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Bound state eigenfunctions of an anharmonic oscillator in one dimension: A Numerov method approach

Research Article

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Abstract: Numerical methods are useful when analytical solutions are difficult to derive. An oscillator is described by the second order differential equation. In this article the numerical method for the special case of differential equation is applied for the solution of the wave function of a harmonic oscillator quantum mechanically in classical as well as non classical region. The Numerov's method is applied for evaluating the wave function with initial condition. The computational flow is explain schematically. The method is further applied to anharmonic oscillator. The evaluated wave function is plotted along with harmonic potential. The possible solution leads to the bound state energy eigen values. The inward and outward integrations are executed to achieve smooth matching at boundaries. The exact bound state solutions are obtained by the numerical integration corresponds to $n=0$ to $n=4$. The numerical approach gives the symmetric and antisymmetric wave functions. Computational issues concerned is energy convergence, which is controlled by the step size h, range of potential x_m and lower bound guessed eigenvalue as well. The present results obtained are also compared with that of Bahttacharya.

MSC: 34L20 • 65L12

Keywords: Numerov method • Anharmonic oscillator • Inward integration• Outward integration

1. Numerov's method

One class of differential equations which often occur in physics are second order differential equations which are independent of the first derivative. An example is the Newton's equation of motion of a particle under the influence of an external force $m\frac{d^2x}{dt^2}=f(x,t)$, where m is the mass of the particle and $f(x,t)$ is the external force. Another example is Schrödinger equation of a quantum system. For a quantum particle of mass m in a potential $V(x)$, the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x)+V(x)\psi(x)=E\psi(x), \tag{1}$$

where $\psi(x)$ is the wave function of the system and E is the energy eigenvalue. Numerov's method is an elegant scheme to solve differential equations which belong to this class[1,2]. The general form of this class of differential equations is

$$\frac{d^2y}{dx^2}=U(x)+V(x)y. \tag{2}$$

The Taylor series expansion of the solution y at $(x-h)$ about x is

$$y(x-h)=y(x)-h\frac{dy(x)}{dx}+\frac{h^2}{2}\frac{d^2y(x)}{dx^2}-\frac{h^3}{6}\frac{d^3y(x)}{dx^3}+\frac{h^4}{24}\frac{d^4y(x)}{dx^4}-\ldots, \tag{3}$$

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and similarly, for the solution at $(x+h)$

$$y(x+h)=y(x)+h\frac{dy(x)}{dx}+\frac{h^2}{2}\frac{d^2y(x)}{dx^2}+\frac{h^3}{6}\frac{d^3y(x)}{dx^3}+\frac{h^4}{24}\frac{d^4y(x)}{dx^4}+\ldots, \tag{4}$$

For simplicity of notation, denote the solution $y(x_n)$ at the nth value of the independent variable x_n as y_n and add Eq.(3) and (4), which gives

$$y_{n+1}+y_{n-1}=2y_n+2\left[\frac{h^2}{2}\frac{d^2y_n}{dx^2}\bigg|_{x_n}+\frac{h^4}{24}\frac{d^4y_n}{dx^4}\bigg|_{x_n}\right]+O(h^6) \tag{5}$$

The form of the equation hints the order of the error, which is $O(h^6)$. For further calculations define $d^2y/dx^2|_{x_n}=F_n$ and after rearranging

$$y_{n+1}=2y_n-y_{n-1}+h^2F_n+\frac{h^4}{12}\frac{d^2F}{dx^2}\bigg|_{x_n}+O(h^6). \tag{6}$$

Replace d^2F/dx^2 in Eq.(6) with the central difference approximation

$$\frac{d^2F}{dx^2}\bigg|_{x_n}=F_n''=\frac{F_{n+1}-2F_n+F_{n-1}}{h^2}, \tag{7}$$

which is of order $O(h^2)$. Then the solution at x_{n+1} is

$$y_{n+1}=2y_n-y_{n-1}+\frac{h^2}{12}(10F_n+F_{n+1}+F_{n-1}). \tag{8}$$

From the general equation in Eq.(2) $F_n=U_n+V_ny_n$, using this expression for F_{n+1} in the above equation

$$y_{n+1}=2y_n-y_{n-1}+\frac{h^2}{12}\left(10F_n+U_{n+1}+V_{n+1}y_{n+1}+F_{n-1}\right). \tag{9}$$

