Quantum information entropies of the eigenstates of the Morse potential

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The position and momentum space information entropies for the Morse potential are numerically obtained for different strengths of the potential. It is found to satisfy the bound obtained by Beckner, Bialynicki-Birula, and Mycielski. Interesting features of the entropy densities are graphically demonstrated.

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I. INTRODUCTION

In quantum mechanics two non-commuting observables cannot be simultaneously measured with arbitrary precision. That is, there is an irreducible lower bound on the uncertainty in the result of a simultaneous measurement of non-commuting observables. This fact, often called the Heisenberg uncertainty principle [1]. The uncertainty principle specified for a given pairs of observables finds its mathematical manifestation as the uncertainty relations. The first rigorous derivation of the uncertainty relation from the quantum mechanical formalism applied for the basic non-commuting observables is due to Kennard [2].

In accordance with the present understanding the quantum system is described by a complex function \( \psi \) which is linked with the function of the probability density of finding a particle at the position \( x \) at the time \( t \) by the equation \( \rho_x (x, t) = |\psi(x, t)|^2 \). On the other hand, the corresponding Fourier transform \( \phi(x, t) \) is connected with the probability of finding a particle with momentum \( p \) at the time \( t \) by the equation \( \rho_p (p, t) = |\phi(p, t)|^2 \).

For the mathematical expression of the uncertainty principle we must more precisely define how to measure the sharpness of the probability density function of an observable. In the mathematical formulation of the uncertainty principle we consider two Hermitian operators \( \hat{A} \) and \( \hat{B} \) which represent physical observables \( A \) and \( B \) in a finite \( N \)-dimensional Hilbert space. Let \( \{|a_j\}\) and \( \{|b_k\}\), \( j, k = 1, 2, ..., N \), be corresponding complete sets of normalized eigenvectors. The probability distribution of the observables \( A \) and \( B \), \( P = \{p_1, p_2, ..., p_N\} \) and \( Q = \{q_1, q_2, ..., q_N\} \) described by the wave-function \( \psi \) are given by the equations

\[
p_j = |\langle a_j | \psi \rangle|^2, \quad q_k = |\langle b_k | \psi \rangle|^2 \tag{1}
\]

respectively. The principle of uncertainty says that if \( A \) and \( B \) are non-commuting observables, then their probability distributions cannot be both arbitrarily peaked. In other words, the uncertainty principle states that two complementary observables cannot have the same eigenfunctions.

The formulation of the uncertainty principle by means of dispersions of non-commuting observables is usually given in the form of the Robertson relation [3]:

\[
\Delta A \Delta B \geq \frac{1}{2} |\langle \psi | [\hat{A}, \hat{B}] | \psi \rangle| \tag{2}
\]

where \( \Delta A \) and \( \Delta B \) denote the standard deviation of distributions (1):

\[
\Delta A = [\langle A^2 \rangle - \langle A \rangle^2]^{1/2}, \quad \Delta B = [(B^2) - \langle B \rangle^2]^{1/2}.
\]

It has been pointed by many authors (See Refs. [4, 5, 6]) that the Robertson form of uncertainty relation has two serious shortcomings; (i) the right-hand side of Eq. (2) is not a fixed lower bound, but depends on the state \( \psi \). If the observables \( A \) and \( B \) is in its eigenstate then \( [A, B] = 0 \) and no restriction on \( \Delta A \) or \( \Delta B \) is imposed by the left-hand side of the inequality (2). (ii) The dispersion may not represent the appropriate measure for the uncertainty of an observables if its probability distribution exhibits some sharp distant peaks.

Therefore, to improve on this situation entropic uncertainty relations have been proposed which rely on the Shannon entropy [7] as a measure of uncertainty. A much more satisfactory measure of quantum uncertainty is given by the information entropy of given probability distribution. An entropic uncertainty relation represents the sum of the entropies of two non-commuting observables \( A \) and \( B \)

\[
S_A + S_B \geq S_{AB} \tag{3}
\]

where \( S_A \) and \( S_B \) denote information entropies of observables \( A \) and \( B \), respectively. The \( S_{AB} \) is a positive constant which represent the lower bound of the right-hand side of the inequality of (3). The information uncertainty relation (3) were first conjectured by Everett [8] in the context of many worlds interpretation of quantum mechanics and Hirschman [9] in 1957, and proved by Bialynicki-Birula and Mycielski [10], and independently by Beckner [11].
For the continuous observables for example \(x\) and \(p\) which are described by the wave-functions \(\psi(x)\) and \(\phi(p)\), position space information entropy \(S_x\) and momentum space information entropy \(S_p\) are defined by

\[
S_x = - \int_{-\infty}^{\infty} |\psi(x)|^2 \ln |\psi(x)|^2 \, dx
\]

