Nonrelativistic Shannon information entropy for Kratzer potential

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The Shannon information entropy is investigated within the nonrelativistic framework. The Kratzer potential is considered as the interaction and the problem is solved in a quasi-exact analytical manner to discuss the ground and first excited states. Some interesting features of the information entropy densities as well as the probability densities are demonstrated. The Bialynicki–Birula–Mycielski inequality is also tested and found to hold for these cases.

Keywords: Schrödinger equation, Kratzer potential, Shannon entropy

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1. Introduction

Interest in the study of wave equations of quantum mechanics has been considerably renewed due to their notable applications in measurement and information technologies. In particular, the entropic uncertainty relations, which provide alternatives to the ordinary Heisenberg uncertainty relation, have been investigated.[1–39] Within the proposed entropies, the Shannon entropy possesses interesting features and is quite an appealing theoretical framework.[1–3] The BBM entropic uncertainty relation, named after Beckner, Bialynicki–Birula, and Mycielski (see, Ref. [4]) is given by

$$S_\rho + S_\gamma \geqslant D\,(1+\log\pi)\,, \tag{1}$$

where D represents the spatial dimension and the position (S_ρ) and momentum (S_γ) information entropies are defined,[40,41] respectively, by

$$\begin{aligned} S_\rho &= -\int |\Psi(\boldsymbol{r})|^2 \log|\Psi(\boldsymbol{r})|^2 \,\mathrm{d}\,\boldsymbol{r}, \\ S_\gamma &= -\int |\Psi(\boldsymbol{p})|^2 \log|\Psi(\boldsymbol{p})|^2 \,\mathrm{d}\,\boldsymbol{p} \end{aligned} \tag{2}$$

with $\Psi(\boldsymbol{r})$ being the normalized eigenfunction in a spatial coordinate and $\Psi(\boldsymbol{p})$ denoting its normalized Fourier transform.

The Shannon entropy has been studied for some quantum systems with exact analytical solutions. Sun *et al.*[42] applied Shannon information entropies to a position-dependent mass Schrödinger problem with a hyperbolic well. They calculated the position and momentum information entropies for six low-lying states. Some interesting features of the information entropy densities were demonstrated and the BBM inequality was also tested.[42] Yáñez-Navarro *et al.* have studied quantum information entropies for position-dependent-mass Schrödinger problems and have demonstrated the behaviors of the position and momentum information entropies. They showed the negative Shannon entropy exits for the probability densities that are highly localized and proved that the mass barrier determines the stability of the system.[43] Rudnicki *et al.* studied the Shannon entropy-based uncertainty relation for D-dimensional central potentials and found that the resulting lower bound does not depend on the specific form of the potential since it only depends on the hyperangular quantum numbers.[44] Song *et al.* studied the Shannon information entropy for an infinite circular well and tested the validity of the BBM inequality.[45] Sun *et al.* studied the Shannon information entropy for a hyperbolic double-well potential and calculated the position and momentum information entropies for the lowest-lying states $n = 1, 2$. They also observed that the position information entropy decreases with an increase in the potential strength but the momentum entropy is contrary to the position entropy. They checked the validity of BBM inequality as well.[46] The particle in a symmetrical squared tangent potential and its Shannon information entropy were well analyzed in Ref. [47]. Massen applied Shannon information entropies in position and momentum space to various s–p and s–d shell nuclei using a correlated one-body density matrix and proposed a method to determine the correlation.[48] Lin *et al.* used Shannon entropy to probe the nature of correlation effects. In addition, they considered the concept in connection with helium-like systems including positronium negative ion, hydrogen negative ion, helium and lithium positive ion.[49] Dehesa *et al.* explicitly obtained the information entropy for a harmonic oscillator and the hydrogen atom in D dimensions. They showed how these entropies are related to entropies involving polynomials.[50] Dehesa *et al.* studied the spreading of the quantum-mechanical probability cloud for the ground-state of the Morse and modified Pöschl-Teller potentials by

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means of global and local information-theoretic measures.[51]

On the other hand the Kratzer potential is amongst the most attractive physical potentials as it contains an inverse square term besides the common Coulomb term which has well accounted for some observed phenomena in atomic, molecular and chemical physics.[52–58] Before focusing on our work, we wish to address the interesting papers[59–68] which discuss various aspects of the field.

