Scaling properties of net information measures for bound states of spherical model potentials confined with finite barrier[#]

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Abstract. Using dimensional analyses, the scaling properties of the Heisenberg uncertainty relationship as well as the various information theoretical *uncertainty-like* relationships are derived for the bound states corresponding to the superposition of the power potential of the form $V(r) = Zr^n + \sum_i Z_i r^{n_i}$, where Z, Z_i, n, n_i are parameters, in the free state as well as in the additional presence of a spherical *penetrable* boundary wall located at radius R . The uncertainty product and *all* other *net* information measures are shown here to depend only on the parameters $[s_i]$ defined by the ratios $Z_i/Z^{(n_i+2)/(n+2)}$. Introduction of a finite potential, V_c at the radial distance $r \geq R$ results in a complete set of scaling parameters given by $[s_i, t_1, t_2]$, where t_1 is given by $RZ^{1/(n+2)}$ and $t_2 = V_c/(Z)^{2/(n+2)}$.

Keywords. Heisenberg uncertainty; information theory; confined potentials.

1. Introduction

The uncertainty relations are the basic properties of quantum mechanics, in particular, we have the Heisenberg uncertainty principle¹ for the product of the uncertainties in position and momentum,

$$\begin{aligned}\sigma_x \sigma_p &\geq \frac{1}{2} \hbar, \\ \sigma_x^2 &< (x - \langle x \rangle)^2, \\ \sigma_p^2 &< (p_x - \langle p_x \rangle)^2,\end{aligned}\quad (1)$$

in terms of Planck's constant. The uncertainty product has many interesting properties for different potentials, for example, the product for bound states in homogeneous, power potentials is independent of the strength of the potentials. While the uncertainty principle is by definition expressed in terms of the quantum mechanical expectation values,² there exist quite a few other interesting uncertainty-like relationships expressed in terms of the information theoretical measures defined in terms of the probability density alone. Here we will consider some general properties for the bound states in superpositions of power potentials with a *finite* barrier. It is observed that the dimensionality and scaling properties lead to interesting properties of the uncertainty product, and densities with implications for entropies and information. The aim of such a study is to ascertain how the parameters in the potential describe the

various information-theoretical uncertainty-like measures expressed through the electron probability density as the key parameter. We would like to mention that the work presented here forms part of a more general review article in a monograph on statistical complexity³ which summarizes the various scaling properties of the uncertainty-like relationships corresponding to a large number of spherical potentials studied by us during the past five years. The work on the superpositions of the power potentials with a *finite* potential barrier is being presented here in a regular journal for the first time.

2. Heisenberg uncertainty relations

Here we analyse some dimensionality properties and their implications for the uncertainty relations for the bound states in superpositions of power potentials with a finite barrier. Similar analysis for a host of spherical model potentials have been reported earlier.⁴ However, the present work provides the first example of a very general class of spherical potential with a finite barrier.

2.1 Superpositions of power potentials with a finite barrier

Consider a potential of the form

$$V(r) = \left[Zr^n + \sum_i Z_i r^{n_i} \right] \theta(R - r) + V_c \theta(r - R), \quad (2)$$

[#]Dedicated to Prof. N Sathyamurthy on his 60th birthday

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where Z, Z_i, n, n_i, R, V_c are parameters (n, n_i may not be integers) with θ being the Heaviside theta function,⁵ in which there are bound states for a particle of mass M . Specifically, we have

$$V_1(r) = [-kr^2 + \lambda r^4]\theta(R - r) + V_c\theta(r - R) \quad (3)$$

for a symmetric double well potential,⁶

$$V_2(r) = \left[\frac{1}{2}kr^2 + \frac{a}{r^2} \right] \theta(R - r) + V_c\theta(r - R) \quad (4)$$

for a modified s. h. o.,⁷ and

$$V_3(r) = \left[-\frac{Z}{r} + \lambda r \right] \theta(R - r) + V_c\theta(r - R) \quad (5)$$

for a hydrogenic system confined under a linear potential.⁸ The Schrödinger equation for the potential in equation 2 is

$$-\frac{\hbar^2}{2M} \nabla^2 \psi + \left[\left(Zr^n + \sum Z_i r^{n_i} \right) \theta(R - r) + V_c \theta(r - R) \right] \psi = E \psi. \quad (6)$$

