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Information Entropy of Isospectral Hydrogen Atom

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Abstract—The position and momentum space information entropies of hydrogen atom are exactly evaluated. Using isospectral Hamiltonian approach, a family of isospectral potentials is constructed having same energy eigenvalues as that of the original potential. The information entropy content is obtained in position space as well as in momentum space. It is shown that the information entropy content in each level can be re-arranged as a function of deformation parameter.

Keywords—Information Entropy, BBM inequality, Isospectral Potential.

I. INTRODUCTION

INFORMATION ENTROPY is an important quantity employed to study quantum mechanical systems. It provide a measure of information about the probability distribution in position and momentum space. The Shannon information entropy of the single particle distribution in position space is

$$S_{pos} = -\int \rho(r) \ln \rho(r) dr \quad (1)$$

and in corresponding momentum space

$$S_{mom} = -\int \rho(p) \ln \rho(p) dp \quad (2)$$

where $\rho(p)$ denote the momentum space particle density. Information entropy plays a crucial role in a stronger formulation of the uncertainty relations. The information theoretic uncertainty relations were first conjectured by Hirschman [1] and Everett [2] in the context of many worlds interpretation and proved by Bialynicki-Birula and Mycielski (BBM) [3]. From the general properties of Fourier transform, it was proved in a d-dimensional system for wave functions normalized to unity,

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

Though S_{pos} and S_{mom} are individually unbounded, their sum is bounded from below. The total sum of information entropy in position space and momentum space is minimum for the ground state of harmonic oscillator. The physical meaning of the inequality is that an increase of S_{mom} corresponds to a decrease of S_{pos} and vice-versa, which indicates that a diffused density distribution $\rho(p)$ in momentum space is associated with a localized density distribution $\rho(r)$ in configuration space. A framework for deriving uncertainty relations of the above type, between general dynamical variables, not necessarily canonically conjugate ones, have been given recently [4-9]. A more general formulation of information theoretic uncertainty relations, which incorporates a pair of arbitrary quantum measurements have also been given [10].

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The position space and momentum space information entropies for various systems like the nuclear density distribution of nuclei, the electron density distribution of atoms and the valence electron density distribution of atomic clusters have been recently studied [11]. It is interesting to know the value of information entropy which is a measure of the spatial spread of the wave function for the various states of different systems.

The analytical determination of the position and momentum space entropies have been carried out only for a few quantum mechanical systems [12-16]. For the simple harmonic oscillator, the information entropies were exactly calculated for the ground state in both coordinate and momentum state, for which the BBM inequality is saturated [17]. The information entropies in various contexts, e.g., information theory, mathematics, mathematical physics, chemical physics and other areas of physics have been extensively analyzed in recent times [18-25].

We use the isospectral Hamiltonian approach to study the isospectral wave functions and their entropies. Two Hamiltonians are said to be strictly isospectral, if they have exactly same energy eigenvalue spectrum and S-matrix [26-28], whereas the wave functions and their dependent quantities are different. Though the idea of generating isospectral Hamiltonians using the Gelfand-Levitan approach or the Darboux procedure were known for some time, the supersymmetric quantum mechanical techniques make the procedure look simpler [29-31]. When one deletes a bound state of a given potential $V(x)$ and reintroduce the state, it involves solving a first order differential equation. Thus, a set of one-dimensional family of potentials $\hat{V}(x, \lambda)$ can be constructed which have the exactly same energy spectrum as that of $V(x)$. In general, for any one dimensional potential with n bound states, one can construct an n-parameter family of strictly isospectral potentials, i.e. potentials with eigenvalues, reflection and transmission coefficients identical to those for original potential. This aspect has been utilized profitably in many physical situations, which are of interest to various fields [32-35]. In this paper, we consider the hydrogen potential and calculate the position and momentum space information entropy exactly for ground state and excited states. Using isospectral Hamiltonian approach (discussed briefly in section 2), the deformed potential and their wave functions are constructed and used to calculate the information entropy for the isospectral potential. In last section, we conclude with brief discussion.