The present article is organized as follows. In the next section, we give the quasi-exact solutions of the nonrelativistic Kratzer potential. In the third section, we first derive the wave functions in momentum space via the Fourier transform and then report the position and momentum information entropy densities, $\rho_{\rm s}(\boldsymbol{r})$ and $\gamma_{\rm s}(\boldsymbol{p})$, respectively. The (radial) probability densities $\rho(\boldsymbol{r})$ and $\gamma(\boldsymbol{p})$ are also discussed. We calculate S_ρ and S_γ for the low-lying one state $n=1$ and the BBM inequality is shown to hold for these cases. Some concluding remarks are given in the last section.

2. Quasi-exact solutions of the Kratzer poential

For an arbitrary external potential $V(r)$, the Schrödinger equation in spherical coordinates is written as

$$\left\{-\frac{\hbar^2}{2\mu}\nabla^2+V(r)\right\}\Psi(r,\theta,\phi)=E\,\Psi(r,\theta,\phi). \tag{3}$$

The standard separation of variables is implemented via

$$\Psi_{n,\ell,\mu}(r,\theta,\phi)=R_{n,\ell}(r)\,\mathrm{Y}_{\ell,\mu}(\theta,\phi). \tag{4}$$

Introducing the Kratzer potential

$$V(r)=\frac{a}{r}+\frac{b}{r^2}+\frac{c}{r^3}+\frac{d}{r^4}, \tag{5}$$

the Schrödinger equation is transformed into the following form:

$$\left\{-\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2\frac{\mathrm{d}}{\mathrm{d}r})+\frac{a}{r}+\frac{b}{r^2}+\frac{c}{r^3}+\frac{d}{r^4}+\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}\right\}R_{n,\ell}(r)=E\,R_{n,\ell}(r). \tag{6}$$

The transformation

$$R_{n,\ell}(r)=\frac{\phi_{n,\ell}(r)}{r} \tag{7}$$

removes the first order derivative and changes the radial equation into

$$\left\{\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{2\mu}{\hbar^2}\left[E-\frac{a}{r}-\frac{b}{r^2}-\frac{c}{r^3}-\frac{d}{r^4}\right]-\frac{\ell(\ell+1)}{r^2}\right\}\phi_{n,\ell}(r)=0. \tag{8}$$

Let

$$\varepsilon=\frac{2\mu E}{\hbar^2},\ A=\frac{2\mu a}{\hbar^2},\ B=\frac{2\mu b}{\hbar^2},\ C=\frac{2\mu c}{\hbar^2},\ D=\frac{2\mu d}{\hbar^2}, \tag{9}$$

then equation (8) will be written more neatly as ($\hbar=\mu=1$)

$$\left\{\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\varepsilon-\frac{A}{r}-\frac{B}{r^2}-\frac{C}{r^3}-\frac{D}{r^4}-\frac{\ell(\ell+1)}{r^2}\right\}\phi_{n,\ell}(r)=0, \tag{10}$$

or via

$$\ell'=-\frac{1}{2}+\sqrt{\left(\ell+\frac{1}{2}\right)^2+B} \tag{11}$$

because

$$\left\{\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\varepsilon-\frac{A}{r}-\frac{\ell'(\ell'+1)}{r^2}-\frac{C}{r^3}-\frac{D}{r^4}\right\}\phi_{n,\ell'}(r)=0. \tag{12}$$

The analogue of this problem has been analyzed by Dong.[69] We choose[69]

$$\phi_{n,\ell'}(r)=f_n(r)\,\mathrm{e}^{g(r)}, \tag{13a}$$

where

$$f_n(r)=\begin{cases}1, & n=0,\\ \prod\limits_{i=1}^{n}(r-\alpha_i^n), & n=1,2,3,\ldots,\end{cases}$$
$$g(r)=\alpha r+\beta\log r+\frac{\gamma}{r},\quad \alpha<0\quad \gamma<0. \tag{13b}$$

Substitution into the proposed ansatz yields

$$\phi''(r)=f(r)\,\mathrm{e}^{g(r)}\left[g''(r)+\left(g'(r)\right)^2+\frac{f''(r)+2f'(r)\,g'(r)}{f(r)}\right]. \tag{14}$$

For $n=0$, we obtain

$$-\frac{\beta}{r^2}+\frac{2\gamma}{r^3}+\alpha^2+\frac{\beta^2}{r^2}+\frac{\gamma^2}{r^4}+\frac{2\alpha\beta}{r}-\frac{2\alpha\gamma}{r^2}-\frac{2\beta\gamma}{r^3}+\varepsilon-\frac{A}{r}-\frac{\ell'(\ell'+1)}{r^2}-\frac{C}{r^3}-\frac{D}{r^4}=0. \tag{15}$$