The variables V_{n+1} and U_{n+1} on the right hand side, from the definitions in Eq.(2), are functions of x_{n+1} only. After rearranging the terms in the equation

$$y_{n+1}=\frac{2y_n-y_{n-1}+\frac{h^2}{12}(U_{n+1}+10F_n+F_{n-1})}{1-\frac{h^2}{12}V_{n+1}}+O(h^6). \tag{10}$$

This is the general expression of the scheme. In practice, if the initial value of the independent variable is x_0, the method is applicable starting from x_2. The solution at this point

$$y_2=\frac{2y_1-y_0+\frac{h^2}{12}(U_2+10F_1+F_0)}{1-\frac{h^2}{12}V_2}+O(h^6). \tag{11}$$

However, in this equation y_1 is an also unknown. To use the method y_1 must be estimated with another scheme to $O(h^5)$ accuracy. The $O(h^5)$ accuracy is essential to maintain the $O(h^6)$ accuracy of the Numerov method. Evaluating y_1 from Taylor series expansion

$$y_1=y_0+hy_0'+\frac{h^2}{2}F_0+\frac{h^3}{3!}F_0'+\frac{h^4}{4!}F_0''+O(h^5), \tag{12}$$

here y_0' is an intial condition. Further, expand F_1 and F_2 in the Taylor series about F_0 up to $O(h^2)$ as

$$F_1=F_0+hF_0'+\frac{h^2}{2}F_0''+O(h^3), \tag{13}$$

$$F_2=F_0+2hF_0'+\frac{2h^2}{2}F_0''+O(h^3). \tag{14}$$

Evaluating $6F_1-F_2$ and rearranging terms in the resulting equation, we get

$$\frac{h^2}{24}7F_0+6F_1-F_2\approx\frac{h^2}{2!}F_0+\frac{h^3}{3!}F_0'+\frac{h^4}{4!}F_0''. \tag{15}$$

Collectively, this is an approximation of F_0, F_0' and F_0'' dependent terms in Eq.(12). Substituting this expression in Eq.(12),

$$y_1=y_0+hy_0'+\frac{h^2}{24}(7F_0+6F_1-F_2)+O(h^5) \tag{16}$$

Noting the earlier definition $F(x,y)=U(x)+V(x)y$, denote $F_1=U_1+V_1y_1$ and $F_2=U_2+V_2y_2$. Substituting F_1, F_2 and rearranging terms the equation is

$$\left(1-\frac{h^2}{4}V_1\right)y_1+\frac{h^2}{24}V_2y_2=y_0+hy_0'+\frac{h^2}{24}(7F_0+6U_1-U_2) \tag{17}$$

In a similar way, rearranging the terms in Eq.(11)

$$-\left(2+\frac{5h^2}{6}V_1\right)y_1+\left(1-\frac{h^2}{12}V_2\right)y_2=-y_0+\frac{h^2}{12}(F_0+10U_1+U_2). \tag{18}$$

These two equations Eq.(17) and (18), are linear algebraic equation with y_1 and y_2 unknowns. In short form, the equation are

$$a_{11}y_1+a_{12}y_2=b_1,$$
$$a_{21}y_1+a_{22}y_2=b_2,$$

where the coefficients and constants are

$$a_{11}=1-V_1\frac{h^2}{4}, \qquad a_{12}=V_2\frac{h^2}{24}, \qquad b_1=y_0+hy_0'+\frac{h^2}{24}(7F_0+6U_1-U_2),$$
$$a_{21}=-2-5V_1\frac{h^2}{6}, \qquad a_{22}=1-V_2\frac{h^2}{12}, \qquad b_2=-y_0+\frac{h^2}{12}(F_0+10U_1+U_2).$$