2.2 Dimensionality and uncertainty relations

The basic dimensional parameters in our Schrödinger equation are $\hbar^2/M, Z, Z_i, R, V_c$. Of these,

$$s_i = \frac{M}{\hbar^2} Z_i \left(\frac{\hbar^2}{MZ} \right)^{\frac{n_i+2}{n+2}}, \quad t_1 = R(MZ/\hbar^2)^{1/(n+2)},$$

$$t_2 = V_c(M/\hbar^2)(\hbar^2/MZ)^{2/(n+2)} \quad (7)$$

are the dimensionless parameters. Now we consider the deviations

$$\sigma_{\vec{r}}^2 = \langle (\vec{r} - \langle \vec{r} \rangle)^2 \rangle, \quad \sigma_{\vec{p}}^2 = \langle (\vec{p} - \langle \vec{p} \rangle)^2 \rangle. \quad (8)$$

For our potential in equation 6, the dimensionality properties imply that the deviations are of the form

$$\sigma_{\vec{r}} = (\hbar^2/MZ)^{1/(n+2)} g_1(s_i, t_i),$$

$$\sigma_{\vec{p}} = \hbar(MZ/\hbar^2)^{1/(n+2)} g_2(s_i, t_i), \quad (9)$$

so that the uncertainty product is

$$\sigma_{\vec{r}} \sigma_{\vec{p}} = \hbar g_1(s_i, t_i) g_2(s_i, t_i),$$

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

$$t_1 = R(MZ/\hbar^2)^{1/(n+2)},$$

$$t_2 = V_c(M/\hbar^2)(\hbar^2/MZ)^{2/(n+2)}. \quad (10)$$

This implies that the uncertainty product depends only on the dimensionless parameters s_i, t_i . It may also be noted that the bound state energies are of the form

$$E = (\hbar^2/M)(MZ/\hbar^2)^{2/(n+2)} g_3(s_i, t_i). \quad (11)$$

These results follow from just the dimensionality properties of the parameters.

It is interesting to note that one can analyse the minimum uncertainty in terms of the scaled parameters. For example, in the case of a hydrogen atom with a finite barrier potential, one can obtain the minimum uncertainty by keeping V_c fixed but varying RZ . Alternatively, one can keep R fixed but vary V_c . These considerations can be extended to the superpositions of power potentials with a finite barrier potential in terms of the scaled variables s_i and t_i .

3. Scaling properties and entropies

We will now consider some scaling properties for bound states in a superposition of power potentials, and their implications for Shannon entropy^{9,10} and other properties.

3.1 Scaling properties

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

$$E : E(\hbar^2/M, Z, Z_i, R, V_c),$$

$$\psi : \psi(\hbar^2/M, Z, Z_i, R, V_c, r). \quad (12)$$

Multiplying equation 6 by $M/\hbar^2$, and introducing a scale transformation

$$\vec{r} = \lambda \vec{r}' \quad (13)$$

one gets

$$-\frac{1}{2} \nabla'^2 \psi + (M/\hbar^2)$$

$$\times \left[Z \lambda^{n+2} r'^n + \sum Z_i \lambda^{n_i+2} r'^{n_i} \right] \theta(R/\lambda - r') \psi$$

$$+ (M/\hbar^2) \lambda^2 V_c \theta(r' - R/\lambda) \psi = (M/\hbar^2) \lambda^2 E \psi. \quad (14)$$

Taking

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

equation (14) leads to

$$\begin{aligned} & -\frac{1}{2}\nabla^2\psi + \left[r'^n + \frac{M}{\hbar^2} \sum Z_i \left(\frac{\hbar^2}{MZ}\right)^{\frac{n_i+2}{n+2}} r'^{n_i}\right] \\ & \times \theta\left(R(MZ/\hbar^2)^{1/(n+2)} - r'\right)\psi \\ & + \frac{M}{\hbar^2}(\hbar^2/MZ)^{2/(n+2)} V_c \theta\left(r' - R(MZ/\hbar^2)^{1/(n+2)}\right)\psi \\ & = \frac{M}{\hbar^2} \left(\frac{\hbar^2}{MZ}\right)^{2/(n+2)} E\psi. \end{aligned} \quad (16)$$