Comparing Eq. (15) with Eq. (12), and equating the corresponding powers on both sides, we can have the following equation set

$$2\alpha\beta-A=0,\quad -\beta+\beta^2-2\alpha\gamma-\ell'\left(\ell'+1\right)=0,\quad 2\gamma-2\beta\gamma-C=0,\quad \gamma^2-D=0,\quad \alpha^2+\varepsilon=0. \tag{16}$$

Therefore, we find restrictions on potential parameters as

$$\alpha = -\sqrt{-\varepsilon}, \quad \alpha \leqslant 0;$$
$$\beta = -\frac{A}{2\sqrt{-\varepsilon}}; \quad \gamma = -\sqrt{D}, \quad \gamma \leqslant 0. \tag{17}$$

From Eq. (16), the energy eigenvalue for $n = 0$ is given as follows:

$$E = \frac{A^2 D}{2\left(2\sqrt{D} - C\right)^2}. \tag{18}$$

By using α, β, and γ, the ground-state radial wave function is given as

$$R_{0,\ell'}(r) = N_{0,\ell'} r^{\beta-1} \mathrm{e}^{\alpha r + \gamma/r}. \tag{19}$$

Therefore the total wavefunction appears in the form

$$\Psi(\boldsymbol{r}) = N_{0,\ell'} r^{\beta-1} \mathrm{e}^{\alpha r + \gamma/r} \mathrm{Y}_{\ell',\mu}(\theta,\phi), \tag{20}$$

where $N_{0,\ell'}$ is the normalization constant. For $n = 1$, we obtain

$$\alpha = -\sqrt{-\varepsilon}, \ \alpha \leqslant 0; \ \beta = \frac{2\sqrt{D} + C}{2\sqrt{D}}; \ \gamma = -\sqrt{D}, \ \gamma \leqslant 0. \tag{21}$$

The wave function takes the following form

$$\Psi(\boldsymbol{r}) = N_{1\ell'}(r - \alpha_1^1) r^{[(2\sqrt{D}+C)/2\sqrt{D}]-1} \times \mathrm{e}^{-\sqrt{-\varepsilon}r - \sqrt{D}/r} \mathrm{Y}_{\ell',\mu}(\theta,\phi). \tag{22}$$

3. Information entropy

The position and momentum space information entropies for three-dimensional potentials can be calculated using Eq. (2). In general, explicit derivations of the information entropy are quite difficult. In particular the derivation of analytical expression for the S_ρ is almost impossible as shown in Refs. [43]–[48] To obtain the information entropy in momentum space, one needs to often use an integral transform, namely the Fourier transform in our case. We represent the position and momentum information entropy densities respectively for $c = 0$ and $d = 0$ by

$$\rho_{\mathrm{s}}(\boldsymbol{r}) = |\Psi(\boldsymbol{r})|^2 \log |\Psi(\boldsymbol{r})|^2$$

and

$$\gamma(\boldsymbol{p}) = |\Psi(\boldsymbol{p})|^2 \log |\Psi(\boldsymbol{p})|^2,$$

since they play a similar role to the probability density $\rho(\boldsymbol{r}) = |\Psi(\boldsymbol{r})|^2$ in quantum mechanics.[50–58,70]

Owing to the difficulty in calculating wave functions in momentum space, we only consider the lowest states $n = 1$. For simplicity, we study the $n = 1$ case in more detail. For the Fourier transform of $n = 1$ we only list the main results in Table 1. We can derive the corresponding representation of $\ell' = 0$ case through the Fourier transform[71]

$$\Psi(\boldsymbol{p}) = \frac{(2p_0)^{5/2}}{\sqrt{8}(p^2 + p_0^2)^2} \mathrm{Y}_{0,0}, \tag{23}$$

with the position and momentum probability density, respectively, being

$$\rho(\boldsymbol{r}) = |\Psi(\boldsymbol{r})|^2 = \varepsilon^6 \mathrm{e}^{-2\varepsilon r} |\mathrm{Y}_{0,0}|^2, \tag{24}$$
$$\gamma(\boldsymbol{p}) = |\Psi(\boldsymbol{p})|^2 = \frac{4p_0^5}{(p^2 + p_0^2)^4} |\mathrm{Y}_{0,0}|^2. \tag{25}$$