II. ISOSPECTRAL HAMILTONIAN APPROACH

The connection between the bound state wave functions and the potential is one of the key ingredients in solving exactly for the spectrum of one dimensional potential problems. Once, we know the ground state wave function (ψ_0) and choose its energy to be zero, we can factorize the Hamiltonian [31] as $H_1 = A^\dagger A$ where (in units $\hbar = 2m = 1$), $A = \frac{d}{dx} + W(x)$ and $A^\dagger = -\frac{d}{dx} + W(x)$ are the supersymmetric operators and $W(x) = -\frac{d}{dx}[\ln \psi_0(x)]$ is called the superpotential. We have

$$H_1\psi_n = A^\dagger A\psi_n = \epsilon_n \psi_n, \tag{4}$$

$$AA^\dagger(A\psi_n) = \epsilon_n(A\psi_n),$$

$$H_2(A\psi_n) = \epsilon_n(A\psi_n). \tag{5}$$

Here H_2 is the supersymmetric partner Hamiltonian of H_1, with eigenfunctions $\chi_n = A\psi_n$. It is obvious that H_2 has the same eigenvalue spectrum as that of H_1, but for the case $A\psi_0 = 0$, which is the case of supersymmetry broken. Explicitly, the relation between Hamiltonians reads,

$$E_n^{(2)} = E_{n+1}^{(1)}; \qquad E_0^{(1)} = 0,$$

$$\psi_n^{(2)} = [E_{n+1}^{(1)}]^{-\frac{1}{2}} A\psi_{n+1}^{(1)},$$

$$\psi_{n+1}^{(1)} = [E_n^{(2)}]^{-\frac{1}{2}} A^\dagger \psi_n^{(2)},$$

The superpotential relates the supersymmetric partner potentials $V_1(x)$ and $V_2(x)$ as

$$V_{1,2}(x) = W^2(x) \mp \frac{dW}{dx}. \tag{6}$$

It is well known that for the potential $V_2(x)$, the original potential $V_1(x)$ is not unique. The argument is as follows. Suppose H_2 has another factorization $BB^\dagger$, where $B = \frac{d}{dx} + \hat{W}(x)$, then, $H_2 = AA^\dagger = BB^\dagger$ but $H_1 = B^\dagger B$ is not $A^\dagger A$ rather it defines a certain new Hamiltonian. For superpotential $\hat{W}(x)$, the partner potential $V_2(x)$ is

$$V_2(x) = \hat{W}^2(x) + \hat{W}'(x). \tag{7}$$

Consider the most general solution as $\hat{W}(x) = W(x) + \phi(x)$, which demands that,

$$\phi^2(x) + 2W(x)\phi(x) + \phi^{'}(x) = 0. \tag{8}$$

The solution of the above equation is $\phi(x) = \frac{d}{dx}\ln[I(x) + \lambda]$, where $I(x) = \int_{-\infty}^{x} \psi_0^2(x^{'})dx^{'}$ and λ is a constant. Therefore, we obtain,

$$\hat{W}(x) = W(x) + \frac{d}{dx}\ln[I(x) + \lambda]. \tag{9}$$

The corresponding one parameter family of potentials $\hat{V}_1(x, \lambda)$ is given as

$$\hat{V}_1(x, \lambda) = V_1(x) - 2\frac{d^2}{dx^2}(\ln(I(x) + \lambda)). \tag{10}$$

The normalized ground state wave function corresponding to the potential $\hat{V}_1(x, \lambda)$ reads

$$\hat{\psi}_0(x, \lambda) = \frac{\sqrt{\lambda(1+\lambda)}\psi_0(x)}{I(x) + \lambda}, \tag{11}$$

where $\lambda \notin (0, -1)$. The eqs. 10, and 11 represent the one parameter family of isospectral potentials and the wave functions which shall be used to obtain the information entropy of hydrogen atom as a function of deformation parameter.

III. Information Entropy of Hydrogen Atom

The one dimensional hydrogen atom is an interesting mathematical and physical problem to study bound states and quantum degeneracy issues. The Hydrogen atom is described by Coulomb potential,

$$V(x) = -\frac{1}{\mid x \mid} \tag{12}$$

The ground state eigenfunction in position space [36,37] is given by

$$\psi(x) = \alpha^{-1/2} e^{-\frac{|x|}{\alpha}} \qquad \alpha \to 0, \tag{13}$$

and for excited states

$$\psi_{even}(x) = \sqrt{\frac{2}{n^5}} e^{-|x|/n} \mid x \mid L_{n-1}^1(2 \mid x \mid /n) \tag{14}$$

$$\psi_{odd}(x) = \sqrt{\frac{2}{n^5}} e^{-|x|/n} x L_{n-1}^1(2 \mid x \mid /n) \tag{15}$$

