Journal of Applied Mathematics and Physics, 2024, 12, 1919-1929
https://www.scirp.org/journal/jamp
ISSN Online: 2327-4379
ISSN Print: 2327-4352

Breakdown of a Commonly Practiced Technique in Quantum Mechanics

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How to cite this paper: Mohazzabi, P., Parker, W.D. and Kveton, P. (2024) Breakdown of a Commonly Practiced Technique in Quantum Mechanics. *Journal of Applied Mathematics and Physics*, **12**, 1919-1929.
https://doi.org/10.4236/jamp.2024.125118

Received: April 21, 2024
Accepted: May 27, 2024
Published: May 30, 2024

Abstract

The dynamically shifted oscillator is investigated quantum mechanically, both analytically and numerically. It is shown that the commonly used method of solving the Schrödinger equation using power series results in incorrect eigenvalues and eigenfunctions.

Keywords

Dynamic, Shift, Oscillator, Quantum, Schrödinger, Solution

1. Introduction

Central to quantum mechanics is the time-independent Schrödinger equation which, for one particle in one dimension, has the form

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+\frac{2m}{\hbar^2}\left[E-V(x)\right]\psi=0 \tag{1}$$

subject to certain constraints on the wavefunction $\psi(x)$ and its derivatives, based on the potential energy function $V(x)$.

Unless the potential energy function is trivial such as a particle in an infinite square potential well, the solution of the Schrödinger equation proceeds by assuming a power series solution of the form

$$\psi(x)=\sum_{n=0}^{\infty}a_n x^n \tag{2}$$

Substitution of this trial solution in the Schrödinger equation and equating the coefficients of same powers of x on both sides of the equation, normally results in a recursion relation with two arbitrary coefficients and two linearly independent power series. The two power series thus obtained, however, usually are not quadratically integrable, therefore, they are not quantum mechanically admissible. To remedy this problem, the common practice is to set one of the coefficients equal to zero to quench one of the series and terminate the other series by setting its coefficients beyond a certain term equal to zero, which results in the energy eigenvalues for the particle.

In doing so, however, sometimes we end up with a recursion relation involving three or more terms. A common example of this is the simple harmonic oscillator, for which the time-independent Schrödinger equation is

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+\frac{2m}{\hbar^2}\left(E-\frac{1}{2}m\omega^2x^2\right)\psi=0 \tag{3}$$

where ω is the classical angular frequency of oscillations. Dividing both sides of the equation by $m\omega/\hbar$ and defining the dimensionless energy ε and dimensionless displacement ξ by

$$\varepsilon=\frac{2E}{\hbar\omega} \quad \text{and} \quad \xi=\left(\frac{m\omega}{\hbar}\right)^{1/2}x \tag{4}$$

the Schrödinger equation reduces to

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2}+\left(\varepsilon-\xi^2\right)\psi=0 \tag{5}$$

Solution of Equation (5) by power series results in a three-term recursion relation. To avoid this, we write the function ψ as

$$\psi\left(\xi\right)=\mathrm{e}^{-\xi^2/2}f\left(\xi\right) \tag{6}$$

which reduces Equation (5) to

$$f''\left(\xi\right)-2\xi f'\left(\xi\right)+\left(2\varepsilon-1\right)f\left(\xi\right)=0 \tag{7}$$

which is the well-known Hermite differential equation [1], solution of which generates two linearly independent power series,

$$f\left(\xi\right)=\sum_{j=0}^{\infty}a_{2j}\xi^{2j}+\sum_{j=0}^{\infty}a_{2j+1}\xi^{2j+1} \tag{8}$$

where the constant coefficients a_0 and a_1 are arbitrary, and the rest are related through the recursion relation

$$a_{j+2}=\frac{2\left(j-\varepsilon\right)+1}{\left(j+2\right)\left(j+1\right)}a_j \qquad j=0,1,2,3,\cdots \tag{9}$$

Therefore,

$$\psi\left(\xi\right)=\mathrm{e}^{-\xi^2/2}\sum_{j=0}^{\infty}a_{2j}\xi^{2j}+\mathrm{e}^{-\xi^2/2}\sum_{j=0}^{\infty}a_{2j+1}\xi^{2j+1} \tag{10}$$