(4)

\[
S_p = - \int_{-\infty}^{\infty} |\phi(p)|^2 \ln |\phi(p)|^2 \, dp
\]

(5)

respectively. For position \(x\) and momentum \(p\) the inequality (3) for \(N\)-dimensional Hilbert space reads

\[
S_x + S_p \geq N(1 + \ln \pi)
\]

(6)

where \(N(1 + \ln \pi)\) is the lower bound for the inequality (3). For \(N = 1\), the entropy sum is bounded from below by the value 2.1447... .

Note that these entropies have been used for numerous practical purposes such as, for example, to measure the squeezing of quantum fluctuation [12] and to reconstruct the charge and momentum densities of atomic and molecular systems [13, 14] by means of maximum-entropy procedures.

II. THE MORSE POTENTIAL

In present study we deal with position and momentum information entropies of the one-dimensional Morse potential as an example, and will discuss whether it satisfy the entropic uncertainty relation (6) or not. The Morse potential, introduced in the 1930's [15], is one of a class of potential [16] for which solutions of the Schrödinger equation are known. The Morse potential is widely used in the literature as a model for bound states, such as the vibrational states of molecules. For the applications the potential is defined as a function of the variable \(x\) which ranges from \(-\infty\) to \(+\infty\), and is given in terms of two parameters \(D\) and \(\alpha\) by

\[
V(x) = De^{-\alpha x}(e^{-\alpha x} - 2)
\]

(7)

where \(D\) is the dissociation energy, \(D > 0\) corresponds to its depth, and \(\alpha\) is related to the range of the potential and \(x\) gives the relative distance from the equilibrium position of the atoms. At the \(x = 0\), it has a negative (attractive) minimum of depth \(D\), and it goes smoothly to zero in the limit of large \(x\). For \(x\) less than \(-\ln 2/\alpha\) this potential becomes positive (repulsive), and as \(x\) decrease even further, the potential becomes increasing large.

The solution of the Schrödinger equation associated with the potential (7) is given by [17]

\[
\Psi_n(\xi) = Ne^{-\xi^2/2}L_n^s(\xi)
\]

(8)

where \(L_n^s(\xi)\) are associated Laguerre functions, the argument \(\xi\) is related to the physical displacement coordinate \(x\) by \(\xi = 2\lambda e^{-\alpha x}\) with \(0 < \xi < \infty\), and \(N\) is normalization constant:

\[
N = \sqrt{\frac{\alpha (2\lambda - 2n - 1) \Gamma(n + 1)}{\Gamma(2\lambda - n)}}
\]

(9)

and \(n = 0, 1, ..., [\lambda - 1/2]\) with \([\rho]\) denoting the largest integer smaller than \(\rho\), so that the total number of bound states is \([\lambda - 1/2]\).

We note that the \(\lambda\) is potential dependent, \(s\) is related to energy \(E\) and by definition \(\lambda > 0\), \(s > 0\). The parameters \(\lambda\) and \(s\) satisfy the constraint condition

\[
s + 2n = 2\lambda - 1
\]

(10)

end they are related to the potential \(D\) and energy \(E\) through

\[
\lambda = \sqrt{\frac{2\mu D}{\alpha^2 \hbar^2}} \quad s = \sqrt{\frac{-8\mu E}{\alpha^2 \hbar^2}}.
\]

(11)

where \(\mu\) is the reduced mass of the molecule. Normalizable states fulfil \(n < s\) and the corresponding eigenvalues (i.e., energy spectrum) are given by

\[
E_n = -\hbar\omega(n + 1/2)
\]

(12)

where \(w = \hbar\alpha^2/2\mu\).

III. THE NUMERICAL RESULTS

The position and momentum space information entropies for the one-dimensional potential can be calculated by using Eqs. (4) and (5), respectively. The analytical derivation of the position and momentum space information entropies for Morse potential is quite cumbersome. However, quite recently position and momentum space information entropies of the Morse have been analytically obtained by Dehesa et al. for the ground state of the wave-function [17]. They also discussed behavior of the ground state entropy for values of the potential parameter \(D\). Therefore, the present article is devoted to the numerical study of the information entropies for Morse potential take into account the parameters of the wave-function (8). Instead evolution of position and momentum space information entropies, we plot entropy densities \(\rho(x) = |\psi(x)|^2 \ln |\psi(x)|^2\) and \(\rho(p) = |\phi(p)|^2 \ln |\phi(p)|^2\) for both position and momentum space, respectively. The entropy densities \(\rho(x)\) and \(\rho(p)\) provide a measure of information about localization of the particle in the respective spaces.

