

Open access Journal International Journal of Emerging Trends in Science and Technology IC Value: 76.89 (Index Copernicus) Impact Factor: 4.219 DOI: https://dx.doi.org/10.18535/ijetst/v4i8.05

# **Information Entropy of Nanostructure systems**

Authors **Anil Kumar<sup>1</sup>, Rajesh Kumar<sup>2</sup>** <sup>1,2</sup>Department of Physics, JC DAV College, Dasuya-144205, Punjab

# Abstract

Systems based on quantum-dot nanostructures could be used as components for quantum information processing devices. One of the possible 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 seemingly inexorable progress of technology appears to promise advanced engineering of quantum dot based structures, thus leading to the fabrication of coupled and scalable quantum dot systems. To use quantum dot devices for quantum computing necessitates the ability to generate and manipulate entanglement within these structures. Using Supersymmetric Quantum mechanics, isospectral Hamiltonian approach is utilized to calculate the information entropy 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 Entropy, nanostructure, Isospectral Hamiltonians.

# 1. Introduction

The quantum information theoretic concepts have found a continuously increasing importance in condensed matter physics, where they offer a new perspective to the structure of complex quantum many-body systems. In quantum dot systems this 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, closely related to thermodynamical entropy, which measures the spread or extent of the 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

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

Information entropy plays a crucial role in a stronger formulation of the uncertainty relations. The information theoretic uncertainty relations were first conjectured by Everett and Hirschman in 1957 and proved by Bialynicki-Birula and Mycielski and independently by Beckner. From the general 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. Though the 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 diffuse density distribution  $\rho(p)$  in momentum space is associated with a localized density distribution  $\rho(\mathbf{r})$  in configuration space[3-12]. In this paper, we investigate the use of the position space information entropy as an indicator of the entanglement for nanostructure system.

#### 2. Isospectral Hamiltonian Approach

The supersymmetric quantum mechanical techniques have been extensively used to study the various concepts in symmetry breaking. Using these concepts, the isospectral Hamiltonian method has been utilized in the generalization of the solutions for different systems [13-17]. The energy spectrum of potential is derived upon utilizing the relationship in eigenfunctions and the potential. The ground state eigenfunction is obtained and choosing its energy equal to zero, the Hamiltonian of the system can be factorized in terms of supersymmetric operators  $A = \frac{d}{dx} + W(x)$  and  $A^{\dagger} = -\frac{d}{dx} + W(x)$  as  $H_1 = A^{\dagger}A$ , where the superpotential W(x) is given as

$$W(x) = -\frac{d}{dx} [\ln \psi_0(x)].$$
(3)

Consider the equation

$$H_{1}\psi_{n} = A^{\dagger}A\psi_{n} = \varepsilon_{n}\psi_{n},$$
(4)

$$AA^{\dagger}(A\psi_{n}) = \varepsilon_{n}(A\psi_{n}),$$

$$H_{2}(A\psi_{n}) = \varepsilon_{n}(A\psi_{n}).$$
(5)

Where  $H_2$  is supersymmetric partner Hamiltonian of  $H_1$  corresponding to the eigenfunction  $\chi_n = A \psi_n$ . The different Hamiltonians are related as,

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

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

The potentials corresponding to partner Hamiltonians are called supersymmetric partner potentials. These are related through the superpotential as

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

(6)

Here, it is stated that corresponding to the partner potential  $V_2(x)$ , the original potential  $V_1(x)$  does not have unique value. If, we consider the factorization for  $H_2$  as  $BB^{\dagger}$ , where  $B = \frac{d}{dx} + \hat{W}(x)$ , then, the Hamiltonian  $H_2 = AA^{\dagger} = BB^{\dagger}$  but  $H_1 = B^{\dagger}B$  is not equal to  $A^{\dagger}A$  and it defines some another Hamiltonian. We have the relation,

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

For a general solution, we obtain

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

which has solution as  $\phi(x) = \frac{d}{dx} \ln[I(x) + \lambda]$ , where  $I(x) = \int_{-\infty}^{x} \psi_0^2(x') dx'$  and  $\lambda$  is a constant. For the superpotential

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

The presence of a constant in these equations define a one-parameter set of isospectral potentials as

$$\hat{V}_{1}(x,\lambda) = V_{1}(x) - 2\frac{d^{2}}{dx^{2}}(\ln(I(x) + \lambda)).$$
(10)

The corresponding ground state eigenfunction is calculated as

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

where  $\lambda \notin (0,-1)$ . The isospectral eigenfunctions corresponding to excited state of the potential have been obtained after some calculations as,

$$\hat{\psi}_{n+1}(x,\lambda) = \psi_{n+1}(x) + \frac{1}{E_{n+1}} \left( \frac{I'(x)}{I(x) + \lambda} \right)$$
$$\times \left( \frac{d}{dx} + W(x) \right) \psi_{n+1}(x).$$
(12)

The one-parameter isospectral potentials and corresponding eigenfunctions derived in above equations have been used to calculate the information density of the nanostructure materials.