The corresponding eigenfunctions in momentum space are

$$\psi_0(p) = \sqrt{\frac{2}{\pi}} \frac{\alpha^{1/2}}{(1 + \alpha^2 p^2)} \qquad \alpha \to 0 \tag{16}$$

$$\psi_n(p) = \sqrt{\frac{2n}{\pi}} \frac{e^{\pm 2in \ \tan^{-1}(np)}}{1 + n^2p^2} \tag{17}$$

The ground state information entropy in position and momentum space is

$$S_{pos} = 1 + \ln \alpha$$

$$S_{mom} = \ln\left(\frac{8\pi}{e^2}\right) - \ln \alpha$$

for excited states

$$S_{pos} = \ln\left(\frac{2n^2}{e^{3n}}\right) - \frac{1}{n^2}(J_2 + J_3/2)$$

$$S_{mom} = \ln\left(\frac{8\pi}{e^2 n}\right)$$

where

$$J_2 = \int_0^\infty t^2 e^{-t} \ln t [L_{n-1}^1(t)]^2 dt$$

$$J_2 = \int_0^\infty t^2 e^{-t} [L_{n-1}^1(t)]^2 \ln[L_{n-1}^1(t)]^2 dt$$

The entropy densities for position and momentum space in different states are plotted in the figure 1 and 2. It is interesting to note that the momentum space information density plot develop a dip at its peak with the increase in value of n. The total information entropy for one dimensional hydrogen atom in ground state is 2.2242 which is above the BBM saturation value 2.1447. For the excited states, the value is higher than ground state.

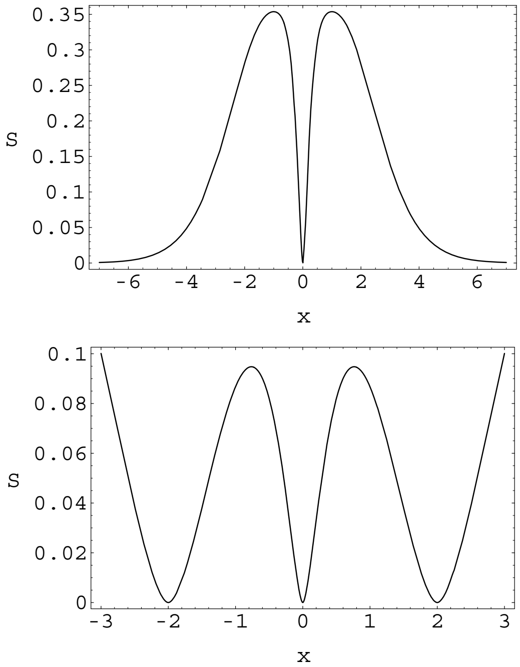

Fig. 1. Position space information densities of hydrogen potential for $n = 1$ and $n = 2$.

IV. Information Entropy of Isospectral Hydrogen Atom

Using isospectral hamiltonian approach, the ground state wave function is obtained as

$$\hat{\psi}_0(x, \lambda) = \frac{2\sqrt{\lambda(\lambda+1)}}{\sqrt{\alpha}} \frac{e^{-\frac{|x|}{\alpha}}}{2(\lambda+1) - e^{-\frac{2|x|}{\alpha}}} \quad (18)$$

The information entropy in position space for ground state of the isospectral potential is obtained after some calculations as

$$\begin{aligned} \hat{S}_0 &= \frac{8\lambda(\lambda+1)}{2(2\lambda+1)(2\lambda+2)} (Log\left[\frac{4\lambda(\lambda+1)}{\alpha}\right] \\ &+ (2\lambda+1)Log[(2\lambda+1)] - 2(2\lambda+2)Log[2\lambda+1] \\ &+ (2\lambda+1)Log[2\lambda+2] - 2) \quad (19) \end{aligned}$$

The excited state isospectral wave function for odd values of n is calculated as

$$\begin{aligned} \hat{\psi}_{n+1}(x, \lambda) &= \sqrt{\frac{2}{n^5}} e^{-\frac{|x|}{n}} [x L^1_{n-1}(\frac{2 \mid x \mid}{n}) \\ & \{1 - \frac{1}{(n+1)^2} \frac{e^{-\frac{2|x|}{n}}}{\alpha^2(\lambda + 1 - \frac{1}{2} e^{-2\frac{|x|}{n}})}\} \\ &- \frac{1}{(n+1)^2} \frac{e^{-\frac{2|x|}{n}}}{\alpha(\lambda + 1 - \frac{1}{2} e^{-\frac{|x|}{n}})} \\ & \{(1 - \frac{x}{n}) L^1_{n-1}(\frac{2 \mid x \mid}{n}) \\ &- \frac{2x}{n} L^2_{n-2}(\frac{2 \mid x \mid}{n})\}] \quad (20) \end{aligned}$$