The solution for y_1 with the required $O(h^5)$ accuracy is

$$y_1=\frac{a_{22}b_1-a_{12}b_2}{a_{11}a_{22}-a_{12}a_{21}}. \tag{19}$$

Then, with this value of y_1 the solution at the next point y_2 is calculated from Eq.(17). The Numerov scheme is then applicable to evaluate the solutions at the other points. An important advantage of the Numerov method is the local error of $O(h^6)$ with one evaluation of U and V per step. Whereas in Runge-Kutta algorithm six function evaluations are needed to achieve the same local error and two previous values of the solution are needed to calculate a new one.

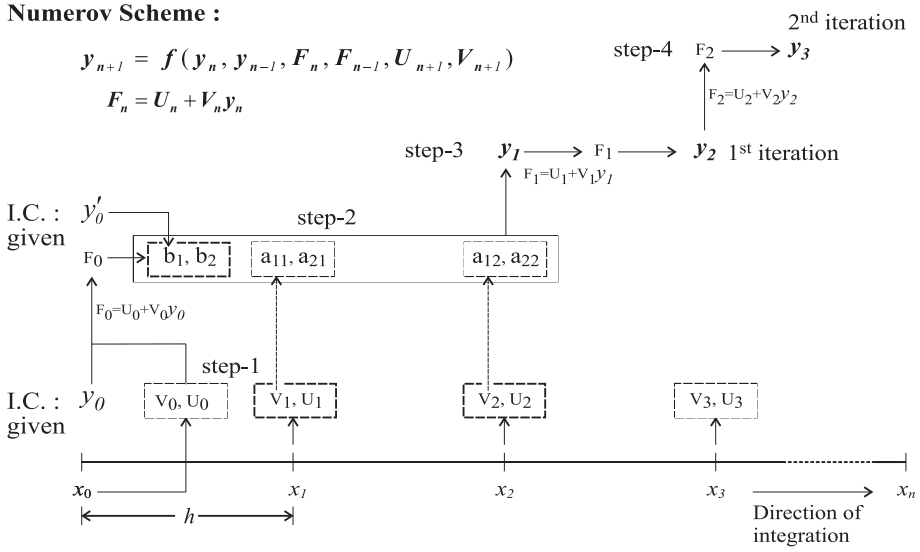

Fig. 1. Sequential steps and direction of arrow show the flow of evaluation of the Numerov's method for simultaneous 1st order ODE. y_n is calculated with the accuracy of the $O(h^5)$ from y_{n-1} with step size h.

2. Eigenfunctions of simple harmonic oscillator

Solution of Schrodinger equation for simple harmonic oscillator potential using Numerov method. Consider realistic case of potential which is continuous functions of position, the simple harmonic oscillator potential $V(x)\propto x^2$.

The simple harmonic oscillator is very important in physics as it is the prototype for any system involving oscillations about a point of stable equilibrium. The potential function must have a minimum at a position of stable equilibrium, thus it can be well approximated by a parabola. Keeping the origin of the x-axis and energy axis at the minimum, we can write

$$V(x)=\frac{C}{2}x^2, \quad C=\text{constant} \tag{20}$$

For an example a particle moving under the potential experiences a linear restoring force, with C being the force constant of the corresponding linear restoring force. Another important feature is the total energy of the particle. Classically it can have any value, whereas quantum mechanics predicts only a discrete set of values. The time-independent Schrodinger equation for simple harmonic oscillator must be solved to find out allowed energy values.

