Information Density of Nanostructure Systems

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ABSTRACT

There has been increasing interest in the studies on information theoretic measures for quantum mechanical systems. The systems based on quantum-dot nanostructures could be used as components for quantum information processing devices. One of the advantages of the use of quantum dots is that the parameters of the system may be changed, allowing the properties of semiconductor nanostructures to be tailored. The development in technology appears to promise advanced engineering of quantum dot based structures leading to the fabrication of quantum dot systems. To use quantum dot devices for quantum computing require the ability to generate and manipulate entanglement within these structures. Using Supersymmetric Quantum mechanics, isospectral Hamiltonian approach is utilized to calculate the information density of the isospectral potential which contains a free parameter. This free parameter can be adjusted to model the complex nanostructure materials and therefore to calculate their entanglement degree.

Keywords: Information Density, Nanostructure, Isospectral Hamiltonians.

1. INTRODUCTION

The quantum information theory has found a continuously increasing importance in condensed matter physics, where they offer a new perspective to the structure of complex quantum systems. In quantum dot systems, the entanglement could be controlled through externally applied electro-magnetic fields or by varying the parameters of the nanostructure. Since the entanglement is considered a key ingredient for quantum information processes, so the availability of entanglement would be useful in designing these nanostructures. However it is practically almost impossible to exactly model complex nanostructures and precisely calculate their entanglement degree. Changing the confinement potential of quantum dot structures influences the spatial entanglement within the nanostructures

[1-2]. Such a property could be exploited to design the nanostructures according to the level of entanglement needed for a specific application.

Boltzmann-Shannon information entropy is a fundamental quantity related to thermodynamical entropy, which measures the extent of single particle density. According to Density Function theory, a many fermion system can be completely characterized by the single particle distribution density, which is denoted by $\rho(r)$ in position space and $\rho(p)$ in momentum space. The position and momentum space information entropies are given by the expression

$$S(pos) = -\int \rho(r) \ln \rho(r) dr$$

$$S(mom) = -\int \rho(\mathbf{p}) \ln \rho(\mathbf{p}) d\mathbf{r}$$
⁽¹⁾

The Information entropy plays an important role in stronger formulation of the uncertainty relations. These uncertainty relations were first given by Everett and Hirschman and then proved by Bialynicki-Birula and Mycielski and independently by Beckner. Using the properties of Fourier transform, it was proved that for wave functions normalized to unity, $S(pos) + S(mom) \ge d(1+ln \pi)$, where *d* is the dimension. These information entropies are individually unbounded but their sum is bounded from below. The minimum value of information entropy is found 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 diffuse density distribution $\rho(p)$ in momentum space is associated with a localized density distribution $\rho(r)$ in configuration space[3-12].

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 eigen value spectrum and S-matrix [13], 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 [14-15]. When one deletes a bound state of a given potential V(x) and re-introduce 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 [16-20]. In this paper, we have performed the model calculations of position space information density for isospectral potential as an indicator of the entanglement for nanostructure system.

2. ISOSPECTRAL HAMILTONIAN APPROACH

The relation between the bound state wave functions and the potential is utilized in solving exactly for the spectrum of one-dimensional potential problems. The supersymmetric partner potentials $V_1(x)$ and $V_2(x)$ are related through superpotential $W(x) = -\frac{d}{dx} [\ln \psi_0(x)]$ as

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

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

$$\hat{V}_{1}(x,\lambda) = V_{1}(x) - 2\frac{d^{2}}{dx^{2}}(\ln(I(x) + \lambda)).$$
(3)

The normalized ground state wave function corresponding to the above potential reads

$$\hat{\psi}_0(x,\lambda) = \frac{\sqrt{\lambda(1+\lambda)}\psi_0(x)}{I(x)+\lambda},\tag{4}$$

where $\lambda \notin (0,-1)$. The excited state eigenfunctions for the potential $\hat{V}_1(x,\lambda)$ are given by [15],

$$\hat{\psi}_{n+1}(x,\lambda) = \psi_{n+1}(x) + \frac{1}{E_{n+1}} \left(\frac{I'(x)}{I(x) + \lambda} \right) \times \left(\frac{d}{dx} + W(x) \right) \psi_{n+1}(x).$$
(5)