Comparing this with equation 6, we obtain

$$\begin{aligned} & E\left(\frac{\hbar^2}{M}, Z, Z_i, R, V_c\right) \\ & = (\hbar^2/M)\lambda^{-2}E(1, 1, Z_i\lambda^{n_i+2}M/\hbar^2, R/\lambda, V_c\lambda^2M/\hbar^2), \\ & \psi\left(\frac{\hbar^2}{M}, Z, Z_i, R, V_c, r\right) \\ & = A\psi(1, 1, Z_i\lambda^{n_i+2}M/\hbar^2, R/\lambda, V_c\lambda^2M/\hbar^2, r'), \\ & r = \lambda r', \quad \lambda = (\hbar^2/MZ)^{1/(n+2)}. \end{aligned} \quad (17)$$

Taking $\psi(1, 1, Z_i\lambda^{n_i+2}M/\hbar^2, R/\lambda, V_c\lambda^2M/\hbar^2, r')$ to be normalized, the normalization of the wave function $\psi(\hbar^2/M, Z, Z_i, R, V_c, r)$ leads to

$$\begin{aligned} 1 & = A^2 \int |\psi(1, 1, Z_i\lambda^{n_i+2}M/\hbar^2, R/\lambda, V_c\lambda^2M/\hbar^2, r')|^2 d^3r, \\ & = A^2 \lambda^3 \Rightarrow A = \lambda^{-3/2} = (MZ/\hbar^2)^{\frac{3}{2(n+2)}}, \end{aligned} \quad (18)$$

so that

$$\begin{aligned} & \psi\left(\frac{\hbar^2}{M}, Z, Z_i, R, V_c, r\right) \\ & = \lambda^{-3/2}\psi(1, 1, Z_i\lambda^{n_i+2}M/\hbar^2, R/\lambda, V_c\lambda^2M/\hbar^2, r'), \\ & \lambda = (\hbar^2/MZ)^{1/(n+2)}, \quad r' = r/\lambda. \end{aligned} \quad (19)$$

For obtaining the wave function in the momentum space, we take the Fourier transform of the wave function in equation (19), leading to

$$\begin{aligned} & f(\hbar^2/M, Z, Z_i, R, V_c, p) \\ & = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3r e^{-i\vec{p}\cdot\vec{r}/\hbar} \psi(\hbar^2/M, Z, Z_i, R, V_c, r). \end{aligned} \quad (20)$$

Using the relation in equation 19 and changing the integration variable to r' , we get

$$\begin{aligned} & f(\hbar^2/M, Z, Z_i, R, V_c, p) \\ & = \lambda^{3/2} f(1, 1, Z_i\lambda^{n_i+2}M/\hbar^2, R/\lambda, V_c\lambda^2M/\hbar^2, p'), \\ & \lambda = (\hbar^2/MZ)^{1/(n+2)}, \quad p' = \lambda p. \end{aligned} \quad (21)$$

From the relations in equations 19 and 21, one has for the corresponding position and momentum densities,

$$\begin{aligned} \rho(\hbar^2/M, Z, Z_i, R, V_c, r) & = \lambda^{-3}\rho(1, 1, s_i, t_1, t_2, r'), \\ \gamma(\hbar^2/M, Z, Z_i, R, V_c, p) & = \lambda^3\gamma(1, 1, s_i, t_1, t_2, p'), \\ \lambda & = (\hbar^2/MZ)^{1/(n+2)}, \quad s_i = \lambda^{n_i+2}MZ_i/\hbar^2, \quad t_1 = R/\lambda \\ t_2 & = V_c\lambda^2M/\hbar^2 \quad r' = r/\lambda, \quad p' = \lambda p, \end{aligned} \quad (22)$$

with s_i, t_i being the scaled parameters.

3.2 Shannon entropy sum

The Shannon entropies⁹ in the position space and momentum space, are

$$\begin{aligned} S_r & = - \int \rho(r) [\ln \rho(r)] d^3r, \\ S_p & = - \int \gamma(p) [\ln \gamma(p)] d^3p. \end{aligned} \quad (23)$$

Using the relations in equation 22, we get for these entropies

$$\begin{aligned} S_r(\hbar^2/M, Z, Z_i, R, V_c) & = 3\ln\lambda + S_r(1, 1, s_i, t_1, t_2), \\ S_p(\hbar^2/M, Z, Z_i, R, V_c) & = -3\ln\lambda + S_p(1, 1, s_i, t_1, t_2), \end{aligned} \quad (24)$$

which imply that the Shannon entropy sum $S_T = S_r + S_p$ satisfies the relation

$$\begin{aligned} S_T(\hbar^2/M, Z, Z_i, R, V_c) & = S_T(1, 1, s_i, t_1, t_2), \\ s_i & = \frac{M}{\hbar^2} Z_i \left(\frac{\hbar^2}{MZ}\right)^{\frac{n_i+2}{n+2}}, \quad t_1 = R(MZ/\hbar^2)^{1/(n+2)}, \\ t_2 & = V_c(M/\hbar^2)(\hbar^2/MZ)^{2/(n+2)}. \end{aligned} \quad (25)$$

Therefore, for given values of the parameters Z, Z_i, R, V_c , the Shannon entropy sum depends only on $Z_i/Z^{(n_i+2)/(n+2)}, t_1, t_2$.

