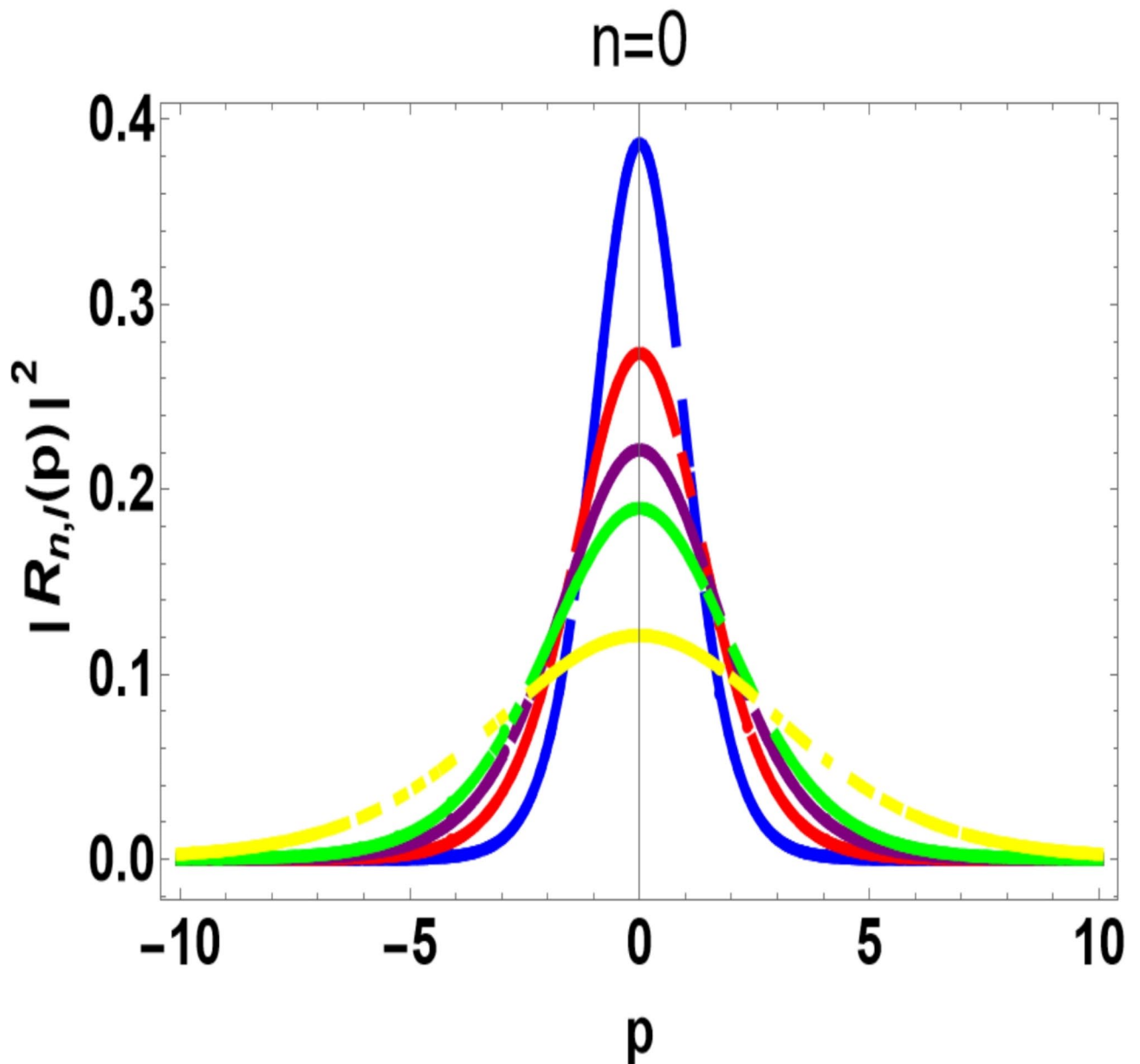


Fig. 3. Momentum space probability density plot for $n=0$.

Data availability

All data generated or analysed during this study are included in this published article.

Appendix A: review of Nikiforov-Uvarov (NU) method

The NU method was proposed by Nikiforov and Uvarov⁵³ to transform Schrödinger-like equations into a second-order differential equation via a coordinate transformation $x_c = x_c(r)$, of the form

$$\psi''(x_c) + \frac{\tilde{\tau}(x_c)}{\sigma(x_c)}\psi'(x_c) + \frac{\tilde{\sigma}(x_c)}{\sigma^2(x_c)}\psi(x_c) = 0 \quad (\text{A1})$$

where $\tilde{\sigma}(x_c)$, and $\sigma(x_c)$ are polynomials, at most second degree and $\tilde{\tau}(x_c)$ is a first-degree polynomial. The exact solution of Eq.(A1) can be obtained by using the transformation.

$$\psi(x_c) = \phi(x_c) y(x_c) \quad (\text{A2})$$

This transformation reduces Eq.(A1) into a hypergeometric-type equation of the form

$$\sigma(x_c) y''(x_c) + \tau(x_c) y'(x_c) + \lambda y(x_c) = 0 \quad (\text{A3})$$

The function $\phi(x_c)$ can be defined as the logarithm derivative

$$\frac{\phi'(x_c)}{\phi(x_c)} = \frac{\pi(x_c)}{\sigma(x_c)} \quad (\text{A4})$$

where $\pi(x_c)$ being at most a first-degree polynomial. The second part of $\psi(x_c)$ in

Eq. (A2) is the hypergeometric function with its polynomial solution given by Rodrigues relation as.

$$y(x_c) = \frac{B_{nl}}{\rho(x_c)} \frac{d^n}{dx_c^n} [\sigma^n(x_c) \rho(x_c)] \quad (\text{A5})$$

where B_{nl} is the normalization constant and $\rho(x_c)$ the weight function which satisfies the condition below;

$$(\sigma(x_c) \rho(x_c))' = \tau(x_c) \rho(x_c) \quad (\text{A6})$$

where also

$$\tau(x_c) = \tilde{\tau}(x_c) + 2\pi(x_c) \quad (\text{A7})$$

For bound solutions, it is required that

$$\tau'(x_c) < 0 \quad (\text{A8})$$

The eigenfunctions and eigenvalues can be obtained using the definition of the following function $\pi(s)$ and parameter λ , respectively:

$$\pi(s) = \frac{\sigma'(s) - \tilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \tilde{\tau}(s)}{2}\right)^2 - \tilde{\sigma}(s) + k\sigma(s)} \quad (\text{A9})$$

and

$$\lambda = k_- + \pi'_-(x_c) \quad (\text{A10})$$

The value of k can be obtained by setting the discriminant in the square root in Eq. (A9) equal to zero. As such, the new eigenvalues equation can be given as

$$\lambda + n\tau'(x_c) + \frac{n(n-1)}{2} \sigma''(x_c) = 0, \quad (n = 0, 1, 2, \dots) \quad (\text{A11})$$

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Author contributions

Inyang E. P., A.E.L. Aouami, and Ali N. formulated the problem, wrote the full manuscript, and presented the results and graphics. Ali N. R., and Endut R. performed computational analysis. Aljunid S.A. progresses by creating the literature, carefully reviewing it, and making essential revisions to the manuscript. All authors have reviewed and endorsed the final manuscript.

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Declarations

Competing interests

The authors declare no competing interests.

Dedication

Dr. Etido P. Inyang respectfully dedicates this research to his late father, who was lead to rest on July 20, 2024.

Additional information

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