# 3. Information Entropy of Isospectral Potential

Using Supersymmetric Quantum mechanics, isospectral Hamiltonian approach can be utilized to calculate the information entropy 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 Poschl-Teller potential

and the corresponding wave functions. The deformed wave functions are used to calculate the information entropy for the isospectral potential. For n-level potential, the one parameter isospectral ground state wave function is obtained as

$$\hat{\psi}_0(x,\lambda) = \frac{\sqrt{\lambda(1+\lambda)\psi_0(x)}}{\int_{-\infty}^x \psi_0^2(x)dx + \lambda} \text{ where } \psi_0(x) \frac{1}{\sqrt{\beta\left(\frac{1}{2},n\right)}} \text{ Sech}^n x$$

$$\hat{\psi}_{0}(x,\lambda) = \frac{\sqrt{\lambda(1+\lambda)}}{\sqrt{\beta\left(\frac{1}{2},n\right)}} \frac{\operatorname{Sech}^{n} x}{\frac{1}{\beta\left(\frac{1}{2},n\right)} \left[\frac{\operatorname{Sinhx}}{2n-1} \left\{\operatorname{Sech}^{2n-1} x + f(x)\right\}\right] + \lambda}$$
(13)

where

$$f(x) = \sum_{k=1}^{n-1} \frac{\left(2^k (n-1)(n-2)\dots(n-k)\right)}{(2n-3)(2n-5)\dots(2n-2k-1)} Sech^{(2n-2k-1)}x + \frac{2}{3}$$

First excited state wave function in position space is given by

$$\psi_1(x) = \frac{1}{\sqrt{\beta\left(\frac{1}{2}, n-1\right) - \beta\left(\frac{1}{2}, n\right)}} \operatorname{Sech}^{n-1} x \tanh x$$

And corresponding deformed excited state wave function is obtained using

$$\hat{\psi}_1(x) = \psi_1(x) + \frac{1}{E_1} \left( \frac{I'}{I+\lambda} \right) \left( \frac{d}{dx} + W(x) \right) \psi_1(x)$$

by puttin  

$$E_1 = \frac{3}{2}, W(x) = -\frac{d}{dx} \ln \psi_0(x), I(x) = \int_{-\infty}^x \psi_1^2(x) dx$$

we obtain

and  $I'(x) = \psi_1^2(x)$ 

by

$$\hat{\psi}_1(x,\lambda) = A \left[ Sech^{n+1}x \tanh x + \frac{2}{3}A^2 \left( \frac{Sech^{2(n-1)}x \tanh x}{I(x) + \lambda} \right) Sech^{n-1}x \right]$$

where

$$I(x) = A^{2} \left\{ Sinh \, x \, Sech^{2n-3}x \left( \frac{1}{2n-3} - \frac{Sech^{2}x}{2n-1} - \frac{2^{n-1}(n-1)!}{(2n-3)!!} \, Sech \, x \right) \right\}$$

The information entropy in *n*-level Poschl-Teller potential for ground state as a function of  $\lambda$  is solved as

$$\hat{S}_0 = -\int_{-\infty}^{\infty} \psi_0^2 \ln \psi_0^2 dx$$

Similarly the information entropy for excited states can be obtained. The position space information entropy for n = 3 is calculated using the isospectral wave functions. In the case of undeformed potential, it has values 0.606, 1.106 and 1.640 for ground state, first excited

ng

state and second excited state respectively but when it is evaluated using  $\hat{\psi}_0(x,\lambda)$ .  $\hat{\psi}_1(x,\lambda)$  and  $\hat{\psi}_2(x,\lambda)$ , it is found that the information entropy content is reduced substantially with the deformation parameter. For  $\lambda = 0.1$ , we have  $S_{0 pos}^{(3)} = 0.52$  and this value increases to 0.606 for large values of  $\lambda$ . Similar results are also obtained for  $S_{1 pos}^{(3)}$ , but for  $S^{(3)}_{2\ pos}$ , the information entropy content first increases from a smaller value and then decreases to the undeformed value for large deformation parameter value. The total information entropy for ground state and first excited state is plotted as a function of deformation parameter, which shows that the total entropy is reduced by choosing smaller values of  $\lambda$ .