In order to demonstrating the entropy distribution in the well, we have plotted position and momentum space entropy densities in Figs. 1(a)-(d) and Figs. 2(a)-(d), respectively, for arbitrary \(n\) and \(\lambda\) values. It seems that in the both figures the number of minima and their depths depend on \(n\) and \(\lambda\). However, entropy distributions
FIG. 1: Plots of the position space entropy densities of the Morse potential for (a) $n=0$ and $\lambda=1, 2, 3$ (b) $n=1$ and $\lambda=2, 3, 4$ (c) $n=2$ and $\lambda=3, 4, 5$ (d) $n=3$ and $\lambda=4, 5, 6$, respectively.

FIG. 2: Plots of the momentum space entropy densities of the Morse potential for (a) $n=0$ and $\lambda=1, 2, 3$ (b) $n=1$ and $\lambda=2, 3, 4$ (c) $n=2$ and $\lambda=3, 4, 5$ (d) $n=3$ and $\lambda=4, 5, 6$, respectively.
TABLE I: Table for BBM inequality for the Morse potential for arbitrary \( n \) and \( \lambda \)

| \( n \) | \( \lambda \) | \( S_x \) | \( S_p \) | \( S_x + S_p \) | \( 1 + \ln \pi \) |
|-----|-----|-----|-----|-----|-----|
| 0   | 1   | 1.5772 | 0.6931 | 2.2694 | 2.1447 |
| 2   | 0.9248 | 1.2692 | 2.1940 | 2.1447 |
| 3   | 0.6475 | 1.5280 | 2.1755 | 2.1447 |
| 4   | 0.4698 | 1.6974 | 2.1672 | 2.1447 |
| 1   | 2   | 1.7218 | 1.2692 | 2.9910 | 2.1447 |
| 3   | 1.1369 | 1.7697 | 2.9066 | 2.1447 |
| 4   | 0.8796 | 1.9736 | 2.8532 | 2.1447 |
| 5   | 0.7117 | 2.1089 | 2.8206 | 2.1447 |
| 2   | 3   | 1.7812 | 1.4081 | 3.1893 | 2.1447 |
| 4   | 1.2347 | 2.0198 | 3.2545 | 2.1447 |
| 5   | 0.9945 | 2.2327 | 3.2272 | 2.1447 |
| 6   | 0.8359 | 2.3621 | 3.1980 | 2.1447 |
| 3   | 4   | 1.8110 | 1.5182 | 3.3183 | 2.1447 |
| 5   | 1.2928 | 2.1809 | 3.4737 | 2.1447 |
| 6   | 1.0662 | 2.4098 | 3.4760 | 2.1447 |
| 7   | 0.9157 | 2.5422 | 3.4579 | 2.1447 |

exhibit interesting behavior, for example, the distribution of the position space entropy density has asymmetric shape as can be seen in Figs. 1(a)-(d), whereas, the distribution of the momentum space entropy density in momentum space are quite symmetric as can be seen in Figs. 2(a)-(d).

In Table 1 we have presented the numerical results of information entropies \( S_x \), \( S_p \) and the entropy sum \( S_x + S_p \) for arbitrary \( n \) and \( \lambda \). It is clearly seen from Table 1 that BBM inequality is satisfied for the Morse potential. For all \( n \) values, as \( \lambda \) increases, the entropy sum \( S_x + S_p \) tends to be saturated to bound value which is defined by BBM inequality. Physically, for increasing \( \lambda \), the depth of the potential increases and it increasingly resembles the oscillator potential, which saturates above inequality. The significance of BBM inequality is that it presents an irreducible lower bound to the entropy sum. The conjugate position and momentum space information entropies have an inverse relationship with each other. A strongly localized distribution in the position space corresponds to widely delocalized distribution in the momentum space. With one entropy increasing, the other entropy decreases but only to the extent that their sum stays above the stipulated lower bound of \((1 + \ln \pi)\).

IV. CONCLUSION

We have studied the information entropies of a class of quantum systems belonging to the Morse potential. Numerical results for the position space entropies and momentum space entropies of the Morse potential are obtained for several potential strengths \( \lambda \) and quantum number \( n \). The entropy densities for the above cases were depicted graphically, for demonstrating the entropy distribution in the well. It is found that these entropies satisfy the Beckner, Bialynicki-Birula and Mycielski (BBM) inequality for the Morse potential.

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