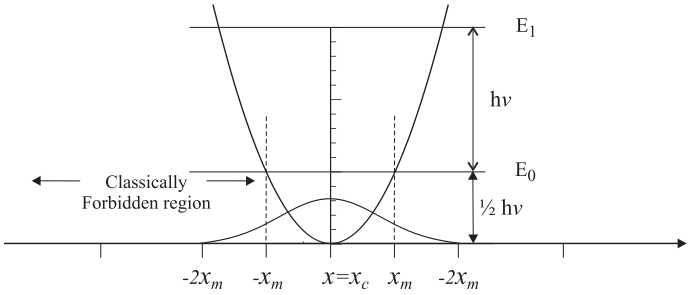

Fig. 2. Simple Harmonic potential well. Solution of Schrodinger equation (Eq. (1)) using Numerov's method. The ground state wave function in classical and non-classical region.

The eigenfunctions are expressed in terms of dimensionless variable[3]

$$u=\left[(Cm)^{1/4}/\hbar^{1/2}\right]x$$

The proportionality constant depends on the properties of the oscillator. In classically allowed region i.e. $E_n < V(x)$, the number of oscillations increases with increasing n, because there are n values of x for which $\psi(x)=0$. The values of x are the locations of the nodes of ψ. Outside the classical regions the eigenfunctions decreases very rapidly. The eigenfunction of lowest allowed energy is of even parity.
The time-independent Schrodinger equation for the potential is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{C}{2}x^2\psi=E\psi \tag{21}$$

The Force constant in terms of the classical oscillation frequency is $\nu=\frac{1}{2\pi}\sqrt{C/m}$ or $\nu^2 2\pi^2 m=C/2$.
The Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+2\pi^2 m\nu^2 x^2\psi=E\psi \qquad \text{or} \qquad \frac{d^2\psi}{dx^2}+\left[\frac{2mE}{\hbar^2}-\left(\frac{2\pi m\nu}{\hbar}\right)^2 x^2\right]\psi=0.$$

Introducing parameters $\alpha=\frac{2\pi m\nu}{\hbar}$ and $\beta=2mE/\hbar^2$

$$\frac{d^2\psi}{dx^2}+(\beta-\alpha^2x^2)\psi=0. \tag{22}$$

Consider dimensionless variable for numerical calculations

$$u=\sqrt{\alpha}x=\left[\frac{2\pi m}{\hbar}\frac{1}{2\pi}\left(\frac{C}{m}\right)^{1/2}\right]^{1/2}x=\frac{(Cm)^{1/4}}{\hbar^{1/2}}x$$

We have

$$\frac{d\psi}{dx}=\frac{d\psi}{du}\frac{du}{dx}=\frac{du}{dx}\frac{d\psi}{du}=\sqrt{\alpha}\frac{d\psi}{du} \qquad \text{and} \qquad \frac{d^2\psi}{dx^2}=\frac{d}{dx}\left(\frac{d\psi}{dx}\right)=\frac{du}{dx}\frac{d}{du}\left(\frac{d\psi}{dx}\right)=\alpha\frac{d^2\psi}{du^2}$$

Finally the Schrodinger equation in terms of variable u becomes

$$\alpha\frac{d^2\psi}{du^2}+(\beta-\alpha u^2)\psi=0 \qquad \text{or} \qquad \frac{d^2\psi}{du^2}+\left(\frac{\beta}{\alpha}-u^2\right)\psi=0 \tag{23}$$

Notice that α and β has unit of length^{-2}. Thus dimensionless Schrodinger equation is

$$\frac{d^2\psi}{du^2}+(\xi-u^2)\psi=0, \qquad \xi=\beta/\alpha=\frac{2E}{h\nu}$$

or

$$\frac{d^2\psi}{du^2}=(u^2-\xi)\psi \tag{24}$$

Theoretically

$$\frac{2E}{h\nu}=2n+1;\ \ n=0,1,2\ldots$$

where E is the eigenvalues of the simple harmonic oscillator. For $n=0$ and given ν $\xi=1$, so the good guess value for ξ may be 0.94 and increment it by very small constant. Similarly for $n=1$, $E=(1+1/2)h\nu \Rightarrow \xi=3.0$ i.e. starting guess value can be 2.4. When ξ will be close to the true value the logarithmic derivatives of the wave function obtained by integration from boundary points to inside using Numerov method match with the required accuracy at the common point $x=x_c$. In the present case because of the symmetric wave function, it could be origin i.e. center of the well. This verifies both correct set of wave functions and a corresponding bound state energy.
Equation (24) is integrated by recurrence relation (9) of Numerov algorithm