It can be shown that the power series in each term of Equation (10) behaves as e^{ξ^2} as $\left|\xi\right|\to\infty$ [2] [3] [4]. Therefore, as $\left|\xi\right|\to\infty$, each term behaves as $\mathrm{e}^{\xi^2/2}$. As a result the function is not quadratically integrable. Therefore, one of the terms should be quenched by setting either $a_0=0$ or $a_1=0$, and terminating the other power series beyond a certain term, say $j=n$, which results in the energy eigenvalue equation for the harmonic oscillator in dimensionless form,

$$\varepsilon_n = n + \frac{1}{2} \quad n = 0, 1, 2, \cdots \tag{11}$$

or

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad n = 0, 1, 2, \cdots \tag{12}$$

The method described above is used by many quantum mechanics books to solve the time-independent Schrödinger equation for the harmonic oscillator [5] [6] [7]. In what follows, we show that this method of solving the Schrödinger equation sometimes fails to produce correct results without warning. As an example, we study the dynamically shifted oscillator, which is a system of interest, both from classical mechanics point of view as well as quantum mechanics, as explained below.

2. Breakdown of the Commonly Practiced Technique

An interesting potential energy function with certain possible applications in physics, such as that experienced by the nitrogen atom in an ammonia molecule [8], is the dynamically shifted oscillator,

$$V(x) = \begin{cases} \frac{1}{2}k(x + x_0)^2, & x \ge 0 \\ \frac{1}{2}k(x - x_0)^2, & x < 0 \end{cases} \tag{13}$$

where the dynamic shift x_0 is a constant, which can be positive or negative. The graphs of this function are shown in **Figure 1**. For $x_0 = 0$, this potential reduces to that of the harmonic oscillator.

Classical behavior of the dynamically shifted oscillator has been studied elsewhere [9] [10]. The quantum mechanical energy eigenvalues of this oscillator have also been investigated, and it has been shown that the system exhibits degeneracy in one dimension [11].

Consider a particle of mass m oscillating in one dimension under the dynamically shifted potential. The time independent Schrödinger equation for the particle is

$$\begin{cases} \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}\left[E - \frac{1}{2}k(x + x_0)^2\right]\psi = 0, & x \ge 0 \\ \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}\left[E - \frac{1}{2}k(x - x_0)^2\right]\psi = 0, & x < 0 \end{cases} \tag{14}$$

Defining the angular frequency $\omega = \sqrt{k/m}$ and dividing both sides of each of Equations (14) by $m\omega/\hbar$, we obtain

$$\begin{cases} \frac{\mathrm{d}^2\psi}{\left(\frac{m\omega}{\hbar}\right)\mathrm{d}x^2} + \left[\frac{2E}{\hbar\omega} - \frac{m\omega}{\hbar}(x + x_0)^2\right]\psi = 0, & x \ge 0 \\ \frac{\mathrm{d}^2\psi}{\left(\frac{m\omega}{\hbar}\right)\mathrm{d}x^2} + \left[\frac{2E}{\hbar\omega} - \frac{m\omega}{\hbar}(x - x_0)^2\right]\psi = 0, & x < 0 \end{cases} \tag{15}$$

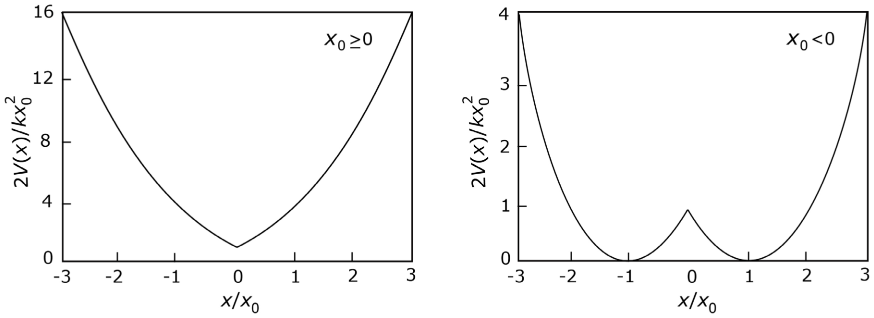

Figure 1. Potential energy function of dynamically shifted oscillator.

