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# A NUMERICAL APPROACH FOR THE SOLUTION OF SCHRÖDINGER EQUATION WITH PSEUDO-GAUSSIAN POTENTIALS

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**Abstract**
The Schrödinger equation with pseudo-Gaussian potential is investigated. The pseudo-Gaussian potential can be written as an infinite power series. Technically, by an ansatz to the wave-functions, exact solutions can be found by analytic approach [12]. However, to calculate the solutions for each state, a condition that will stop the series has to be introduced. In this way the calculated energy values may suffer modifications by imposing the convergence of series. Our presentation, based on numerical methods, is to compare the results with those obtained in the analytic case and to determine if the results are stable under different stopping conditions.

## 1. Introduction

The solution of the fundamental equation of quantum mechanics, namely the Schrödinger equation (SE) has continued to attract interest of physicists and mathematicians. Solving this equation is not always an easy task, thus different methods have been developed to solve it. One of these is the numeric approach which has a long history, but recently SE has been the subject of a great activity to achieve a fast and reliable algorithm that generates a stable numerical solution. SE is a differential equation of type:

$$\frac{d}{dx^2}\psi(x) = (V(x) - E)\psi(x), \tag{1}$$

and there is a real need to be able to solve it by any method. In the above equation $\psi(x)$ is a complex valued square integrable function, $V(x)$ a real valued function, named

potential, and $E$ stands for energy values of the physical system. These, energy values, are real numbers iff the Hamiltonian is a hermitic operator on the space of functions $\psi(x)$. SE cannot be solved exactly for any potential function, except for a small number of potentials, which are nevertheless of extreme theoretical importance. For most potential function the equation has to be solved by different suitable ways. Several lines of approach have been followed in the study of SE for different types of potentials such as: variational [1, 2] and perturbational schemes [3], also combined with direct numerical methods [4] and series solutions [5] as well as the recently approach to solve SE into momentum representation [6]. Also there is a geometic approach to solve SE, known as geometric quantisation [7]. There is a class of potentials which allows to obtain the spectrum algebraically under certain conditions, or at least a finite part of the eigenvalues are obtained algebraically while the rest must be obtained numerically. The polynomial potentials belong to this class and these systems are referred to as quasi-exactly solvable ones [8].

In a previous work [12], we have found that the pseudo-Gaussian potential belongs to quasi-exactly solvable systems. We have shown that the pseudo-Gaussian potential expands into an infinite power series, that converges due to the asymptotic behavior. The general analytical solution of SE with this potential has been proposed as an infinite power series. A general condition was imposed in order to have a convergent solution. This provides the quantification rule for energy levels. In order to write down the solution for a specific energy level (particular quantum number, 0.1....). it was shown that the general solution has to be truncated. In this condition there are a finite number of terms in the analytical solution. The purpose of this presentation is to investigate the stability for the values of energy levels considering different numbers of terms in the analytical solution and comparing them with those obtained by computational technique. We have chosen the finite difference methods for computing approximate eigenvalues of equation (1). In this case of quasi-exactly solvable systems a numerical verification upon the convergence of the solution is required.

In the next section we present the main features of pseudo-Gaussian system, known as pseudo-Gaussian oscillator (PGO) [9, 10, 11]. In the last section we talk about numerical method and the obtained results are presented.

## 2. The physical model. General solutions

Let us consider the radial part of the three-dimensional Schrödinger's time-independent equation, $\mathbf{H}\psi = E\psi$, the square-integrable complex functions $\psi$ of real variable are called eigenfunctions and the numbers $E$ are called eigenvalues of the energy. The Hamiltonian operator $\mathbf{H}$, acting on the space of eigenfunctions, given in atomic units, $\mathbf{H} = -\frac{1}{2}\Delta + V(r)$, introduces the central real valued potential $V(r)$ on Euclidean real space with spherical coordinates as:

$$V^s_{\lambda,\mu}(r) = \left(\lambda + \sum_{k=1}^{s} C_k r^{2k}\right) \exp(-\mu r^2)\,, \tag{2}$$

having the coefficients $C_k$, [11]:

$$C_k = \frac{(\lambda + k)\mu^k}{k!}\,. \tag{3}$$

The properties of this model are completely determined by the dimensionless parameters $\lambda \in \mathbb{R}$, $\mu \in \mathbb{R}_+$ and the positive integer $s = 1, 2, ...$, named the *order* of PGO. We note that the genuine Gaussian potential corresponding to the order $s = 0$ is not included in this family. The potentials defined by the eqs. (2) and (3) have the remarkable property to approach to the HO potential when $r \to 0$ and together with Gaussian asymptotic behavior, i.e. $\lim_{r\to\infty} V^s_{\lambda,\mu}(r) = 0$. We also have to notice that, for each order, $s$, the Taylor expansion of these potentials does not have terms proportional with $r^4, r^6, ..., r^{2s}$.