$$\psi_{i+1}=\frac{2\psi_i-\psi_{i-1}+\frac{h^2}{12}(U_{i+1}+10F_i+F_{i-1})}{1-\frac{h^2}{12}V_{i+1}} \tag{25}$$

where $U=0$, $V=u^2-\xi$ and $F=(u^2-\xi)\psi(u)$. For starting the solution ψ_0,ψ_1 are needed, where ψ_0 is the initial condition and $\psi_1=\epsilon$, where ϵ is a small constant. It is typically sufficient to have about 5 significant figures of accuracy, so that $\epsilon=10^{-6}$ is a reasonable choice. But it reduces magnitude of ψ, so consider $\epsilon=0.001$ in the calculation.
It is very important to start the Numerov iterations deep inside a classically forbidden region, where the true solution decreases. Then integrate out towards lower potential energy region. Because the truncation error accumulation in forbidden region would not be dominant in the solution. The trick is to integrate the solution in the direction of increasing magnitude.

2.1. Outward-Inward integration

Starting from the left side of the common matching point with step height $+h$. The acceptable behavior of the wave function is $\psi(x)=0$ as $|x|\to\infty$. The potential well is bounded here by the region $[-u_m,u_m]$, where its center is origin. Since the true solution decays exponentially, the wave function can safely be set to zero at a point that is deep enough in to the classically forbidden region. Assume the distance $-2u_m$ and $2u_m$ corresponds to infinite region where $\psi(x)\to 0$. Thus outward integration begins from $x=-2u_m$ where $\psi(x)=0$ (initial condition).

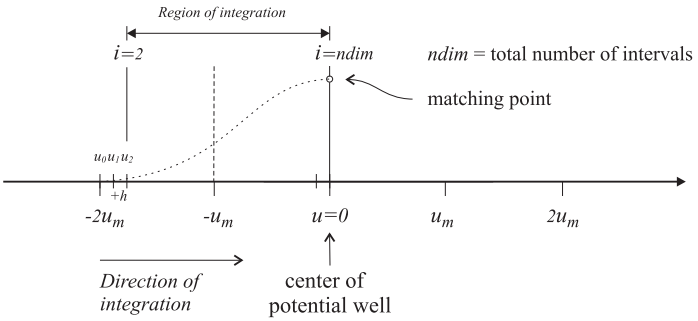

Fig. 3. Outward integration (left to right) by Numerov method from $-\infty=-2u_m$ to the matching point (origin $u=0$), with positive step height.

Starting from $x=2u_m$, the right side of the well, where $\psi(x)\big|_{x=2u_m}=0$ (initial condition) up to the matching point with step height $-h$.

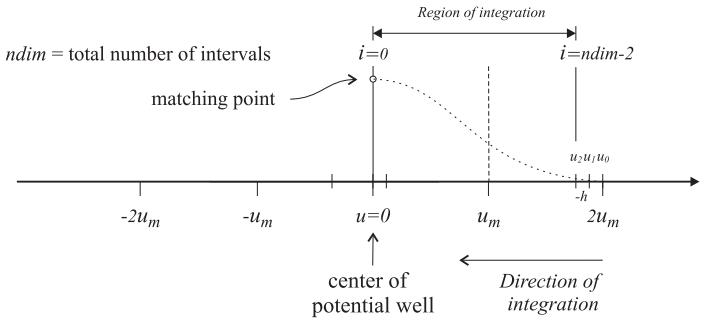

Fig. 4. inward integration (right to left) by Numerov method from $+\infty = +2u_m$ to the matching point (origin $u = 0$), with nagative step height.

