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Calculation of moments and uncertainty in position space

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Abstract
The moments are calculated for some levels of Pöschl-Teller potentials. Using isospectral Hamiltonians, the calculations are extended to deformed wave functions and their properties are graphically demonstrated. Two Hamiltonians are said to be strictly isospectral, if they have exactly same eigenvalue spectrum and S-matrix. The wave functions and their dependent quantities are different but related. This property is utilized to obtain the uncertainty in position space. Due to the presence of a deformation parameter, the uncertainty in position space is rearranged.

1. Introduction

The studies of molecular properties with high accuracy require the treatment of electron correlation effects. The calculation of electron transition moments have been performed using various methods. Some relations have been derived in N-dimensional space which connects the moments of the ground state density to the lowest multipole excitation energy [1-4]. The present method for these calculations includes a free parameter which can be adjusted without disturbing the energy eigenvalues. Applying supersymmetric quantum mechanical techniques [5-11], the isospectral Hamiltonian approach has been used to calculate the moments for some levels of Pöschl-Teller potential. Although the idea of generating isospectral Hamiltonians using the Gelfand-Levitan approach [12] or the Darboux procedure [13] were known for some time, the supersymmetric quantum mechanical techniques make the procedure look simpler. When one deletes a bound state of a given potential *V(x)* and re-introduces the state, it involves solving a first order differential equation, which admits a free parameter. 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)*. For any one dimensional potential (full line or half-line) with *n* bound states, one can construct an n-parameter family of strictly isospectral potentials, i.e. potentials with eigen values, reflection and transmission coefficients identical to those for original potential [8]. This aspect has been utilized profitably in many physical situations, which are of interest to various fields [14-21].

2. 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. If the ground state wave function (ψ_0) is known and its energy is chosen to be zero, the Hamiltonian can be factorized as $H_1 = A^{\dagger}A$, (in units $\hbar = 2m = 1$), where $A = \frac{d}{dx} + W(x)$ 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

$$H_1\psi_n = A^\dagger A\psi_n = \varepsilon_n\psi_n, \quad (1)$$

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

$$H_2(A\psi_n) = \varepsilon_n(A\psi_n). \quad (2)$$

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. The relation between Hamiltonians reads,

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

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

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

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

$$V_{1,2}(x) = W^2(x) \mp \frac{dW}{dx}. \quad (3)$$

For the potential $V_2(x)$, the original potential $V_1(x)$ is not unique [6,7]. 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

$$V_2(x) = \hat{W}^2(x) + \hat{W}'(x). \quad (4)$$

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

$$\varphi^2(x) + 2W(x)\varphi(x) + \varphi'(x) = 0. \quad (5)$$

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

$$\hat{W}(x) = W(x) + \frac{d}{dx}\ln[I(x) + \lambda]. \quad (6)$$

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

$$\hat{V}_1(x,\lambda) = V_1(x) - 2\frac{d^2}{dx^2}(\ln(I(x) + \lambda)). \quad (7)$$

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

$$\hat{\psi}_0(x,\lambda) = \frac{\sqrt{\lambda(1+\lambda)}\psi_0(x)}{I(x) + \lambda}, \quad (8)$$

where $\lambda \notin (0,-1)$. The eqs. (7) and (8) represent the one-parameter family of isospectral potentials and wave functions, which shall be used to obtain the moments for some states of the potential.

3. Calculation of Moments

The moments are calculated for different states of the 3-level Pöschl-Teller potential. For undeformed potential, the calculation of odd moments gives the null result, whereas the even moments result in some particular value. We start with Schrödinger equation for hyperbolic Pöschl-Teller potential, which is reflectionless and admits *n* bound states,

$$[-\tfrac{d^2}{dx^2} + (\tfrac{n^2 - n(n+1)seh^2x}{2})]\,\Psi_m^{(n)}(x) = E_m\Psi_m^{(n)}(x). \quad (9)$$

The normalized ground state wave function in position space reads

$$\psi_0 = \frac{1}{\sqrt{\beta\left(\frac{1}{2}, n\right)}}\sec h^n x \quad (10)$$

where β is the beta function. The first excited state wave function in position space is given as

$$\psi_1 = \frac{1}{\sqrt{\beta\left(\frac{1}{2}, n-1\right) - \beta\left(\frac{1}{2}, n\right)}}\sec h^{n-1}x\tanh x \quad (11)$$

