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Quantum Information Entropies for the Morse Potential

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Abstract

Quantum information entropies for the one dimensional Morse potential are discussed in position and momentum space. These entropies for different strengths of the potential well are numerically obtained. Interesting features of the entropy densities are also graphically demonstrated and it is shown that the position and momentum space information entropies satisfy the bound which is obtained by Beckner, Bialynicki-Birula, and Mycielski.

Key Words: Information entropy, BBM inequality, Morse potential.

1. Introduction

The one-particle position and momentum probability densities are the basic elements for the quantum mechanical description of the physical and chemical properties of the natural systems according to the density functional theory (DFT) initiated by Hohenberg and Kohn [1]. Indeed, all the fundamental and/or experimentally accessible quantities of these systems may be calculated by means of these densities in position and momentum spaces. However, its determination from the (wavefunction-based) Schrodinger equation of the system or even by means of the much simpler (density-based) Kohn-Sham equations of the DFT is an impossible analytical task [2]. For this reason, often attention is focused on deriving not the densities themselves but certain specific properties of them (e.g., the spreading) directly from the Hamiltonian of the system. Nowadays it is commonly accepted [3, 4] that the spreading of the quantum probability densities in both position and momentum spaces are best measured not by the standard deviation but by the quantum i.e, Boltzmann-Shannon information entropy. Moreover the uncertainty relation based on the information entropy of the densities (the entropic uncertainty relation) is valid for any quantum probability density, contrary to the Heisenberg uncertainty principle (which is based on the standard deviation of the densities) or any of its generalizations based on moments other than the standard deviation which yield non useful information or no information at all in certain cases [5].

The quantum information entropy S_{pos} in the position space is defined by

$$S_{pos} = \int dx \left|\psi\left(x\right)\right|^2 \ln\left|\psi\left(x\right)\right|^2 \tag{1}$$

and the corresponding momentum space counterpart is given by

$$S_{mom} = \int dp \left|\widetilde{\psi}\left(p\right)\right|^2 \ln\left|\widetilde{\psi}\left(p\right)\right|^2 \tag{2}$$

where $\psi(x)$ is the wave function of the particle and $\widetilde{\psi}(p)$ denotes the fourier transform of the wave function.

The entropic sum of this system, which the joint position-momentum uncertainty is bounded from below according to the so-called entropic uncertainty relation of this system is

$$S_{pos} + S_{mom} \geq d\,(1 + \ln \pi)\,. \tag{3}$$

which is a consequence of a well-known inequality in Fourier analysis, first conjectured by Everett [6] in the context of many worlds interpretation of quantum mechanics and Hirschman [7] in 1957, and then proved by Bialynicki-Birula and Mycielski [8], and independently by Beckner [9]. This inequality strongly generalizes and improves [8, 10] the Heisenberg-Kennard-Robertson uncertainty principle $\Delta x.\Delta p \geq \hbar/2$.

In this paper we will consider the one dimensional Morse potential as an example, and we will give the result of our numerical studies on the Shannon information entropy integral of the Morse potential in the position space and momentum space.

2. Solution of the Morse potential

The one dimensional Morse potential has the following form [11]:

$$V(x) = De^{-\alpha x}(e^{-\alpha x} - 2) \tag{4}$$

where $D > 0$ corresponds to its depth, α is related to the range of the potential and x gives relative distance from the equilibrium position of the atom.

The solution of the Schrödinger equation associated with the potential (4) is given by [11]

$$\Psi_n^s(y) = Ny^{s-n}e^{-y/2}L_n^{2(s-n)}(y) \tag{5}$$

where $L_n^{2(s-n)}(y)$ are associated Laguerre functions, the argument y is related to the physical displacement coordinate x by $y = (2s+1)e^{-\alpha x}$, and N is normalization constant

$$N = \sqrt{\frac{\alpha\,(2s-2n)\,\Gamma\,(n+1)}{\Gamma\,(2s-n+1)}} \tag{6}$$

where n is a non-negative integer, and s is a real positive value. They are related to the potential and energy through

$$2s+1 = \sqrt{\frac{8\mu D}{\alpha^2\hbar^2}} \qquad s-n = \sqrt{\frac{-2\mu E}{\alpha^2\hbar^2}} \tag{7}$$

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

$$E_n(s) = -\hbar\omega(n-s)^2 \qquad n = 0, 1, ..., [s] \tag{8}$$

where $[s]$ denotes the largest integer that is smaller than s, and $w = \hbar\alpha^2/2\mu$ Eq. (8) indicates that the number of bound states (normalizable eigenstates) is equal to the integer part of $[s]+1$.

3. Numerical Results

Using Eq. (5) position space entropy density and momentum space entropy densities have been evaluated. The position space entropy density were plotted versus position in Figures 1(a)-(b) for arbitrary n and s values ($\alpha = \hbar = 2\mu = 1$), respectively. As seen in Figure1, the position space entropy densities have quite asymmetric shape depending on n and s values. The figures clearly indicate that the number of the minimas and their depths are also depend on n and s values. Also, the momentum space entropy densities are plotted versus momentum space in Figures 2(a)-(b) for arbitrary n and s values, respectively. In contrary to position space entropy density plots, as seen in Figure 2, the momentum space entropy density plots in momentum

