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Scaling properties of net information measures for superpositions of power potentials: Free and spherically confined cases

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Abstract

The dimensional analyses of the position and momentum variances based *quantum mechanical* Heisenberg uncertainty measure, along with several *entropic* information measures are carried out for the *superposition* of the power potentials of the form $V(r) = Zr^n + \sum_i Z_i r^{n_i}$ where Z, Z_i, n, n_i are parameters yielding *bound states* for a particle of mass M. The uncertainty product and *all* other *net* information measures for given values of the parameters Z, Z_i, are shown to depend only on M and the ratios $Z_i/Z^{(n_i+2)/(n+2)}$. Under the imposition of a spherical impenetrable boundary of radius R over the polynomial potential, an *additional* parametric dependence on $RZ^{1/(n+2)}$ is derived. A representative set of numerical results are presented which support the validity of such a general scaling property.

Keywords: Heisenberg uncertainty relation; Shannon entropy; Fisher information measure; Rényi entropy; Tsallis entropy; Power potentials; Polynomial potentials; Spherically confined system

1. Introduction

The uncertainty relations are the basic properties of quantum mechanics. In particular, we have the Heisenberg uncertainty principle [1] for the product of the uncertainties in position and momentum, expressed in terms of Planck's constant. For a one-dimensional system defined over $-\infty \leqslant x \leqslant \infty$, it is given by the product of the corresponding variances, $(\Delta x) = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$, and $(\Delta p) = \sqrt{\langle p^2\rangle - \langle p\rangle^2}$, according to

$$(\Delta x)(\Delta p) \geqslant \frac{1}{2}\hbar. \tag{1}$$

The Heisenberg uncertainty product (HUP), $(\Delta x)(\Delta p)$, has many interesting properties for different potentials. For example, HUP for the bound states in homogeneous, power potentials is independent of the strength of the potentials [2]. For several other numerical studies on HUP we refer to the published literature [3]. For such potentials similar interesting related properties are also displayed [4] through the various information measures such as the Shannon information entropy sum [5–8], the Fisher information product [9–12], Onicescu energy [13], Rényi [14,15], and Tsallis entropy [16,17], respectively. In this Letter we will consider some general scaling properties for the bound states arising out of the *superpositions* of power potentials of the form

$$V(r) = Zr^n + \sum_i Z_i r^{n_i}, \tag{2}$$

where Z, Z_i, n, n_i are parameters (n, n_i may not be integers), in which there are bound states for a particle of mass M. Specifically, in addition to the Lennard–Jones type isotropic potentials, we have

$$V_1(r) = -kr^2 + \lambda r^4 \tag{3}$$

for a symmetric double well potential [18],

$$V_2(r) = \frac{1}{2}kr^2 + \frac{a}{r^2} \tag{4}$$

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for a modified isotropic harmonic oscillator [19], and

$$V_3(r) = -\frac{Z}{r} + \lambda r \tag{5}$$

for a confined hydrogenic system [20] and the static quarkonium potential [21]. The Schrödinger equation for the potential in Eq. (2) is

$$-\frac{\hbar^2}{2M}\nabla^2\psi + \Big[Zr^n + \sum Z_i r^{n_i}\Big]\psi = E\psi. \tag{6}$$

We note here that the generalized cosine exponential screened Coulomb potentials [22] which are the natural extensions of the Yukawa [23] and Hulthén [24] potentials can be expressed, to a good approximation, as polynomial potentials when the screening parameter assumes very small values [25]. This is also true of the truncated Coulomb potentials [26] with the truncation parameter $\to 0$. Due to the widespread applications of the polynomial potentials [18–21,25,27–29] several numerical studies dealing with the eigenvalue spectrum have been reported previously [30,31]. For the sake of clarity of presentation this Letter is structured as follows. In Section 2, some general properties corresponding to the Heisenberg uncertainty product, HUP, are derived for the potential $V(r)$. In Section 3, the scaling property of the associated position and momentum space densities is derived following which it is shown how the scaling property of the Shannon information entropy sum [5–8], the Fisher information product [9] and other information measures [13,14,16] can be obtained from it. Further, in Section 3 we have considered the scaling properties of the potential $V(r)$ under the specific condition of confinement inside an impenetrable spherical boundary wall defined by a radius R. In Section 4, we present numerical results, in atomic units, which support the analytic results derived in this work. Finally, a summary of the main results is presented in Section 5.

