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Deformation parameter's effects on quantum information measures

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Abstract
This study explores the influence of deformation parameters on quantum information measures using the q-deformed Hulthén-quadratic exponential-type potential. By solving the Schrödinger equation with the parametric Nikiforov-Uvarov (pNU) method, the energy spectrum and wavefunctions were derived. Quantum information measures, including Shannon entropy and Fisher information, were analyzed for ground states in position and momentum spaces. The results validate the Berkner, Bialynicki-Birula, and Mycieslki, and Stam-Cramér-Rao inequalities, underscoring their consistency with quantum principles. These findings deepen our understanding of deformation effects on quantum systems and offer potential applications in astrophysics and quantum chemistry, advancing the exploration of molecular systems and quantum information theory.

Keywords: Schrödinger equation; parametric Nikiforov-Uvarov method; Energy equation; Information Metrics

1. Introduction

Shannon entropy and Fisher information, which are rooted in foundational contributions to information theory [1], serve as essential metrics in quantum information theory. Their importance has increased notably in recent years due to their broad applications in physics and chemistry [2-4]. In addition to Shannon entropy, global measures such as Tsallis entropy, Rényi entropy, and Onicescu energy [5] play a crucial role in analyzing the uncertainties associated with probability distributions.

The entropic relation in position and momentum spaces, derived by Berkner, Bialynicki-Birula, and Mycieslki, is expressed as $S(\rho)+S(\gamma)\geq D(1+\ln\pi)$ where D represents the spatial dimension [6]. This relation mirrors the Heisenberg uncertainty principle but accommodates higher-order considerations. In these spaces, Shannon entropy characterizes the system's localization and delocalization behavior, while Fisher information, a local measure, captures changes in probability density [7]. For central potentials, Fisher information, expressed in terms of probability density, is validated through the Stam-Cramér-Rao inequalities [8].

Quantum information-theoretic measures have been widely applied in molecular, atomic, and reactive systems. For example, Yamano [9] examined the intrinsic information of solitary wave profiles in nonlinear Schrödinger equations (SE), focusing on Shannon entropy and Fisher information. The study revealed soliton-specific variations, providing novel insights into the structure and dynamics of solitons, emphasizing the utility of these measures in understanding solitary wave behavior. Similarly, Boumali et al. [10] studied the Fisher and Shannon information parameters for the Feshbach-Villars oscillator (FVO), a model describing spin-0 particles. Their research employed the Feshbach-Villars framework, which, unlike the Klein-Gordon equation, provides a positive probability density. This framework enabled them to analyze the sensitivity of probability distributions to changes in system parameters.

Omugbe et al. [11] investigated bound-state solutions of the SE under a deformed hyperbolic potential, exploring correlations between information measures, and system variance. Their study revealed the inverse relationship between these measures, aligning with theoretical predictions and simplifying entropy calculations for complex potentials.

Moreover, Onate et al. [8] extended these investigations by exploring the combined effects of pseudoharmonic and Kratzer potentials via the radial SE. Their supersymmetric and shape-invariance approach demonstrated how potential constants influence energy eigenvalues, expectation values, and Fisher information. Also, Santana-Carrillo et al. [12] studied Shannon entropies in position and momentum spaces within the fractional SE for a hyperbolic double-well potential. They found that decreasing fractional derivative values led to more localized position entropy density, offering insights into fractional quantum systems. Njoku et al. [13] investigated quantum information measures and complexity in the modified Möbius squared plus Eckart (MMSE) potential. Using the parametric Nikiforov-Uvarov (pNU) method, they demonstrated shifts in radial and momentum probability densities influenced by the screening parameter. The study validated several quantum measures, including Shannon entropy, Onicescu energy, Fisher information, and the Heisenberg uncertainty principle. Additionally, Njoku et al. [14] solved the Dirac equation under spin and pseudospin symmetry limits for the inversely quadratic Hellmann potential, advancing the understanding of spinor systems. Finally, Moreira and Ahmed [15] explored topological defects caused by spiral dislocations in a quantum harmonic oscillator. Their analysis of eigenvalues and entropy information revealed the significant impact of defect-induced perturbations on system properties, bridging quantum harmonic systems with broader physical contexts. Despite these advancements, exponential-type potential models remain underexplored, motivating this study. To the best of our knowledge, the q-deformed Hulthén-quadratic exponential-type potential (q-HQP) has not been investigated for quantum information-theoretic measures, which forms the basis of our work.