2.2. Matching Criteria

The acceptable solution of the Schrodinger equation, the wave function and its first derivative must be continuous at all the points of region $[-2u_m, 2u_m]$, so as at the matching point $u = 0$, for selected ξ. The matching is confidently done by comparing the logarithmic derivative of both the solutions[4]. If $\gamma = \psi'/\psi$ and if $x = x_c$ is the matching point, then matching condition is

$$\gamma_l\big|_{x_c} = \gamma_r\big|_{x_c} \qquad \text{or} \qquad |\gamma_l - \gamma_r| < \delta \tag{26}$$

where γ_l and γ_r are the logarithmic derivative of solutions starting from left and right regions respectively. Increment in ξ from the guess value must be small, as an example if $|\gamma_l - \gamma_r| \le 0.0001$, then required increment is $\xi = \xi + 0.0001$. In the case of antisymmetric wave function $\psi_1 = -\epsilon$ and matching condition at origin $x = x_c$ would be

$$\frac{1}{\gamma_l}\bigg|_{x=x_c} = \frac{1}{\gamma_r}\bigg|_{x=x_c}$$

In addition to ψ, its fist derivative is also required at $x = x_c$ for matching. One can use the central difference formula of order $O(h^4)$.

$$f'(x_0) = \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h}$$

$$\text{or} \qquad \psi'(x_c) = \frac{-\psi\big|_{x_c+2h} + 8\,\psi\big|_{x_c+h} - 8\,\psi\big|_{x_c-h} + 8 + \psi\big|_{x_c-2h}}{12h} \tag{27}$$

The integration must be continued up to two more points after the matching boundary. Note that direction in which derivative is evaluated for both the wave functions from outward and inward integration must be the same.
It is obvious from the figure that width of the potential must cover the bound energy level, therefore x_m should be such that $V(x_m) \ge E_n$. Thus, range of the dimensionless independent variable u is $[-u_m, u_m]$, where $u_m = \sqrt{\alpha}\, x_m$.
For the case $n = 0 : V(x_m) > \frac{1}{2} h\nu$ i.e. $u_m^2 > \xi$ or $u_m > \sqrt{\xi}$

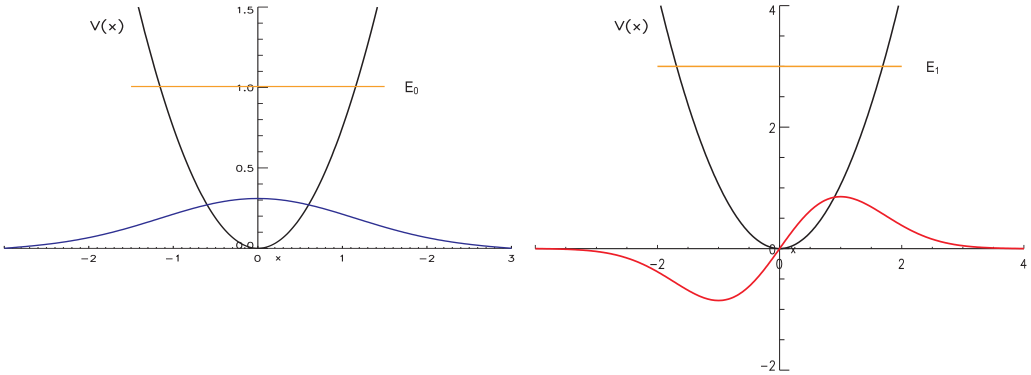

Fig. 5. Simple harmonic potential wave functions and associated eigenvalues for $n = 0$ (left) and $n = 1$ (right).