We also computed the two parameter wave functions and calculated the information entropy content for different positive and negative values of deformation parameter  $\lambda_0$  and  $\lambda_1$ . The results are shown in Figure for ground state and first excited state respectively. For large values of  $\lambda_0$ and  $\lambda_1$ , the value of deformed information entropy approaches the undeformed value. The variation of double deformed information entropy in ground state with  $\lambda_0$  is shown for large, intermediate and small values of  $\lambda_1$ . In this case, the value of information entropy is reduced from 0.606 to 0.1

or even less for smaller values of  $\lambda_0$ . In first

excited state, for small  $\lambda_1$ , the value of information entropy increases with increase in  $\lambda_0$ , but it become constant below the undeformed value. For large  $\lambda_1$ , the value of information entropy first decreases and then increases and becomes constant at the value of undeformed information entropy.



Figure 1: One parameter deformed ground state information entropy as a function of deformation parameter.



Figure 2: One parameter deformed first excited state information entropy as a function of deformation parameter.





function of  $\lambda_0$  for different (large, intermediate, and small), values of  $\lambda_1$ . For solid line  $\lambda_1 = 10.0$  for broken line  $\lambda_1$ 

=1.0 and for dotted line  $\lambda_1 = 0.65$ 

### Conclusion

Using Supersymmetric Quantum mechanics, isospectral Hamiltonian approach is utilized to calculate the information entropy 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.

#### References

- Coe JP, Abdullah S, D'Amico I. Geometry induced entanglement transitions in nanostructures. J Appl Phy 2010:107:09E110.
- Coe JP, Franca VV, D'Amico I. Entanglement and position-space information entropy: Hubbard model as an approximation to nanostructure systems. J Phy: Conf Series 2011:303:012110.
- Pooja, Kumar R, Kumar G, Kumar R, Kumar A. Quantum Information Entropy of Eckart Potential. Int J Quantum Chem. 2016:116:1413-1418.
- Atre R, Kumar A, Kumar CN, Panigrahi PK. Quantum-Information Entropies of the Eigenstates and the Coherent State of the Poschl-Teller Potential. Phys Rev A. 2004:69:052107(1-6).
- Bouvrie PA, Angulo JC, Dehesa JS. Entropy and complexity analysis of Dirac-delta-like quantum potentials Physica A.

2011:390:2215.

- Kumar A. Information Entropy of Isospectral Poschl-Teller Potential. Ind J Pure & App Phys. 2005:43:958-963.
- Kumar A, Pooja. Information Density of Isospectral Potential. Int J Pure and App Phys, 2017:13(1):27-33.
- Deutsch D. Uncertainty in quantum measurements. Phys Rev Lett. 1983:50:631-633.
- Pooja, Sharma A, Gupta R, Kumar A. Quantum Information Entropy of Modified Hylleraas plus Exponential Rosen-Morse Potential and Squeezed States. Int J Quantum Chem. 2017:117:e25368.
- Sun GH, Aoki MA, Dong SH. Quantum Information Entropies of the Eigenstates for the Pöschl-Teller-like Potential. Chin Phys B. 2013:22(5):050302(1-5).
- Jizba P, Dunningham JA, Joo J. Role of Information Theoretic Uncertainty Relations in Quantum Theory. Annals Phys. 2015:355:87-114.
- March NH, Angilella GGN, Pucci R. Natural Orbitals in Relation to Quantum Information Theory: From Model Light Atoms Through to Emergent Metallic Properties. Int J Mod Phys B. 2013:27:133021(1-26).
- Pursey DL. New Families of Isospectral Hamiltonians. Phys Rev D. 1986:33:1048-1055.
- Cooper F, Khare A, Sukhatme U. Supersymmetry and Quantum Mechanics. Phys Rep. 1995:251:267-385.
- 15. Kumar A. Calculation of Moments and

Uncertainty in Position Space. Am J Sci Tech. 2014:1(5):283-287.

- Kumar A. Generalization of Soliton Solutions. Int J Nonlin Sc. 2012:13(2):170-176.
- Kumar A, Kumar CN. Calculation of Franck-Condon factors and r-centroids using isospectral Hamiltonian approach. Ind J Pure & App Phys. 2005:43:738-742.