The potential is defined as follows [16]

$$V(r_z) = -\frac{V_z e^{-\alpha_z r_z}}{1-qe^{-\alpha_z r_z}} + \frac{V_{zz}\left(a_z + b_z e^{-\alpha_z r_z} + c_z e^{-2\alpha_z r_z}\right)}{\left(1-qe^{-\alpha_z r_z}\right)^2} \quad (1)$$

where V_z and V_{zz} are the potential strengths, α_z is the screening parameter, a_z, b_z and c_z are the adjusted parameter and q is the deformation parameter. The q-HQP has significant applications in physics, particularly in quantum mechanics, where it effectively models atomic and molecular interactions with remarkable precision. The inclusion of a deformation parameter provides flexibility for simulating bound-state properties, scattering phenomena, and quarkonium systems [17-20]. This capability enhances the study of energy spectra, thermodynamic properties, and quantum information measures.

This research article focuses on two main objectives. First, the SE is solved for the q-HQP using the pNU method. Second, the effects of the deformation parameter on information metrics, such as Shannon entropy and Fisher information, are thoroughly investigated.

2. The theory

To solve the radial SE for the q-HQP, we express the SE with the radial potential V(r) as follows [21,22]

$$\frac{d^2\psi_{nl}}{dr_z^2} + \left(\frac{2\mu_z}{\hbar^2}E_{nl} - \frac{2\mu_z}{\hbar^2}V(r_z) - \frac{l(l+1)}{r_z^2}\right)\psi_{nl}(r_z) = 0 \quad (2)$$

where l is the angular momentum quantum number, μ_z is the reduced mass , r_z is the particle distance, and $\hbar$ is the reduced Planck constant.

Inserting Eq. (1) into (2) gives

$$\frac{d^2\psi_{nl}}{dr_z^2} + \left(\frac{2\mu_z}{\hbar^2}E_{nl} - \frac{2\mu_z}{\hbar^2}\left(-\frac{V_z e^{-\alpha_z r_z}}{1-qe^{-\alpha_z r_z}} + \frac{V_{zz}\left(a_z + b_z e^{-\alpha_z r_z} + c_z e^{-2\alpha_z r_z}\right)}{\left(1-qe^{-\alpha_z r_z}\right)^2}\right) - \frac{l(l+1)}{r_z^2}\right)\psi_{nl}(r_z) = 0, \quad (3)$$

To address the centrifugal term in Equation (3), the Greene-Aldrich approximation [23, 24] is introduced. This method provides an accurate solution to the centrifugal problem for $\alpha_z << 1,$, resulting in the following expression

$$r_z^{-2} \approx \alpha_z^2 e^{-\alpha_z r_z}\left(1-qe^{-\alpha_z r_z}\right)^{-2}. \quad (4)$$

We perform a convenient change of variables by setting $y_z = e^{-\alpha_z r_z}$ and incorporate this ansatz, along with Equation (4), into Equation (3). After some simplifications, the resulting radial equation takes the Schrödinger form, and we obtain

$$\frac{d^2\psi(y_z)}{dy_z^2} + \frac{1-qy_z}{y_z(1-qy_z)}\frac{d\psi(y_z)}{dy_z} + \frac{1}{y_z^2(1-qy_z)^2}\begin{bmatrix}-\left(\varepsilon_z q^2 + \beta_z q + \delta_{3z}\right)y_z^2 + \\ \left(2\varepsilon_z q + \beta_z - \delta_{2z} - \gamma_z\right)y_z - \left(\varepsilon_z + \delta_{1z}\right)\end{bmatrix}\psi(y_z) = 0, \quad (5)$$

where

$$\left.\begin{aligned} -\varepsilon_z &= \frac{2\mu_z E_{nl}}{\alpha_z^2\hbar^2}, \\ \beta_z &= \frac{2\mu_z V_z}{\alpha_z^2\hbar^2}, \quad \delta_{1z} = \frac{2\mu_z a_z V_{zz}}{\alpha_z^2\hbar^2}, \\ \delta_{2z} &= \frac{2\mu_z b_z V_{zz}}{\alpha_z^2\hbar^2}, \\ \delta_{3z} &= \frac{2\mu_z c_z V_{zz}}{\alpha_z^2\hbar^2}, \quad \gamma_z = l(l+1) \end{aligned}\right\}. \quad (6)$$