Using the similar procedure, the two-parameter ground state wave function can be obtained as

$$\hat{\psi}_{0}(x,\lambda_{0},\lambda_{1}) = \frac{1}{\phi_{0}(x,\lambda_{0},\lambda_{1})} = \frac{\psi_{0}(x)}{\hat{A}_{1}(\lambda_{1})A_{1}(I_{0}(x)+\lambda_{0})}.$$
(6)

The equations (3), (4) and (5) represent the one-parameter family of isospectral potentials and wave functions, which shall be used to calculate the information density. Further, the system can also be studied using two parameters using equation (6).

3. INFORMATION DENSITY OF ISOSPECTRAL HYDROGEN POTENTIAL

Using Supersymmetric Quantum mechanics, the isospectral Hamiltonian approach can be utilized to calculate the information density of the isospectral potential which contains a free parameter. This free parameter can be adjusted to model the complex nanostructure materials and therefore precisely calculate their entanglement degree. The isospectral Hamiltonian approach is used to construct the isospectral Hydrogen potential and the corresponding wave functions. The deformed wave functions are used to calculate the information density for the isospectral potential. The one dimensional hydrogen atom is an interesting problem to study the bound states. It is described by the Coulomb potential,

$$V(x) = -\frac{1}{|x|}$$
(7)

The ground state wave function is given by [21, 22],

$$\psi(x) = \alpha^{-\frac{1}{2}} e^{-\frac{|x|}{\alpha}}$$
(8)

For excited states

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

$$\psi_{odd}(x) = \sqrt{\frac{2}{n^5}} e^{-\frac{|x|}{n}} x L_{n-1}^1(\frac{2|x|}{n})$$
(9)

The corresponding eigenfunctions in momentum space are

$$\psi_0(p) = \sqrt{\frac{2}{\pi}} \frac{\alpha^2}{(1+p^2 \alpha^2)} \tag{10}$$

$$\psi_n(p) = \sqrt{\frac{2n}{\pi}} \, \frac{e^{\pm 2in} \tan^{-1}(n\,p)}{(1+p^2\,n^2)} \tag{11}$$

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

$$\psi_0(x,\lambda) = \frac{2\sqrt{\lambda(\lambda+1)}}{\sqrt{\alpha}} \frac{e^{-\frac{|x|}{\alpha}}}{\frac{2(\lambda+1)-e^{-\frac{2}{\alpha}}}{\alpha}}$$
(12)

After some calculation, the excited state isospectral wave function for odd values of n is calculated as

$$\psi_{n+1}(x,\lambda) = \sqrt{\frac{2}{n^5}} e^{-\frac{|x|}{n}} \left[x \, \mathrm{L}_{n-1}^{1}(\frac{2|x|}{n}) \right] \left\{ 1 - \frac{e^{\frac{2|x|}{n}}}{(n+1)^2 \alpha^2 \left(\frac{\lambda+1-\frac{1}{2}e^{-\frac{2|x|}{n}}}{n} \right)} - \frac{e^{\frac{2|x|}{n}}}{(n+1)^2 \alpha \left(\frac{\lambda+1-\frac{1}{2}e^{-\frac{|x|}{n}}}{n} \right)} \left(1 - \frac{x}{n} \right) \, \mathrm{L}_{n-1}^{1}\left(\frac{2|x|}{n} \right) - \frac{2x}{n} \, \mathrm{L}_{n-2}^{2}(\frac{2|x|}{n}) \right]$$
(13)