The isospectral Hamiltonian approach is used to construct the isospectral Pöschl-Teller potential and the corresponding wave functions. The deformed wave functions are used to calculate the moments for the isospectral potential. For n-level potential, the one parameter isospectral ground state wave function is calculated as,

$$\hat{\psi}_0(x,\lambda) = \frac{\sqrt{\lambda(1+\lambda)}}{\sqrt{\beta\left(\frac{1}{2}, n\right)}}\;\frac{\sec h^n x}{\frac{1}{\beta\left(\frac{1}{2}, n\right)}\left[\frac{\sinh x}{2n-1}\left\{\sec h^{2n-1}x + f(x)\right\}\right] + \lambda} \quad (12)$$

$$where\ f(x) = \sum_{k=1}^{n-1}\frac{\left(2^k(n-1)(n-2).....n-k)\right)}{(2n-3)(2n-5).....(2n-2k-1)}\sec h^{(2n-2k-1)}x + \frac{2}{3}$$

and the deformed first excited state wave function is obtained using the relation

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

$$\hat{\psi}_1(x,\lambda) = A\left[\sec h^{n+1}x \tanh x + \frac{2}{3}A^2\left(\frac{\sec h^{2(n-1)}x \tanh x}{I(x)+\lambda}\right)\sec h^{n-1}x\right] \quad (13)$$

where

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

The normalized ground state, first excited state and the second excited state wave functions for 3-level potential reads,

$$\psi_0 = \frac{\sqrt{15}}{4}\sec h^3 x \quad (14)$$

$$\psi_1 = \sqrt{\frac{15}{2}}\sec h^2 x \tan h\, x \quad (15)$$

$$\Psi 2(x) = \sqrt{3}\,(\sec hx - \tfrac{5}{4}\sec h3x) \quad (16)$$

The values obtained for the ground state, first excited state and second excited state square moments are 0.20, 0.82 and 2.70 respectively. The values of the square moments for the ground state and first excited state of the Pöschl-Teller potential as a function of the number of bound states (n) are plotted in figures 1 and 2. As the number of bound states in the potential increases, the values of the ground state and first excited state square moments go on decreasing. When we consider the deformed wave functions, we also obtain some non zero value for the odd moments as a function of the deformation parameter. The deformed moments are plotted for different states of the Pöschl-Teller potential as a function of the deformation parameter λ, in figures 3-8.

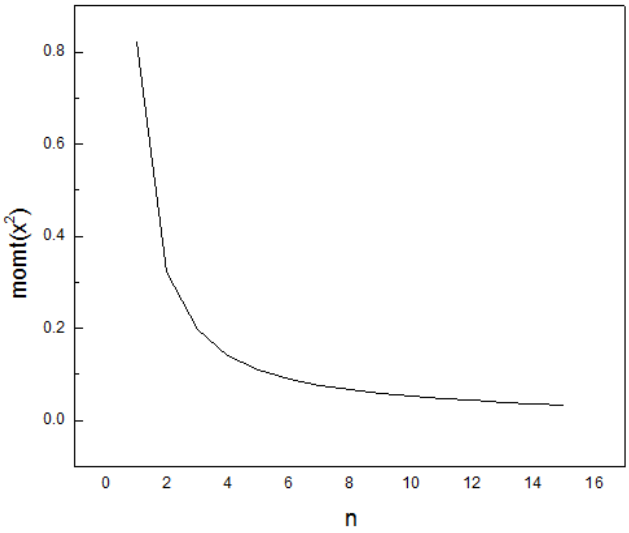

Figure 4.1. *The square moments for the ground state of the Pöschl-Teller potential as a function of the number of bound states of the potential (n).*