As in the case of harmonic oscillator, using the following dimensionless quantities,

$$\xi = \left(\frac{m\omega}{\hbar}\right)^{1/2} x, \quad \xi_0 = \left(\frac{m\omega}{\hbar}\right)^{1/2} x_0, \quad \varepsilon = \frac{E}{\hbar\omega} \tag{16}$$

Equations (15) reduce to

$$\begin{cases} \dfrac{d^2\psi}{d\xi^2} + \left[2\varepsilon - \left(\xi + \xi_0\right)^2\right]\psi = 0, & \xi \geq 0 \\ \dfrac{d^2\psi}{d\xi^2} + \left[2\varepsilon - \left(\xi - \xi_0\right)^2\right]\psi = 0, & \xi < 0 \end{cases} \tag{17}$$

We now solve these equations for $\xi \geq 0$ and $\xi < 0$ separately, using the standard method described in the previous section.

Defining $u = \xi + \xi_0$, the first of Equations (17) becomes

$$\frac{d^2\psi}{du^2} + \left(2\varepsilon - u^2\right)\psi = 0, \quad u \geq \xi_0 \tag{18}$$

As in the case of harmonic oscillator, to avoid a three-term recursion relation which is hard to work with, we make the substitution

$$\psi(u) = e^{-u^2/2} f(u) \tag{19}$$

which, not only results in a two-term recursion relation, but also its functional form is suggested by examining the limiting behavior of $\psi(u)$ as $u \to \pm\infty$ and as $u \to 0$ [6]. Therefore, Equation (18) reduces to

$$f''(u) - 2uf'(u) + (2\varepsilon - 1) f(u) = 0 \quad u \geq \xi_0 \tag{20}$$

which is the Hermite differential equation as in the case of harmonic oscillator [1]. The general solution is

$$f(u) = \sum_{j=0}^{\infty} a_{2j} u^{2j} + \sum_{j=0}^{\infty} a_{2j+1} u^{2j+1} \tag{21}$$

where the constant coefficients a_0 and a_1 are arbitrary, and the rest are related through the recursion relation

$$a_{j+2} = \frac{2(j - \varepsilon) + 1}{(j+2)(j+1)} a_j \quad j = 0, 1, 2, 3, \cdots \tag{22}$$

Therefore,

$$\psi(u) = \mathrm{e}^{-u^2/2} \sum_{j=0}^{\infty} a_{2j} u^{2j} + \mathrm{e}^{-u^2/2} \sum_{j=0}^{\infty} a_{2j+1} u^{2j+1} \tag{23}$$

Substituting back for u, we have

$$\psi_+(\xi) = \mathrm{e}^{-(\xi+\xi_0)^2/2} \sum_{j=0}^{\infty} a_{2j} (\xi+\xi_0)^{2j} + \mathrm{e}^{-(\xi+\xi_0)^2/2} \sum_{j=0}^{\infty} a_{2j+1} (\xi+\xi_0)^{2j+1} \quad \xi \geq 0 \tag{24}$$

In exactly the same way, by using $u = \xi - \xi_0$, it can be shown that the solution of the second of Equations (17) is

$$\psi_-(\xi) = \mathrm{e}^{-(\xi-\xi_0)^2/2} \sum_{j=0}^{\infty} b_{2j} (\xi-\xi_0)^{2j} + \mathrm{e}^{-(\xi-\xi_0)^2/2} \sum_{j=0}^{\infty} b_{2j+1} (\xi-\xi_0)^{2j+1} \quad \xi < 0 \tag{25}$$

where, as in the previous case, the constant coefficients b_0 and b_1 are arbitrary, and the rest are related through the recursion relation

$$b_{j+2} = \frac{2(j-\varepsilon)+1}{(j+2)(j+1)} b_j \quad j = 0,1,2,3,\cdots \tag{26}$$