$$V^s_{\lambda,\mu}(r) = \lambda + \mu r^2 + O(r^{2s+2}) \tag{4}$$

In figure (1) it is shown the graph of both PGO and HO, one can see their similar shape in a vicinity of origin and the Gaussian asymptotic behavior of PGO beside HO, which goes to infinity.

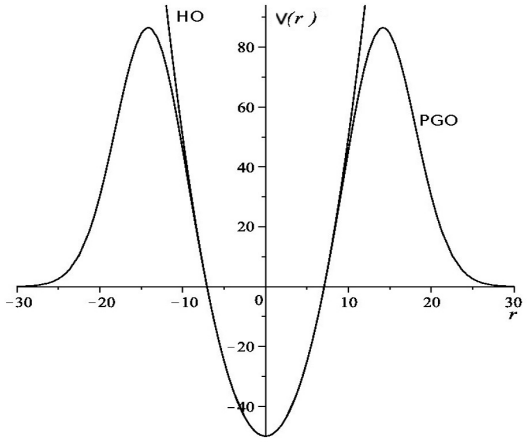


Figure 1: The pseudo-Gaussian oscillator potential graph ($s = 3$) compared with harmonic oscillator potential one.

Taking into consideration that $l(l + 1)$ represents the eigenvalue of the square of the angular-momentum operator $\mathbf{L}^2$, the radial part of the Schrödinger equation for the stationary states can be written as:

$$\left[\frac{d^2}{dr^2} + \frac{(2)}{r}\frac{d}{dr} + (E - V(r)) - \frac{l(l+1)}{r^2}\right]\psi(r) = 0, \tag{5}$$

with $\psi(r)$ the radial wave-function. Considering the potential (2) we can study the radial three dimensional Schrödinger eigenvalue problem. We can eliminate the first derivative by setting

$$\psi(r) \equiv r^{-1}R(r) \tag{6}$$

and (5) becomes:

$$\left[\frac{d^2}{dr^2} + (E - V(r)) - \frac{l(l+1)}{r^2}\right]R(r) = 0. \tag{7}$$

We can calculate the series (4) of potential (2) with coefficients (3), and after some algebra we get the form:

$$V^s_{\lambda,\mu}(r) = \lambda + \mu r^2 + \sum_{k=s+1} \hat{C}_k r^{2k}, \tag{8}$$

with coefficients $\hat{C}_k$ coming from the Taylor expansion and having the following form:

$$\hat{C}_k \propto (-1)^{s+k} \left( \frac{1}{(k-1)!} + \frac{\lambda}{k!} \right) (k-s)^{\frac{k}{2}}. \tag{9}$$

The potential (2) with terms grouped as in (8), allows us to recognize that it is basically made up by a term representing the HO potential $V_{HO} = \lambda + r^2$, with $\lambda$ an arbitrary energy level and an additional term, which is actually a power series, $V_{int} = \sum_{k=s+1} \hat{C}_n r^{2k}$.

The analytical solutions were developed in [12]

$$\psi_n(r) = N_n \, r^{l(l+1)-1} \exp[p_n(r)]. \tag{10}$$

$N_n$ denotes a polynomial of degree n, whose coefficients $a_i$ are determined from the normalization condition, this means the eigenfunctions obey the condition of square-integrable functions,

$$\int_0^\infty |\psi_n(r)|^2 \, r^2 dr = 1. \tag{11}$$

The condition of stopping the power series yields the quantification condition. This means that the power series, coming from potential, has to be finite too. The potential will be a polynomial of finite degree. We compare energy values obtained numerically with those obtained analytically for different polynomial.