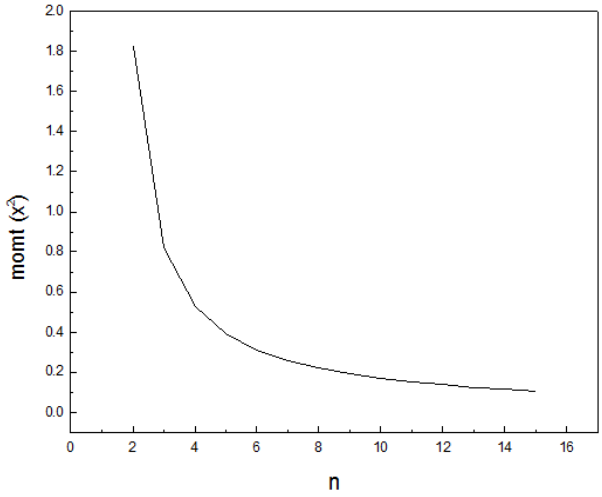

Figure 4.2. *The square moments for the first excited state of the Pöschl-Teller potential as a function of number of bound states of the potential (n).*

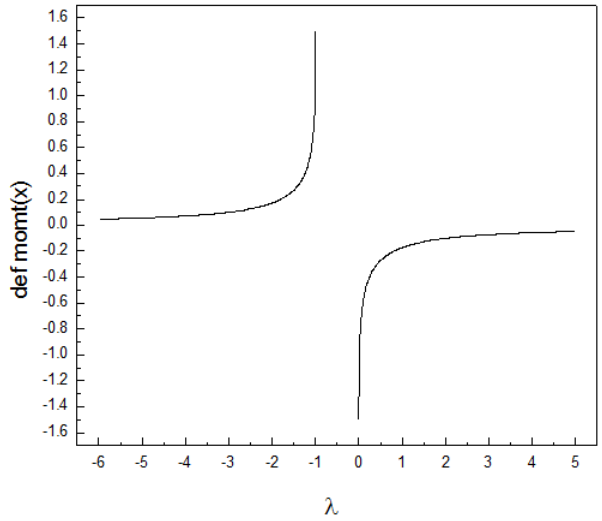

Figure 4.3. *The moments for the ground state of the Pöschl-Teller potential as a function of the deformation parameter (λ).*

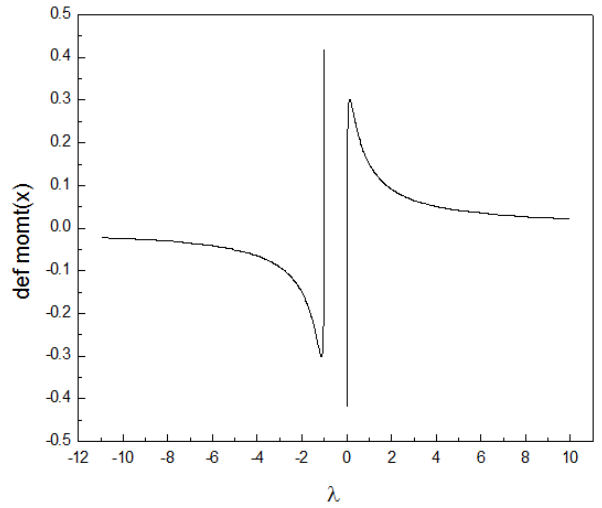

Figure 4.4. *The moments for the first excited state of the Pöschl-Teller potential as a function of the deformation parameter (λ).*

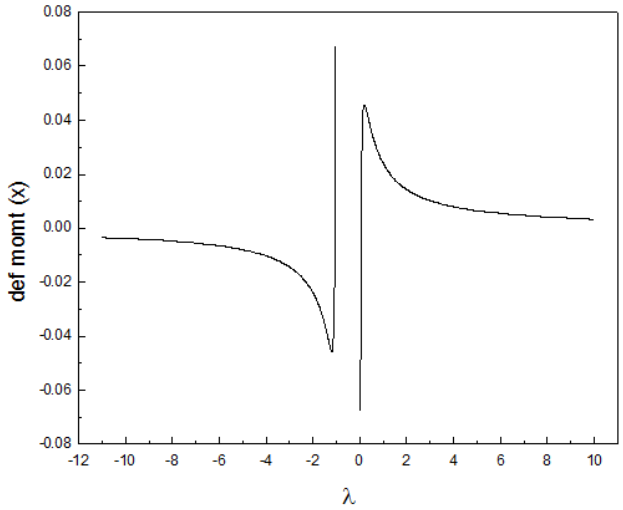

Figure 4.5. *The moments for the second excited state of the Pöschl-Teller potential as a function of the deformation parameter (λ).*