and for even n, we have

$$\psi_{n+1}(x,\lambda) = \sqrt{\frac{2}{n^5}} e^{-\frac{|x|}{n}} \left| |x| L_{n-1}^1(\frac{2|x|}{n} \left\{ 1 - \frac{e^{-\frac{2|x|}{n}}}{(n+1)^2 \alpha^2} \left(\lambda + 1 - \frac{1}{2} e^{-\frac{2|x|}{n}} \right) \right\} - \frac{e^{-\frac{2|x|}{n}}}{(n+1)^2 \alpha} \left\{ \frac{e^{-\frac{2|x|}{n}}}{(n+1)^2 \alpha} \left(\frac{\lambda + 1 - \frac{1}{2} e^{-\frac{2|x|}{n}}}{(n+1)^2 \alpha} \right) \left\{ \left(1 - \frac{|x|}{n} \right) L_{n-1}^1(\frac{2|x|}{n}) - \frac{2|x|}{n} L_{n-2}^2(\frac{2|x|}{n}) \right\} \right\}$$
(14)

In momentum space, the ground state isospectral wave function is calculated after some lengthy but straight forward calculations as

$$\psi_{0}(p,\lambda) = \sqrt{72 \pi \alpha \lambda(\lambda+1)} \frac{1}{[3\pi(2\lambda+1)(1+\alpha^{2}p^{2})+t_{1}]}$$
(15)
$$t_{1} = 6(1+\alpha^{2}p^{2}) \tan^{-1}(\alpha p) + p$$

The excited state isospectral wave function in momentum space reads,

$$\psi_{n}(p,\lambda) = \frac{Exp\left[2\,i\,n\,\tan^{-1}(n\,p)\right]\,\sqrt{\frac{2}{\pi}}\left[n^{2}\left(1+n^{2}p^{2}\right)^{3}+t_{2}\right]}{n^{\frac{3}{2}}\left(1+n^{2}p^{2}\right)^{4}}$$

$$t_{2} = \frac{4\,a\left(-p\,\alpha^{2}+n^{2}\left(p-i\left(1+\alpha^{2}p^{2}\right)\right)\right)}{\left(1+\alpha^{2}p^{2}\right)\left(n+\lambda\,\pi+2\,\tan^{-1}(n\,p)\right)}$$
(16)

Using isospectral wave functions, the information density is calculated for different states and their characteristic features are graphically demonstrated for some levels of the potential. The Figs. 1 and 2 demonstrates the variation of information density as a function of deformation parameter in position and momentum space respectively. In Figs. 3 and 4, the information density is analyzed with the variation in parameter α in addition to the deformation parameter.



Fig 1: Information density in position space for isospectral Hydrogen potential with $\alpha = 1$ and deformation parameter (a) $\lambda = 0.1$, (b) $\lambda = 0.22$, (c) $\lambda = 0.25$, (d) $\lambda = 0.3$



Fig 2: Information density in momentum space for isospectral Hydrogen potential with $\alpha = 1$ and deformation parameter (a) $\lambda = 0.3$, (b) $\lambda = 0.5$, (c) $\lambda = 0.8$, (d) $\lambda = 2$



Fig 3: Information density in position space for isospectral Hydrogen potential with α and deformation parameter (a) α =0.1, λ = 0.2, (b) α = 0.2, λ =0.3, (c) α = 0.3, λ = 0.4, (d) α = 0.4, λ = 0.45



Fig 4: Information density in momentum space for isospectral Hydrogen potential with α and deformation parameter (a) α =1.5, λ = 0.15, (b) α =2, λ =0.2, (c) α =3, λ =0.3, (d) α =4, λ =0.4

The momentum probability density function of the hydrogen potential exhibits sharp distant peaks. The dip in the momentum density function changes with the parameter α . As seen in figures 1 and 3, the position space entropy densities have quite asymmetric shape which depends on the values of different parameters. It is interesting to observe the development of sharp dip on the peaks of density functions which increases with the deformation parameter characterizing specific properties of the potential. The momentum density function shown in Figs. 2 and 4 as function of different parameters also possess different behavior for various values of the parameter.

4. Conclusion

Using Supersymmetric Quantum mechanics, isospectral Hamiltonian approach is utilized to calculate the information density of the isospectral potential which contains a free parameter. This free parameter can be adjusted to model the complex nanostructure materials and therefore precisely calculate their entanglement degree.

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