Now we derive their position and momentum information entropy S_ρ and S_γ by discussing their analytical expressions. Characteristic features of the position and momentum information entropies $\rho_{\mathrm{s}}(\boldsymbol{r})$ and $\gamma_{\mathrm{s}}(\boldsymbol{p})$ are shown in Figs. 1 and 2 for the lowest state $\ell' = 0$ and three different values of parameter a. The probability densities $\rho(\boldsymbol{r})$ and $\gamma(\boldsymbol{p})$ are shown in Figs. 3 and 4. We find that $\gamma(\boldsymbol{p})$ first decreases and then increases to zero with the increase of momentum which implies the local behavior of the momentum. In addition, we find that the maxima of $\rho_{\mathrm{s}}(\boldsymbol{r})$ and $\rho(\boldsymbol{r})$ increase with the increase of parameter a, which is closely related to the energy of the system. However, the behavior of the maximum amplitude of the $|\gamma_{\mathrm{s}}(\boldsymbol{p})|$ is contrary to that of $\rho_{\mathrm{s}}(\boldsymbol{r})$.

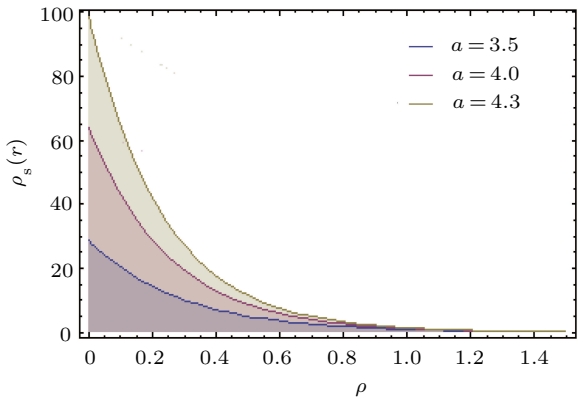


Fig. 1. (color online) Plots of the position space entropy densities for $n = 1$.

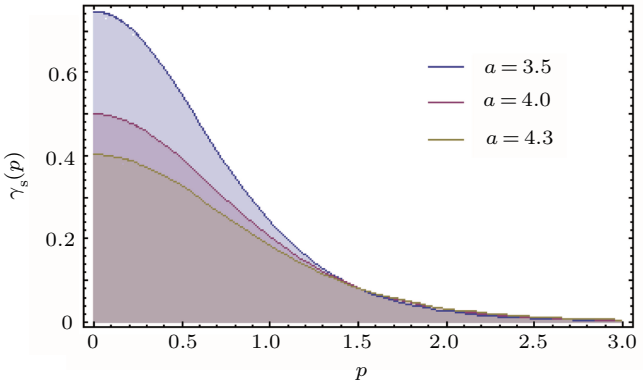


Fig. 2. (color online) Plots of the momentum space entropy densities for $n = 1$.

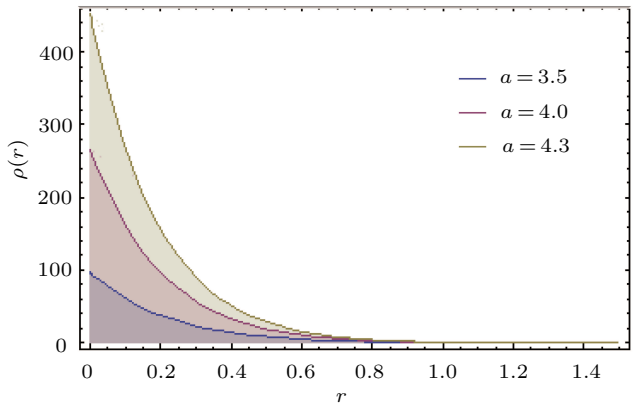


Fig. 3. (color online) Plots of the position space probability density for $n=1$.

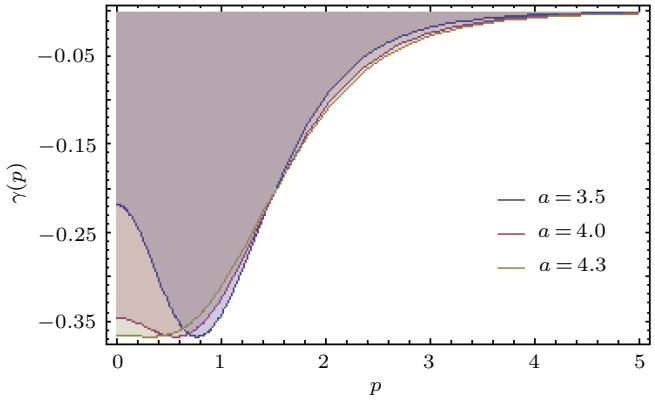


Fig. 4. (color online) Plots of the momentum space probability density for $n=1$.