3. Eigenfunctions of Anharmonic Oscillator

First two eigenfunctions and eigenvalues for a harmonic oscillator are evaluated by solving Schrödinger equation with the Numerov method as shown in fig.5. Now the numerical derivation of an *anharmonic oscillator* is followed by the potential energy of the form $V(x) = \frac{C}{2}x^2 + \frac{D}{2}x^4$. The Schrodinger equation for the anharmonic potential is followed from Eq.(22) will be of the form

$$\frac{d^2\psi}{dx^2} + (\beta - \alpha^2 x^2 - \frac{D}{2}x^4)\,\psi = 0 \tag{28}$$

Considering dimensionless variable $u = \sqrt{\alpha}\,x$

$$\alpha\frac{d^2\psi}{du^2} + (\beta - \alpha u^2 - \frac{D}{2}\frac{u^4}{\alpha^2})\psi = 0$$
$$\frac{d^2\psi}{du^2} + (\xi - u^2 - \delta u^4)\psi = 0\,; \quad \delta = \frac{D}{2\alpha^3}$$

or

$$\frac{d^2\psi}{du^2} = (u^2 + \delta u^4 - \xi)\psi. \tag{29}$$

3.1. Result and Discussion

The numerical procedure discussed in previous section is tested in sequential executions of corresponding code. It is obvious that the particular value of δ is constant for the differential equation (29). The independent variable is u and ξ is the parameter results from guessed energy eigenvalue. The eigenvalue selected through iterative process which satisfy proper matching of logarithmic derivatives while developing eigenfunction about the origin. Thus eigenvalues and corresponding eigenfunctions are executed from IDL 0.7 code based on the above Numerov approach prepared by the author. The graph of eigenfunctions are generated within the code. The plotted graphs has the same y-axis to compare wave functions and related potential widths. The height of the wave functions is proportionally reduce for perfect matching. The horizontal lines along y-axis represents energy eigenvalues which is combined together with their respective wave functions.

Table 1. Ground state energies of quartic anharmonic oscillator evaluated by Numerov method and compared with that of Bhattacharya

δ	Numerov Method	Ranjan Bhattacharya
0.1	1.0674000	1.06529
0.2	1.1192000	1.11829
1.0	1.3923000	1.3923
4.0	1.9031000	1.9031
10.0	2.4491000	2.4491
50.0	4.0039000	4.00399

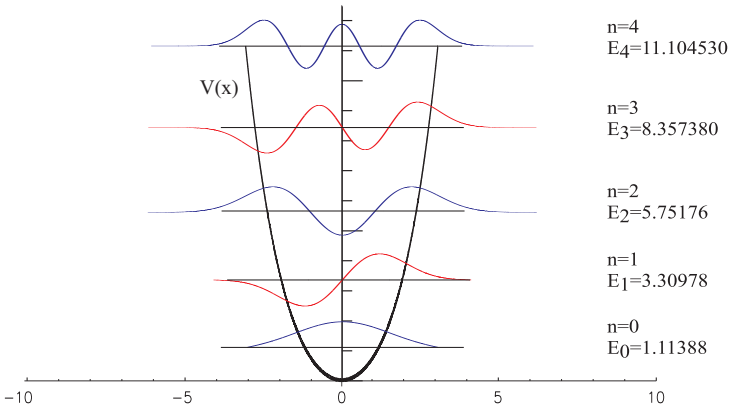

Fig. 6. Anharmonic potential and wave functions for $n = 0$ to $n = 4$ generated by Numerov method with $\delta = 0.10$.

The results of ground state energies of anharmonic oscillator are obtained by R. Bhattcharya solving polynomial equation[5]. By the application of Numerov method the energy eigenvalues evaluated exactly by taking care of energy convergence in the present work. The graphical representation of anharmonic potential along with corresponding bound states and their wave functions within a single graph clarify distribution of wave function along the effective range of potential and its nature. The input parameters have been playing major role in the computational task are mentioned here.

1. The guessed eigenvalue should be the lower bound value to stop the divergence.
2. The search for eigenvalue is restricted to energy region where the wave function has same number of nodes about the origin.
3. x_m will be different for different states.
4. Accuracy of the solution depends on the step size h and choice of x_m. These parameters must be varied till energy convergence is achieved.

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