Tezcan and Sever [25] showed that the pNU method allows for the straightforward derivation of both the energy equation and the wave function. The pNU method is particularly effective due to its simplicity and has provided more accurate solutions for wave equations involving various potential energy functions. According to these authors, the standard equation is expressed as

$$\psi''(s)+\frac{(x_1-x_2 s)}{s(1-x_3 s)}\psi'(s)+\frac{1}{s^2(1-x_3 s)^2}\left[-p_0 s^2+p_1 s-p_2\right]\psi(s)=0 \tag{7}$$

By applying Eq. (7), the authors derived the condition for the energy equation along with the associated wave function as

$$x_2 n-(2n+1)x_5+\left[2x_8+n(n+1)\right]x_3+x_7+(2n+1)\sqrt{x_9}+\sqrt{x_8}\left[2\sqrt{x_9}+x_3(2n+1)\right]=0 \tag{8}$$

$$\psi(s)=N_{nl}s^{x_{12}}(1-x_3 s)^{-x_{12}-\frac{x_{13}}{x_3}}p_n^{\left(x_{10}-1,\frac{x_{11}}{x_3}-x_{10}-1\right)}(1-2x_3 s) \tag{9}$$

The values of the parametric constants in Eqs. (8) and (9) are calculated as follows

$$\left.\begin{aligned}
&x_1=x_2=x_3=1, x_4=0.5(1-x_1), x_5=0.5(x_2-2x_3),\\
&x_6=x_5^2+p_0, x_7=2x_4x_5-p_1,\\
&x_8=x_4^2+p_2, x_9=x_3(x_7+x_3x_8)+x_6,\\
&x_{10}=x_1+2x_4+2\sqrt{x_8},\\
&x_{11}=x_2-2x_5+2\left(\sqrt{x_9}+x_3\sqrt{x_8}\right),\\
&x_{12}=x_4+\sqrt{x_8},\\
&x_{13}=x_5-\left(\sqrt{x_9}+x_3\sqrt{x_8}\right)
\end{aligned}\right\} \tag{10}$$

Upon Matching Eq. (5) with Eq. (7), the parametric constants in Eq. (10) take the form

$$\left.\begin{aligned}
&p_0=\varepsilon_z q^2+\beta_z q+\delta_{3z}\\
&p_1=2\varepsilon_z q+\beta_z-\delta_{2z}-\gamma_z\\
&p_2=\varepsilon_z+\delta_{1z}\\
&\text{and}\\
&x_1=1, x_2=x_3=q, x_4=0, x_5=-0.5q,\\
&x_6=\frac{q^2}{4}+\varepsilon_z q^2+\beta_z q+\delta_{3z},\\
&x_7=-2\varepsilon_z q-\beta_z+\delta_{2z}+\gamma_z\\
&x_8=\varepsilon_z+\delta_{1z},\\
&x_9=\frac{q^2}{4}+\delta_{2z}q+\gamma_z q+\delta_{1z}q^2+\delta_{3z},\\
&x_{10}=1+2\sqrt{\varepsilon_z+\delta_{1z}},\\
&x_{11}=2\left[q+\left(\sqrt{\frac{q^2}{4}+\delta_{2z}q+\gamma_z q+\delta_{1z}q^2+\delta_{3z}}+q\sqrt{\varepsilon_z+\delta_{1z}}\right)\right],\\
&x_{12}=\sqrt{\varepsilon_z+\delta_{1z}},\\
&x_{13}=-\frac{q}{2}-\left(\sqrt{\frac{q^2}{4}+\delta_{2z}q+\gamma_z q+\delta_{1z}q^2+\delta_{3z}}+q\sqrt{\varepsilon_z+\delta_{1z}}\right)
\end{aligned}\right\} \tag{11}$$

By inserting Eqs. (6) and (11) into Eqs. (8) and (9), respectively, the energy eigenvalue and its associated wave function are obtained as follows