Therefore, collectively we have

$$\psi(\xi) = \begin{cases} \mathrm{e}^{-(\xi+\xi_0)^2/2} \left(\sum_{j=0}^{\infty} a_{2j} (\xi+\xi_0)^{2j} + \sum_{j=0}^{\infty} a_{2j+1} (\xi+\xi_0)^{2j+1} \right) & \xi \geq 0 \\ \mathrm{e}^{-(\xi-\xi_0)^2/2} \left(\sum_{j=0}^{\infty} b_{2j} (\xi-\xi_0)^{2j} - \sum_{j=0}^{\infty} b_{2j+1} (\xi-\xi_0)^{2j+1} \right) & \xi < 0 \end{cases} \tag{27}$$

where the recursion relations for the coefficients in each series are given by Equations (22) and (26).

These equations are the general solutions of Equations (17). However, for these functions to be quantum mechanically admissible for the given potential, they have to remain finite as $|\xi| \to \infty$. But, as in the case of the harmonic oscillator, it can be shown that each sum in Equations (27) behaves as $\mathrm{e}^{(\xi\pm\xi_0)^2}$ for large $|\xi|$ [2] [3] [4], consequently, each term in these equations behaves as $\mathrm{e}^{(\xi\pm\xi_0)^2/2}$ for large $|\xi|$. Therefore, in accord with the general practice in quantum mechanics, in each branch of the solution one of the series should be eliminated and the other series should be terminated setting all coefficients beyond $j = n$ equal to zero, which results in the possible energy eigenfunctions for the problem. Thus, in the first equation of (27), we set $a_0 = 0$ or $a_1 = 0$ to eliminate one of the series. If we set $a_0 = 0$, the first term drops out and we get

$$\psi_+(\xi) = \mathrm{e}^{-(\xi+\xi_0)^2/2} \sum_{j=0}^{\infty} a_{2j+1} (\xi+\xi_0)^{2j+1} \quad \xi \geq 0 \tag{28}$$

or if we set $a_1 = 0$, we get

$$\psi_+(\xi) = \mathrm{e}^{-(\xi+\xi_0)^2/2} \sum_{j=0}^{\infty} a_{2j} (\xi+\xi_0)^{2j} \quad \xi \geq 0 \tag{29}$$

Similarly, in the second of Equations (27), if we set $b_0 = 0$ or $b_1 = 0$, we obtain the following results

$$\psi_-(\xi) = \mathrm{e}^{-(\xi-\xi_0)^2/2} \sum_{j=0}^{\infty} b_{2j+1} (\xi - \xi_0)^{2j+1} \quad \xi < 0 \tag{30}$$

or

$$\psi_-(\xi) = \mathrm{e}^{-(\xi-\xi_0)^2/2} \sum_{j=0}^{\infty} b_{2j} (\xi - \xi_0)^{2j} \quad \xi < 0 \tag{31}$$

respectively.

Because the dynamically shifted potential energy is an even function, the eigenfunctions can be chosen to be either even or odd [5]. Therefore, the function in Equations (28)-(31) should be paired as,

$$\psi_{even}(\xi) = \begin{cases} \mathrm{e}^{-(\xi+\xi_0)^2/2} \sum_{j=0}^{\infty} a_{2j} (\xi + \xi_0)^{2j} & \xi \ge 0 \\ \mathrm{e}^{-(\xi-\xi_0)^2/2} \sum_{j=0}^{\infty} b_{2j} (\xi - \xi_0)^{2j} & \xi < 0 \end{cases} \tag{32}$$

and

$$\psi_{odd}(\xi) = \begin{cases} \mathrm{e}^{-(\xi+\xi_0)^2/2} \sum_{j=0}^{\infty} a_{2j+1} (\xi + \xi_0)^{2j+1} & \xi \ge 0 \\ \mathrm{e}^{-(\xi-\xi_0)^2/2} \sum_{j=0}^{\infty} b_{2j+1} (\xi - \xi_0)^{2j+1} & \xi < 0 \end{cases} \tag{33}$$