## 3. Computing methods and results

Let us introduce a finite set of grid points, considering a domain $[a, b]$ and $r_i = a+(i-1)h$, $i = 1 \ldots n$ with $h = (b-a)/(n-1)$, $n \geq 5$. We shall also designate $R_i = R(r_i)$, $V_i = V(x)$. The method described hereafter are based on the central difference formula:

$$R_{i-1} - 2R_i + R_{i+1} = h^2 R_i^{(2)} \tag{12}$$

By replacing $R_i^{(2)}$ using (1) with the potential (8), the system of linear equations (12) can be written in the matrix form:

$$(\mathbf{J} + h^2 \mathbf{V}) \, \mathbf{R} = \mathbf{E} h^2 \, \mathbf{R} \tag{13}$$

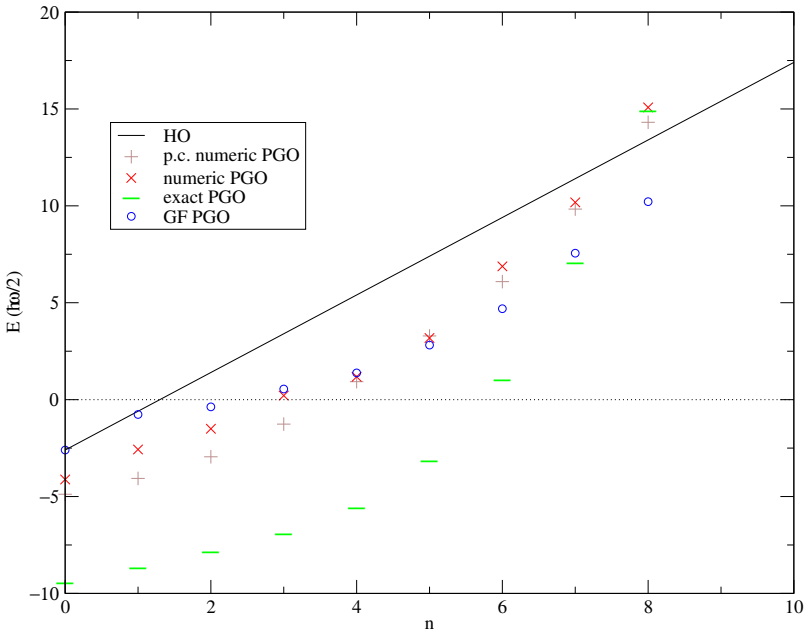


Figure 2: The eigenvalues given by finite difference, implicit and also predictor corrector method.

where $\mathbf{J} = (j_{n,m})$ is a tridiagonal matrix such that:

$$j_{n,n} = 2 \quad n = 0 \ldots N, \tag{14}$$

$$j_{0,1} = 0 \quad \text{odd-parity solutions},$$

$$j_{n,m} = -1 \quad |n-m| = 1, \;\; n = 1 \ldots N. \tag{15}$$

The matrix $V$ is diagonal:

$$\mathbf{V} = diag[v_0, v_1, \ldots p_N]$$

and

$$\mathbf{R} = diag[r_0, r_1, \ldots r_N]^T$$

In this way our equation can be expressed as an algebraic eigenvalue one. To solve this algebraic eigenvalue problem, we first transform the matrix $\mathbf{J}$ into a symmetric one. Due to the already special form of $\mathbf{J}$, this can be done by means of one similarity transformation.We then reduce this matrix to a tridiagonal one by transformations described in Wilkinson [14]. To compute eigenvalues and eigenvectors of this symmetric, tridiagonal matrix, we have used our Mapple subroutine. Finally we expand the eigenfunctions

$$R(r) = \sum_{i=0}^{N} < R_i | u_i > u_i(r) \tag{16}$$

in terms of the harmonic oscillator eigenfunctions, $u_i$

$$u_i(r) = r^{l+1} e^{-\nu r^2} L_k^{l+1/2}(2\nu r^2) \tag{17}$$

Where $L_k^{l+1/2}$ are Laguerre polynomial and $\nu = m\omega/2\hbar$. We present in figure (2) the values for eigenvalues given by finite difference using implicit and also predictor corrector

method.

As can be observed the eigenvalues for energy levels are in good accordance with the theory prediction. Unlike the generating function method [9, 10, 11], it is obtained a better prediction starting from the first energy levels. The results being more accurate with a predictor-corrector improvement of the method. The numbers $< R_i|u_i >$, obtained from numerical subroutine, are the coefficients of the projection of eigenfunctions (16) on the HO basis (17).

In this presentation we have shown that the solution of quasi-exactly PGO system presented in [12] is stable and it is in concordance with both the numerical approximation presented here and with generting functional aproach presentedin [9].

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