$$E_{nl}=V_z a_z-\frac{\alpha_z^2\hbar^2}{8\mu_z}\left[\frac{\left(n+\frac{1}{2}+\sqrt{\frac{1}{4}-\frac{2\mu_z b_z V_{zz}}{q\alpha_z^2\hbar^2}+\frac{l(l+1)}{q}+\frac{2\mu_z V_{zz}a_z}{\alpha_z^2\hbar^2}-\frac{2\mu_z c_z V_{zz}}{q^2\alpha_z^2\hbar^2}}\right)^2+\frac{2\mu_z c_z V_{zz}}{q^2\alpha_z^2\hbar^2}+\frac{2\mu_z a_z V_{zz}}{\hbar^2\alpha_z^2}-\frac{2\mu_z V_z}{q\hbar^2\alpha_z^2}}{n+\frac{1}{2}+\sqrt{\frac{1}{4}-\frac{2\mu_z b_z V_{zz}}{q\alpha_z^2\hbar^2}+\frac{l(l+1)}{q}+\frac{2\mu_z V_{zz}a_z}{\alpha_z^2\hbar^2}-\frac{2\mu_z c_z V_{zz}}{q^2\alpha_z^2\hbar^2}}}\right]^2. \tag{12}$$

The wave function is obtain as;

$$\psi(s)=N_{nl}s^{\sqrt{\varepsilon_z+\delta_{1z}}}(1-s)^{\frac{1}{2}+\frac{1}{2}\left(\sqrt{\frac{1}{4}-\frac{\delta_{2z}}{q}+\frac{\gamma_z}{q}+\delta_{1z}-\frac{\delta_{3z}}{q^2}}\right)} \\ p_n^{\left(2\sqrt{\varepsilon_z+\delta_{1z}},\left(2\sqrt{\frac{1}{4}-\frac{\delta_{2z}}{q}+\frac{\gamma_z}{q}+\delta_{1z}-\frac{\delta_{3z}}{q^2}}\right)\right)}(1-2s) \tag{13}$$

where N_{nl} is normalization constant and can be evaluated using Eq.(14)

$$\int_0^\infty |\psi_{nl}(r_z)|^2\, dr_z = 1 \tag{14}$$

3. Shannon entropy

The Shannon entropy, representing logarithmic probability density, offers insights into a system's probability distribution [1]

$$S(\rho)=-\int \rho(r_z)\ln\rho(r_z)dr_z \tag{15}$$

,

and

$$S(\gamma)=-\int \gamma(p)\ln\gamma(p)dp\,, \tag{16}$$

In this context, $S(\rho)$ refers to the Shannon entropy in position space, and $S(\gamma)$ represent the Shannon entropy in momentum space. Equations (17) and (18) describe the probability densities (PD) in the position and momentum spaces, respectively

$$\rho(r_z)=|\psi(r_z)|^2 \tag{17}$$

and

$$\gamma(p)=|\psi(p)|^2 \tag{18}$$

$\psi(p)$ represents the wave function in momentum space, which is derived by applying the Fourier transform (FT) to $\psi(r_z)$. The concept was explored by Berkner, Bialynicki-Birula, and Mycieslki (BBM) [6], who established the connection between momentum and position spaces as $D(1+\ln\pi)\geq S(\rho)+S(\gamma)$, with D representing the number of spatial dimensions.

4. Fisher information

In contrast, Fisher Information is a local measure of information entropy, factoring in differential components that make it sensitive to local variations in probability density. Recognized as a fundamental measure of information entropy, it is vital in determining the localization of probability densities. Additionally, Fisher information can be viewed as a measure of the oscillator's degree, relevant in quantum mechanical kinetic energy calculations. It is expressed in both position and momentum spaces as [7]

$$I(\rho)=\int \frac{|\nabla\rho_{nl}(r_z)|^2}{\rho_{nl}(r_z)}dr_z \tag{19}$$

$$I(\gamma)=\int \frac{|\nabla\rho_{nl}(p)|^2}{\rho_{nl}(p)}dp\,. \tag{20}$$

In Fisher information theory, higher Fisher information indicates better precision in predicting the system's localization, leading to increased fluctuations. For any central potential model with an arbitrary angular momentum quantum number, the product of Fisher information in both position and momentum spaces must comply with the Stam-Cramér-Rao inequality $I(\rho)I(\gamma)\geq 4$ [4,5,8].

We use Mathematica 13 software to solve Equations (19) and (20) because they are difficult to solve analytically due to the integral's complex form.