3.3 Fisher information

The Fisher information measures^{11–14} for position and momentum are

$$I_r = \int \frac{[\vec{\nabla}\rho(r)]^2}{\rho(r)} d^3r, \quad I_p = \int \frac{[\vec{\nabla}\gamma(p)]^2}{\gamma(p)} d^3p. \quad (26)$$

Using the relations in equation 22, one obtains

$$\begin{aligned} I_r(\hbar^2/M, Z, Z_i, R, V_c) &= \frac{1}{\lambda^2} I_r(1, 1, s_i, t_1, t_2), \\ I_p(\hbar^2/M, Z, Z_i, R, V_c) &= \lambda^2 I_p(1, 1, s_i, t_1, t_2). \end{aligned} \quad (27)$$

which together imply that the Fisher information product $I_r I_p$ satisfies the relation

$$\begin{aligned} I_{rp}(\hbar^2/M, Z, Z_i, R, V_c) &= I_{rp}(1, 1, s_i, t_1, t_2), \\ I_{rp} &= I_r I_p, \\ s_i &= \frac{M}{\hbar^2} Z_i \left(\frac{\hbar^2}{MZ} \right)^{\left(\frac{n_i+2}{n+2} \right)}, \quad t_1 = R(MZ/\hbar^2)^{1/(n+2)}, \\ t_2 &= V_c(M/\hbar^2)(\hbar^2/MZ)^{2/(n+2)}. \end{aligned} \quad (28)$$

Here, for given values of the parameters Z, Z_i, R, V_c , the Fisher information product depends only on $Z_i/Z^{(n_i+2)/(n+2)}, t_1, t_2$.

3.4 Rényi entropy

The Rényi entropies¹⁵ in position and momentum spaces are

$$\begin{aligned} H_\alpha^{(r)} &= \frac{1}{1-\alpha} \ln \int [\rho(r)]^\alpha d^3r, \\ H_\alpha^{(p)} &= \frac{1}{1-\alpha} \ln \int [\gamma(p)]^\alpha d^3p. \end{aligned} \quad (29)$$

With the relations in equation 22, we get for these entropies,

$$\begin{aligned} H_\alpha^{(r)}(\hbar^2/M, Z, Z_i, R, V_c) &= 3\ln\lambda + H_\alpha^{(r)}(1, 1, s_i, t_1, t_2), \\ H_\alpha^{(p)}(\hbar^2/M, Z, Z_i, R, V_c) &= -3\ln\lambda + H_\alpha^{(p)}(1, 1, s_i, t_1, t_2), \end{aligned} \quad (30)$$

which imply that the Rényi entropy sum $H_\alpha^{(T)} = H_\alpha^{(r)} + H_\alpha^{(p)}$ satisfies the relation

$$\begin{aligned} H_\alpha^{(T)} \left(\frac{\hbar^2}{M}, Z, Z_i, R, V_c \right) &= H_\alpha^{(T)}(1, 1, s_i, t_1, t_2), \\ s_i &= \frac{M}{\hbar^2} Z_i \left(\frac{\hbar^2}{MZ} \right)^{\left(\frac{n_i+2}{n+2} \right)}, \quad t_1 = R(MZ/\hbar^2)^{1/(n+2)}, \\ t_2 &= V_c(M/\hbar^2)(\hbar^2/MZ)^{2/(n+2)}. \end{aligned} \quad (31)$$

Therefore, as in other cases, for given values of the parameters Z, Z_i, R, V_c , the Rényi entropy sum depends on $Z_i/Z^{(n_i+2)/(n+2)}, t_1, t_2$.