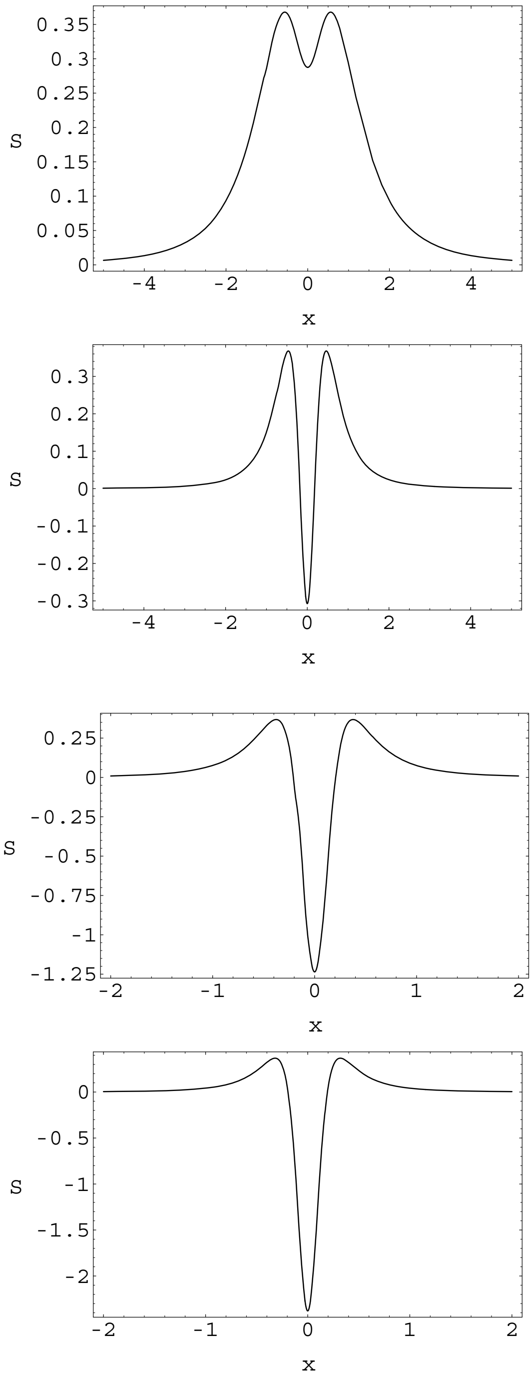

Fig. 2. Momentum space information densities of hydrogen potential for (a) $n = 1$, (b) $n = 2$, (c) $n = 3$ and (d) $n = 4$.

and for even n, we have

$$\begin{aligned}\hat{\psi}_{n+1}(x,\lambda) &= \sqrt{\frac{2}{n^5}}e^{-\frac{|x|}{n}}[| x | L^1_{n-1}(\frac{2 | x |}{n}) \\ &\{1-\frac{1}{(n+1)^2}\frac{e^{-\frac{2|x|}{n}}}{\alpha^2(\lambda+1-\frac{1}{2}e^{-2\frac{|x|}{n}})}\} \\ &- \frac{1}{(n+1)^2}\frac{e^{-\frac{2|x|}{n}}}{\alpha(\lambda+1-\frac{1}{2}e^{-\frac{|x|}{n}})} \\ &\{(1-\frac{| x |}{n})L^1_{n-1}(\frac{2 | x |}{n}) \\ &- \frac{2 | x |}{n}L^2_{n-2}(\frac{2 | x |}{n})\}] \qquad (21)\end{aligned}$$