5. Results and Discussion

This study explores the approximate analytical solutions of the Schrödinger equation using the q-HQP. By applying Equations (15) and (16), the Shannon entropies in both position and momentum spaces are calculated, confirming the validity of the BBM uncertainty relation as presented in Table 1. A key implication of the BBM inequality is its establishment of a lower bound for the sum of Shannon entropies, reinforcing the quantum uncertainty principles that govern molecular behavior. Table 2 presents the numerical calculation of Fisher information in position and momentum spaces for various values of the deformation parameter (q = 10, 20, 30, 40, 50, 60, 70, 80, 90, and 100), using Eqs. (19) and (20). The findings confirm the satisfaction of the Stam-Cramér-Rao inequality, illustrating the inverse relationship between Fisher information in both spaces. This alignment underscores the quantum mechanical constraints that govern these systems, offering a deeper understanding of how the strength of deformation affects the distribution of information in position and momentum spaces. Figures 1(a) and 1(b) explore the behavior of Shannon entropy as a function of the screening parameter α in both position and momentum spaces, respectively. As α increases, Shannon entropy increases in position space, while simultaneously decreasing in momentum space. This inverse relationship between entropies in the two spaces reflects the uncertainty principle, where a decrease in uncertainty (or entropy) in one space results in an increase in the other. An increase in the screening parameter α leads to a rise in position-space entropy and a corresponding decline in momentum-space entropy. This behavior highlights the quantum mechanical uncertainty principle, with Shannon entropy serving as a measure of uncertainty in the system. The decrease in momentum-space entropy, shown in figure 1(b), reflects greater uncertainty in momentum. Figures 2(a) and 2(b) analyze variations in Fisher information with respect to α. In both position and momentum spaces, Fisher information exhibits increasing and decreasing trends, respectively, as α increase. Fisher information, which measures the sensitivity of a system to parameter changes, suggests that the system becomes more responsive to changes in α. In figure 2(b), the increasing trend in Fisher information reveals the system's heightened sensitivity to parameter variations, while in figure 2(a), the decreasing Fisher information suggests reduced sensitivity to these changes. Figures 3(a) and 3(b) illustrate the wave function and probability density in position space across various deformation parameters. In figure 3(a), the wave function exhibits an increase in amplitude and complexity for various deformation parameters, with multiple sinusoidal patterns representing distinct quantum states. This behavior reflects the quantum mechanical principle of wave function evolution with increasing energy levels. Figure 3(b) shows the probability density for various deformation parameters, displaying normal distribution curves with multiple peaks that correspond to distinct quantum states. These peaks reflect improved precision in predicting particle localization and suggest increased stability within the quantum system.

6. Conclusions

This study explores the influence of deformation parameters on quantum information measures, such as Shannon entropy and Fisher information, within the framework of the q-HQP. By solving the Schrödinger equation using the pNU method, energy eigenvalues and wavefunctions were determined. For ground states, Shannon entropy and Fisher information were calculated in both position and momentum representations. The findings validate the BBM inequality for Shannon entropy and the Stam-Cramér-Rao inequality for Fisher information, consistent with fundamental quantum mechanical principles. These results provide valuable insights, with potential applications in fields like astrophysics and quantum chemistry.

AVAILABILITY OF DATA AND MATERIALS

All data generated during this study are fully referenced within the paper.

COMPETING INTERESTS

The author declares no conflicts of interest.

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Author contribution:

E.P.I prepared the original draft and validated the results.

Table 1: Shannon entropy for the various deformation parameters in ground state $a_z = 0.009, b_z = 0.1, c_z = -0.1, \mu_z = \hbar = 1, \alpha_z = 0.1, V_{zz} = 19.9, V_z = -0.001$

q	S_γ	S_p	$S_T \geq 2.14473$
10	1.91856	0.44885	2.36741
20	1.92361	0.33608	2.25969
30	1.95664	0.29196	2.24860
40	1.97077	0.27345	2.24422
50	1.97874	0.26311	2.24185
60	1.98389	0.25649	2.24038
70	1.98749	0.25187	2.23936
80	1.99016	0.24847	2.23863
90	1.99221	0.24585	2.23806
100	1.99384	0.24378	2.23762

Table 2: Fisher information for the various deformation parameters in ground state $a_z = 0.009, b_z = 0.1, c_z = -0.1, \mu_z = \hbar = 1, \alpha_z = 0.1, V_{zz} = 19.9, V_z = -0.001$

q	I_γ	I_p	$I_\gamma I_p \geq 4$
10	0.30413	13.18549	4.01391
20	0.30306	13.19501	4.00077
30	0.30296	13.21285	4.00051
40	0.29790	13.69283	4.08684
50	0.29209	13.75304	4.01014
60	0.27992	14.36422	4.01868
70	0.26304	15.28201	4.01865
80	0.24136	16.66674	4.01906
90	0.21519	18.71638	4.02793
100	0.20638	19.54378	4.02856