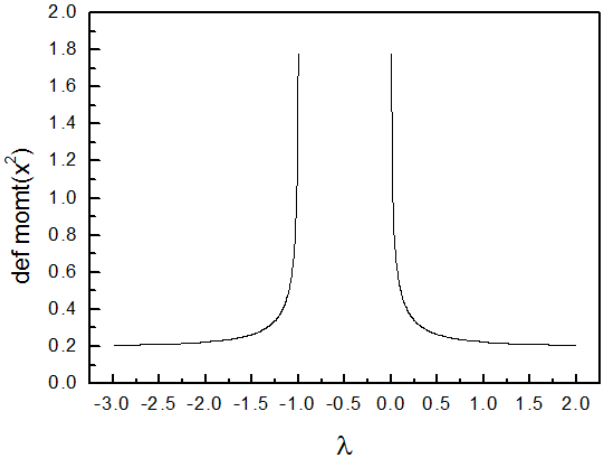

Figure 4.6. *The square moments for the ground state of the Pöschl-Teller potential as a function of the deformation parameter (λ).*

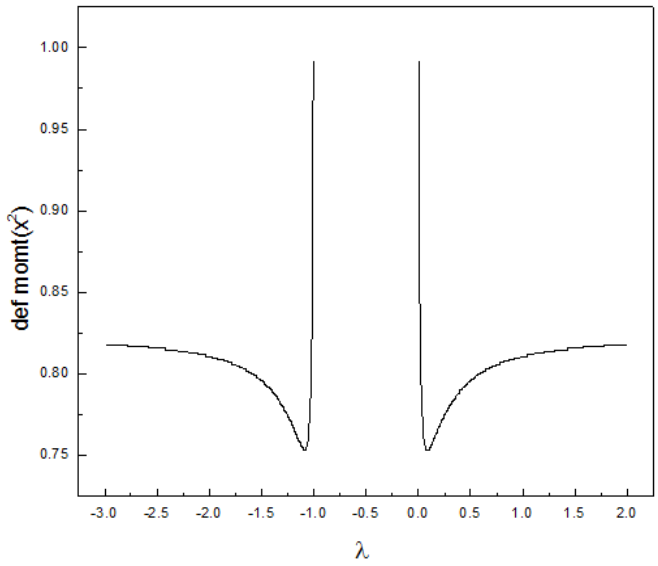

Figure 4.7. *The square moments for the first excited state of the Pöschl-Teller potential as a function of the deformation parameter (λ).*

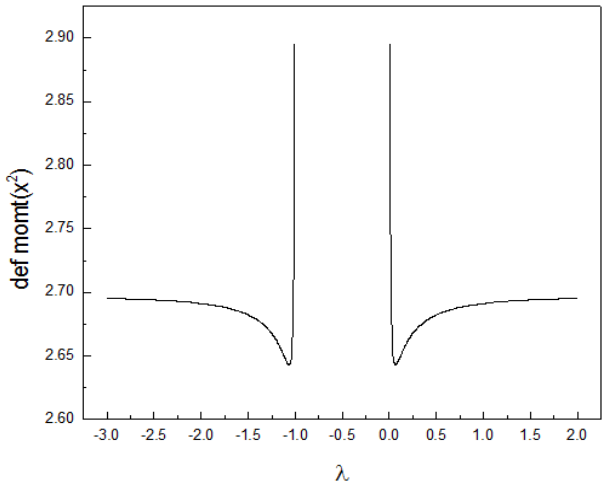

Figure 4.8. *The square moments for the second excited state of the Pöschl-Teller potential as a function of λ.*

4. Uncertainty in Position Space

These calculations are further used to obtain uncertainty in the position space and the isospectral Hamiltonian approach is utilized in reducing the uncertainty in the position space. The uncertainty in position space is given by $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$ which can be calculated for each level of three level potential. For the undeformed case, it is straightforward to check that $\langle x \rangle = 0$, so uncertainty in position space is equal to $\langle x^2 \rangle$. This is calculated for ground state, first excited state and second excited state to be 0.20, 0.82 and 2.70 respectively. When we consider the deformed wave functions, then $\langle x^2 \rangle$ increases for smaller values of λ and we also get contribution from $\langle x \rangle^2$ for smaller values of λ and the uncertainty in position space get reduced for smaller values of deformation parameter.

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