The excited state information entropy in position space is obtained as

$$\hat{S}_{n+1}(x) = -\frac{2}{n^5}J_1 - \frac{4}{n^5}J_2 \qquad (22)$$

where

$$J_1 = \int e^{-\frac{2|x|}{n}} J_3^2 Log[\frac{2}{n^5}e^{-2\frac{|x|}{n}}]dx$$

$$J_2 = \int e^{-\frac{2|x|}{n}} Log[J_3]dx$$

and for odd n

$$J_3 = xL^1_{n-1}(\frac{2 | x |}{n})\{1-\frac{1}{(n+1)^2}\frac{e^{-\frac{2|x|}{n}}}{\alpha^2(\lambda+1-\frac{1}{2}e^{-2\frac{|x|}{n}})}\}$$

$$-\frac{1}{(n+1)^2}\frac{e^{-\frac{2|x|}{n}}}{\alpha(\lambda+1-\frac{1}{2}e^{-\frac{|x|}{n}})}$$

$$\{(1-\frac{x}{n})L^1_{n-1}(\frac{2 | x |}{n}) - \frac{2x}{n}L^2_{n-2}(\frac{2 | x |}{n})\}$$

whereas for even n,

$$J_3 =| x | L^1_{n-1}(\frac{2 | x |}{n})\{1-\frac{1}{(n+1)^2}\frac{e^{-\frac{2|x|}{n}}}{\alpha^2(\lambda+1-\frac{1}{2}e^{-2\frac{|x|}{n}})}\}$$

$$-\frac{1}{(n+1)^2}\frac{e^{-\frac{2|x|}{n}}}{\alpha(\lambda+1-\frac{1}{2}e^{-\frac{|x|}{n}})}$$

$$\{(1-\frac{| x |}{n})L^1_{n-1}(\frac{2 | x |}{n}) - \frac{2 | x |}{n}L^2_{n-2}(\frac{2 | x |}{n})\}$$

In momentum space, the ground state isospectral wave function is calculated as

$$\hat{\psi}_0(p,\lambda) = \sqrt{72\pi\alpha\lambda(\lambda+1)}\frac{1}{[3\pi(2\lambda+1)(1+\alpha^2p^2)+t_1]} \qquad (23)$$

where

$$t_1 = 6(1+\alpha^2p^2)tan^{-1}(\alpha p) + p$$

The ground state information entropy is calculated numerically using the above wave function and plotted in figure 3 as a function of deformation parameter. The information entropy increases with deformation parameter to 1.2377 for $\lambda = 0.57$ and then gets saturated to 1.22 for large values of the of λ. The excited state isospectral wave function in momentum space reads,

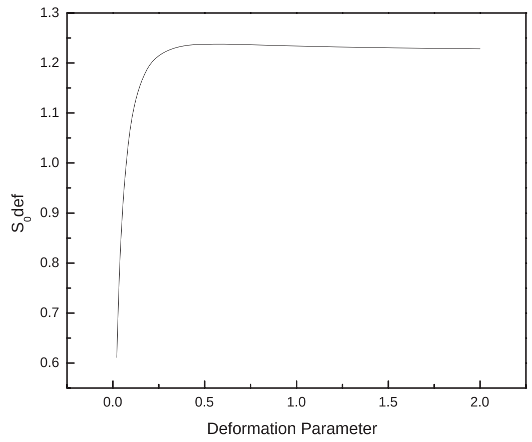

Fig. 3. Momentum space information entropy of hydrogen atom in the ground state as a function of deformation parameter.

$$\hat{\psi}_n(p,\lambda) = \frac{Exp[2i\ n\tan^{-1}(np)]\sqrt{\frac{2}{\pi}}\left[n^2(1+n^2p^2)^3+t_2\right]}{n^{3/2}(1+n^2p^2)^4} \qquad (24)$$

where

$$t_2 = \frac{4\alpha(-p\alpha^2+n^2(p-i(1+p^2\alpha^2)))}{(1+p^2\alpha^2)(\pi+\lambda\pi+2\tan^{-1}(np))}.$$

Using above wave function, information entropy in momentum space can be obtained in any excited state for different values of deformation parameter. For first excited state, information entropy is 0.59 for $\lambda = .001$, 1.13 for $\lambda = 1$ and approaches to 1.22 for $\lambda = 8$. The information entropy in different states is rearranged as a function of deformation parameter.

V. Conclusion

The information entropy of quantum mechanical systems is a great scientific challenge of present time as it provides a deeper insight into the internal structure of the systems. The information entropies of a class of systems is obtained, which belong to the hydrogen potential. In position space, the information entropy for isospectral potential is exactly calculated for all the energy levels. The expression for momentum space isospectral wave function are obtained analytically for the ground state as well as excited states which is used to calculate the information entropy in momentum space. It is found that the information entropy is reduced for the smaller values of deformation parameter. For lower information entropy, the wave function will be more concentrated and the accuracy in predicting the localization of the particle will be higher. This approach can also be applied in the reduction of Heisenberg's uncertainty in position space.

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