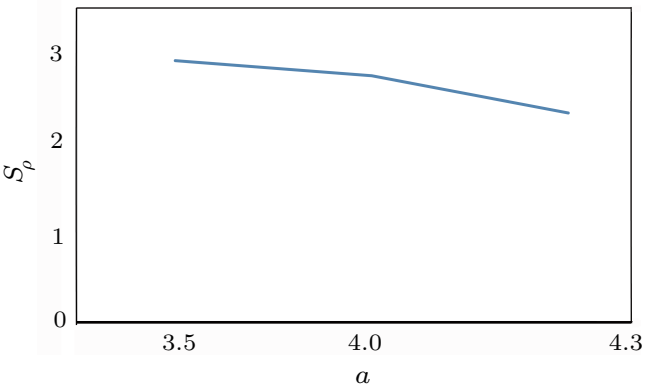


Fig. 5. (color online) Plot of the position space entropy for $n=1$.

In Figs. 5 and 6, we show the position information entropy S_γ and momentum space entropy S_ρ each as a function of parameter a respectively. We find that S_γ decreases with the increase of parameter a. Notice that the S_ρ decreases with the increase of parameter a. With increasing a, the mass barrier becomes narrower, thus the passing time becomes shorter and the system becomes more stable. The behavior of S_γ is contrary to that of S_ρ. With parameter a fixed, the S_ρ decreases with the energy level increasing. That is to say, when the energy of the system decreases, the quantum system becomes stable. It is notable that S_γ increases with the increase of parameter a.

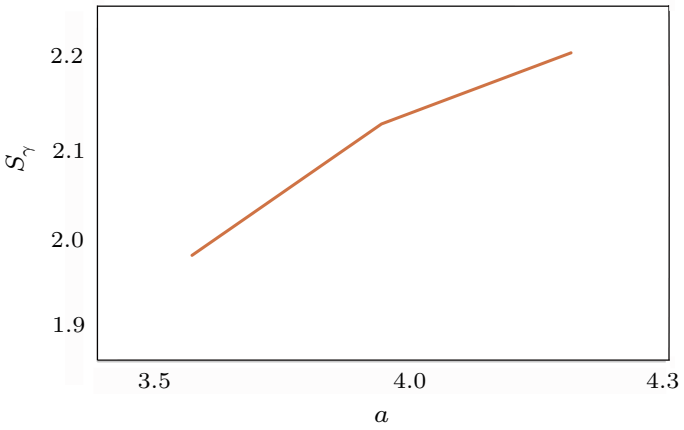


Fig. 6. (color online) Plot of the momentum space entropy for $n=1$.

In Table 1, we present the numerical results of the information entropies S_ρ and S_γ and their sum for the lowest states $n=1$ with parameter a values of 3.5, 4, and 4.3 for $\ell'=0$. It should be noted that the sum of the entropies, consistent with the BBM inequality, possesses the stipulated lower bound $3\,(1+\log\pi)$.

Table 1. Information entropies of the $n=1$ eigenstates for $\ell'=0$.

ε	a	S_ρ	S_γ	$S_\rho+S_\gamma$	$3(1+\log\pi)$
1.75	3.5	2.91192	1.97741	4.88933	4.49145
2	4	2.74428	2.13472	4.879	4.49145
2.15	4.3	2.33109	2.21992	4.55101	4.49415

4. Concluding remarks

We present the Shannon entropy for the position and momentum eigenstates of the Schrödinger equation with the Kratzer potential. The position S_ρ and momentum S_γ information entropies are calculated for $n=1$. Particularly, the S_ρ entropy for the lowest state is derived analytically, and also some numerical calculations for S_γ are presented. We find that the position information entropy S_ρ decreases with the increase of parameter a, but the behavior of S_γ is contrary to that of the S_ρ. The influence of parameter a on the stability of the system is shown in detail. Some interesting features of the information entropy densities, $\rho_s(\boldsymbol{r})$ and $\gamma_s(\boldsymbol{p})$, are demonstrated via various figures and one table. The consistency with the BBM inequality is also verified for a number of states.

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