3.5 Onicescu energies

The Onicescu energies¹⁷ in position and momentum spaces are

$$E_r = \int [\rho(r)]^2 d^3r, \quad E_p = \int [\gamma(p)]^2 d^3p. \quad (32)$$

Using the relations in equation 22, we get

$$\begin{aligned} E_r(\hbar^2/M, Z, Z_i, R, V_c) &= \frac{1}{\lambda^3} E_r(1, 1, s_i, t_1, t_2), \\ E_p(\hbar^2/M, Z, Z_i, R, V_c) &= \lambda^3 E_p(1, 1, s_i, t_1, t_2), \end{aligned} \quad (33)$$

which imply that the Onicescu energy product $E_{rp} = E_r E_p$ satisfies the relation

$$\begin{aligned} E_{rp}(\hbar^2/M, Z, Z_i, R, V_c) &= E_{rp}(1, 1, s_i, t_1, t_2), \\ s_i &= \frac{M}{\hbar^2} Z_i \left(\frac{\hbar^2}{MZ} \right)^{\left(\frac{n_i+2}{n+2} \right)}, \quad t_1 = R(MZ/\hbar^2)^{1/(n+2)}, \\ t_2 &= V_c(M/\hbar^2)(\hbar^2/MZ)^{2/(n+2)}. \end{aligned} \quad (34)$$

In this case also, for given values of the parameters Z, Z_i, R, V_c , the Onicescu energy product depends on $Z_i/Z^{(n_i+2)/(n+2)}, t_1, t_2$.

3.6 Tsallis entropy

The Tsallis entropies¹⁶ in position and momentum spaces are

$$\begin{aligned} T_r &= \frac{1}{q-1} \left[1 - \int [\rho(r)]^q d^3r \right], \\ T_p &= \frac{1}{m-1} \left[1 - \int [\gamma(p)]^m d^3p \right], \quad \frac{1}{q} + \frac{1}{m} = 2. \end{aligned} \quad (35)$$

We consider the integral terms

$$\begin{aligned} J_r(\hbar^2/M, Z, Z_i, R, V_c) &= \int [\rho(r)]^q d^3r, \\ J_p(\hbar^2/M, Z, Z_i, R, V_c) &= \int [\gamma(p)]^m d^3p. \end{aligned} \quad (36)$$

Using the relations in equation 22, we get

$$\begin{aligned} J_r(\hbar^2/M, Z, Z_i, R, V_c) &= \lambda^{3-3q} J_r(1, 1, s_i, t_1, t_2), \\ J_p(\hbar^2/M, Z, Z_i, R, V_c) &= \lambda^{3m-3} J_p(1, 1, s_i, t_1, t_2). \end{aligned} \quad (37)$$

Then one obtains for the ratio,

$$\begin{aligned} J_{p/r}(\hbar^2/M, Z, Z_i, R, V_c) &= J_{p/r}(1, 1, s_i, t_1, t_2), \\ J_{p/r} &= \frac{J_p^{1/2m}}{J_r^{1/2q}}, \quad \frac{1}{m} + \frac{1}{q} = 2, \\ s_i &= \frac{M}{\hbar^2} Z_i \left(\frac{\hbar^2}{MZ} \right)^{\frac{n_i+2}{n+2}}, \quad t_1 = R(MZ/\hbar^2)^{1/(n+2)}, \\ t_2 &= V_c(M/\hbar^2)(\hbar^2/MZ)^{2/(n+2)}. \end{aligned} \quad (38)$$

Therefore in this case also, for given values of the parameters Z, Z_i, R, V_c , the ratio of Tsallis entropies depends on $Z_i/Z^{(n_i+2)/(n+2)}, t_1, t_2$.

4. Summary

For the bound states corresponding to the superposition of the power potential of the form $V(r) = Zr^n + \sum_i Z_i r^{n_i}$, where Z, Z_i, n, n_i are parameters, in the free state as well as in the additional presence of a spherical penetrable boundary wall located at radius R , the quantum mechanical uncertainty product and *all other net information measures* are shown here to depend only on the parameters $[s_i]$ defined by the ratios $Z_i/Z^{(n_i+2)/(n+2)}$. Further, we have shown that the introduction of a finite potential, V_c at the radial distance $r \geq R$ results in a complete set of scaling parameters given by $[s_i, t_1, t_2]$, where t_1 is given by $RZ^{1/(n+2)}$ and $t_2 = V_c/(Z)^{2/(n+2)}$. It is significant to note that the uncertainty like measures scale with the finite barrier as given by the parameter t_2 .

Acknowledgements

One of the authors, SHP acknowledges support from AICTE (All India Council for Technical Education) as Emeritus Fellow. KDS is grateful to the Department of Science and Technology for the award of JC Bose National Fellowship during 2009–2014.

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