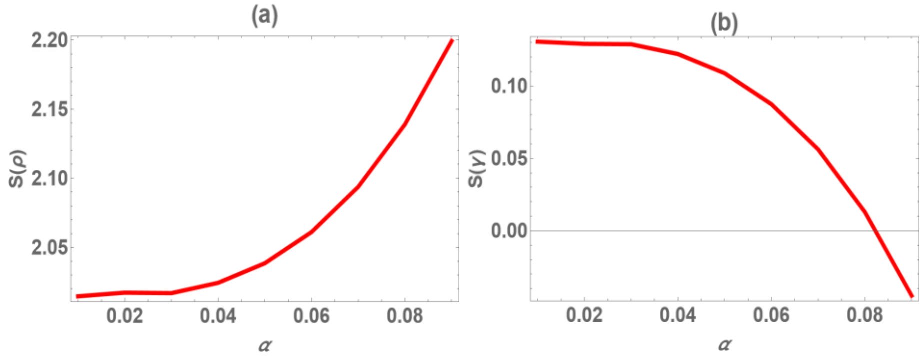


Figure 1(a, b). Variations of Shannon entropies with α parameter

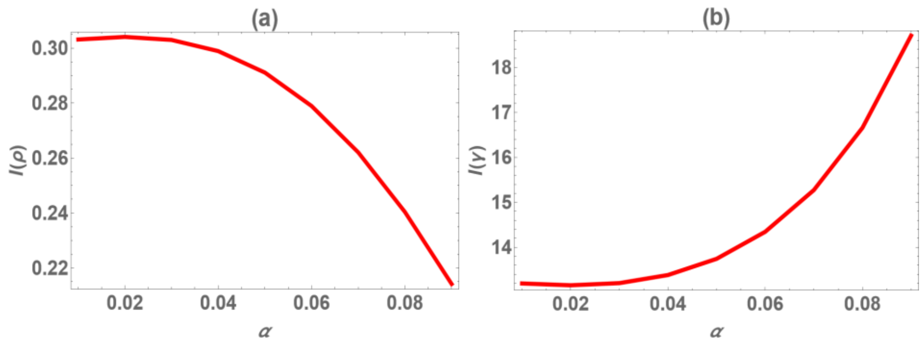
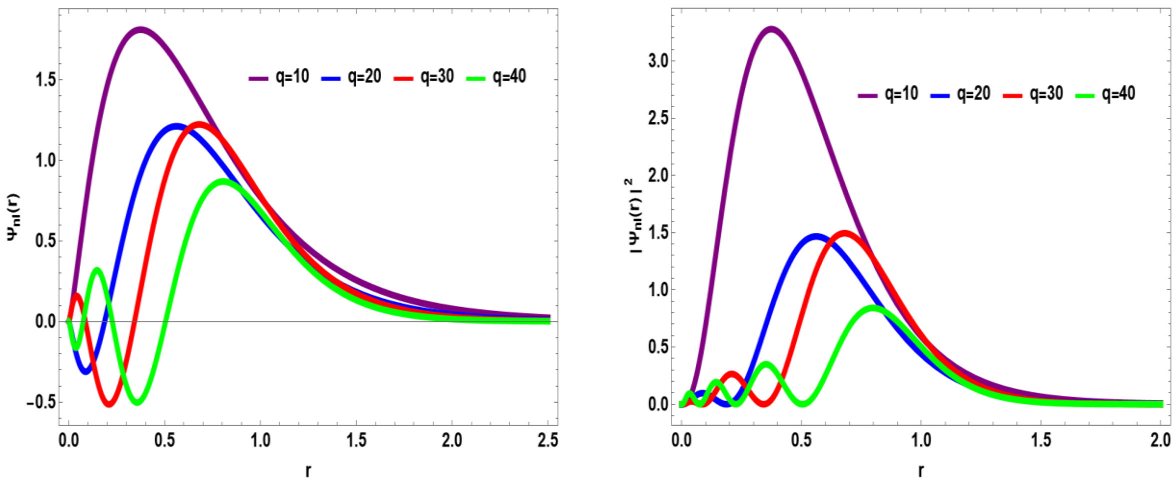


Figure 2 (a,b). Variations of Fisher information with α parameter



(a) (b)

Figure 3 (a,b). The wave function and probability density in position space for different values of the deformation parameter.

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