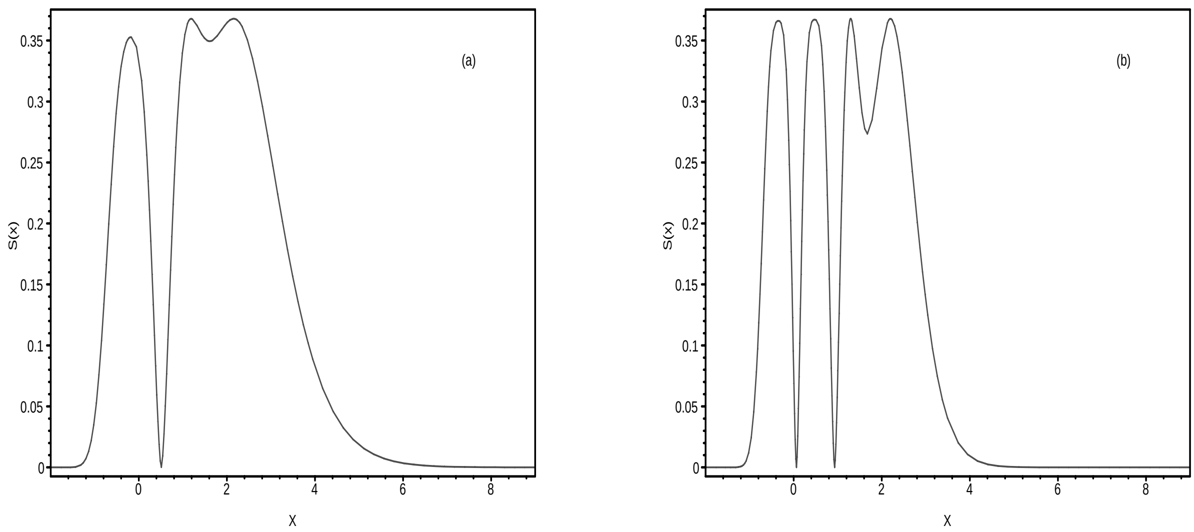

Figure 1. The position space entropy densities of the Morse potential for (a) $n = 1$, $s = 2$ (b) $n = 2$, $s = 4$ for $\alpha = \hbar = 2\mu = 1$.

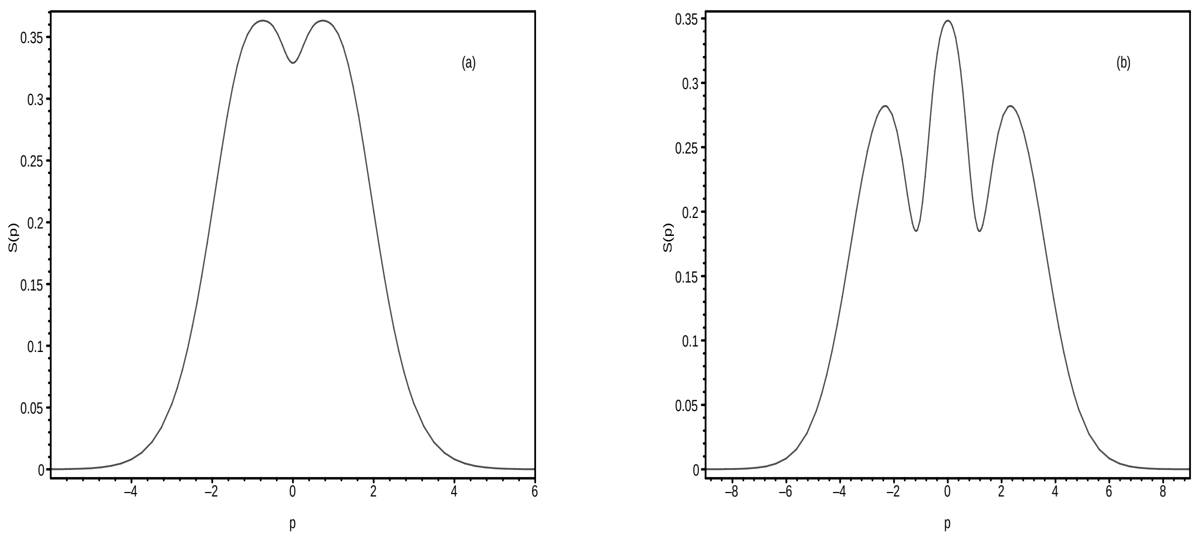

Figure 2. The momentum space entropy densities of the Morse potential for (a) $n = 1$, $s = 2$ (b) $n = 2$, $s = 4$ for $\alpha = \hbar = 2\mu = 1$.

space are quite asymmetric shapes for arbitrary n and s values. The number of the minimas and their depths are also depend on n and s values like in Figure 1.

It is clearly seen from Table 1 that BBM inequality for arbitrary n and s values are satisfied for the Morse potential. Table 1, depicts the BBM inequality as a function of n and s. One sees that as the values of n and s increases the sum of the entropies increase. Physically, for increasing n and s, the depth of the potential decreases and it decreasingly resembles the oscillator potential, which satisfy the above inequality.

It is seen that sum of the entropies approach to BBM bound. This may be a result of interest, since so

Table 1. Table for BBM inequality for the Morse potential for arbitrary n and s ($\alpha = \hbar = 2\mu = 1$)

n	s	S_{pos}	S_{mom}	$S_{pos} + S_{mom}$	$(1 + \ln \pi)$
0	1	1.1544	1.0609	2.2153	2.1447
0	2	0.7673	1.4153	2.1826	2.1447
1	2	1.3458	1.6009	2.9467	2.1447
1	3	0.9915	1.8848	2.8763	2.1447
2	3	1.4283	1.8236	3.2519	2.1447
2	4	1.0993	2.1432	3.2425	2.1447
3	4	1.4752	1.9653	3.4405	2.1447
3	5	1.1652	2.3149	3.4801	2.1447

far it has been believed in the literature that the lower bound can be reached only by a class of Gaussian wave packets. It is also seen that in Table 1, n and s values increase the sum of the entropies tends towards a saturation value higher than the ground state value.

4. Results and Conclusions

In 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 s 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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