2. Dimensionality and uncertainty relations

In this section we shall derive some dimensionality properties and discuss their implications on the uncertainty relations for the bound states resulting from superpositions of the isotropic power potentials.

The basic dimensional parameters in our Schrödinger equation in Eq. (6) are $\hbar^2/M$, Z, Z_i. Of these,

$$s_i = \frac{M}{\hbar^2} Z_i \left(\frac{\hbar^2}{MZ}\right)^{(\frac{n_i+2}{n+2})} \tag{7}$$

are the dimensionless parameters. Now we consider the standard deviations

$$(\Delta_{\vec r})^2 = \big\langle \big(\vec r - \langle \vec r\rangle\big)^2\big\rangle, \qquad (\Delta_{\vec p})^2 = \big\langle \big(\vec p - \langle \vec p\rangle\big)^2\big\rangle. \tag{8}$$

For our potential in Eq. (2), the dimensionality properties imply that the deviations are of the form

$$\Delta_{\vec r} = \big(\hbar^2/MZ\big)^{1/(n+2)} g_1(s_i),$$
$$\Delta_{\vec p} = \hbar\big(MZ/\hbar^2\big)^{1/(n+2)} g_2(s_i), \tag{9}$$

so that the uncertainty product is

$$\Delta_{\vec r}\Delta_{\vec p} = \hbar g_1(s_i) g_2(s_i), \qquad s_i = \frac{M}{\hbar^2} Z_i \left(\frac{\hbar^2}{MZ}\right)^{(\frac{n_i+2}{n+2})}. \tag{10}$$

This implies that the HUP depends only on the dimensionless parameters s_i. The quantity s_i, according to Eq. (7) includes M and in general HUP depends on M. Our numerical results presented in Section 4 are reported in a.u. whereby it is implied that $M = 1$. Under this assumption, the parameter s_i would be completely characterized by $Z_i/Z^{(n_i+2)/(n+2)}$. Thus, for the potential $V_1(r)$ in Eq. (3), HUP depends only on $\lambda k^{-3/2}$, and for the potential $V_2(r)$ in Eq. (4), it depends only on a. It may also be noted that the bound state energies are of the form

$$E = \big(\hbar^2/M\big)^{n/(n+2)} Z^{2/(n+2)} g_3(s_i). \tag{11}$$

These results follow from just the dimensionality properties of the parameters and the exact expressions of $g_i(s_i)$ in Eqs. (9)–(11) are not obtained.

3. Scaling properties of net information measures

We will now consider some scaling properties for bound states in a superposition of power potentials, and their implications for Shannon entropy and other properties.

3.1. Scaling properties

For the Schrödinger equation in Eq. (6), the energy E and eigenfunction ψ are functions of the form

$$E:\quad E\big(\hbar^2/M, Z, Z_i\big), \qquad \psi:\quad \psi\big(\hbar^2/M, Z, Z_i, r\big). \tag{12}$$

Multiplying Eq. (6) by $M/\hbar^2$, and introducing a scale transformation

$$\vec r = \lambda \vec r\,' \tag{13}$$

one gets

$$-\frac{1}{2}\nabla'^2\psi + \big(M/\hbar^2\big)\Big[Z\lambda^{n+2}r'^n + \sum Z_i\lambda^{n_i+2}r'^{n_i}\Big]\psi$$
$$= \big(M/\hbar^2\big)\lambda^2 E\psi. \tag{14}$$

Taking

$$\lambda = \left(\frac{\hbar^2}{MZ}\right)^{1/(n+2)}, \tag{15}$$

it leads to

$$-\frac{1}{2}\nabla'^2\psi + \left[r'^n + \frac{M}{\hbar^2}\sum Z_i\left(\frac{\hbar^2}{MZ}\right)^{(\frac{n_i+2}{n+2})} r'^{n_i}\right]\psi$$
$$= \frac{M}{\hbar^2}\left(\frac{\hbar^2}{MZ}\right)^{2/(n+2)} E\psi. \tag{16}$$

Comparing this with Eq. (6), we obtain

$$E\left(\frac{\hbar^2}{M}, Z, Z_i\right)$$
$$= \big(\hbar^2/M\big)\lambda^{-2} E\big(1, 1, Z_i\lambda^{n_i+2}M/\hbar^2\big),$$