where Equations (32) and (33) give the even and the odd eigenfunctions, respectively. Furthermore, since in the case of even eigenfunctions, we have $\psi(-\xi) = \psi(\xi)$, we must have $b_{2j} = a_{2j}$. Similarly since for odd eigenfunctions, we have $\psi(-\xi) = -\psi(\xi)$, we must have $b_{2j+1} = a_{2j+1}$. Therefore, Equations (32) and (33) reduce to

$$\psi_{even}(\xi) = \begin{cases} \mathrm{e}^{-(\xi+\xi_0)^2/2} \sum_{j=0}^{\infty} a_{2j} (\xi + \xi_0)^{2j} & \xi \ge 0 \\ \mathrm{e}^{-(\xi-\xi_0)^2/2} \sum_{j=0}^{\infty} a_{2j} (\xi - \xi_0)^{2j} & \xi < 0 \end{cases} \tag{34}$$

and

$$\psi_{odd}(\xi) = \begin{cases} \mathrm{e}^{-(\xi+\xi_0)^2/2} \sum_{j=0}^{\infty} a_{2j+1} (\xi + \xi_0)^{2j+1} & \xi \ge 0 \\ \mathrm{e}^{-(\xi-\xi_0)^2/2} \sum_{j=0}^{\infty} a_{2j+1} (\xi - \xi_0)^{2j+1} & \xi < 0 \end{cases} \tag{35}$$

with the recursion relation given by Equation (22).

We now terminate each series by setting all coefficients of the series beyond $j = n$ equal to zero. Thus, from the recursion relations (22), we get

$$2(n - \varepsilon) + 1 = 0 \tag{36}$$

which gives the energy eigenvalue equation,

$$\varepsilon_n = n + \frac{1}{2} \quad n = 0, 1, 2, 3, \cdots \tag{37}$$

and the eigenfunctions become

$$\psi_{2n}(\xi)=\begin{cases} e^{-(\xi+\xi_0)^2/2}\sum_{j=0}^{n}a_{2j}(\xi+\xi_0)^{2j} & \xi\ge 0\\ e^{-(\xi-\xi_0)^2/2}\sum_{j=0}^{n}a_{2j}(\xi-\xi_0)^{2j} & \xi<0\end{cases}\quad n=0,1,2,3,\cdots \tag{38}$$

and

$$\psi_{2n+1}(\xi)=\begin{cases} e^{-(\xi+\xi_0)^2/2}\sum_{j=0}^{n}a_{2j+1}(\xi+\xi_0)^{2j+1} & \xi\ge 0\\ e^{-(\xi-\xi_0)^2/2}\sum_{j=0}^{n}a_{2j+1}(\xi-\xi_0)^{2j+1} & \xi<0\end{cases}\quad n=0,1,2,3,\cdots \tag{39}$$

In these equations, a_0 and a_1 are used to normalize the eigenfunctions and the rest of the coefficients are obtained through the recursion relation (22). However, these results are wrong!

According to Equation (37), the energy eigenvalues of the dynamically shifted oscillator are the same as those for the simple harmonic oscillator, which is not correct. In fact, numerical solution of the Schrödinger equations (17) show that the correct eigenvalues are quite different from those for the harmonic oscillator, both for positive and negative values of the dynamic shift ξ_0. Furthermore, the odd eigenfunctions from Equations (39) are discontinuous at $\xi=0$. For example, for $n=0$, from Equations (39) we have

$$\psi_1(\xi)=\begin{cases} a_1 e^{-(\xi+\xi_0)^2/2}(\xi+\xi_0) & \xi\ge 0\\ a_1 e^{-(\xi-\xi_0)^2/2}(\xi-\xi_0) & \xi<0\end{cases} \tag{40}$$

A plot of this function for $\xi_0=1$ and $a_1=1$ is shown in Figure 2. Therefore, they are not quantum mechanically admissible. Again, numerical solution of Equations (17) show that those given by Equations (38) and (39) are not the correct eigenfunctions.

Numerical Results

We solve Equations (17) numerically by bracketing the energy eigenvalues ε

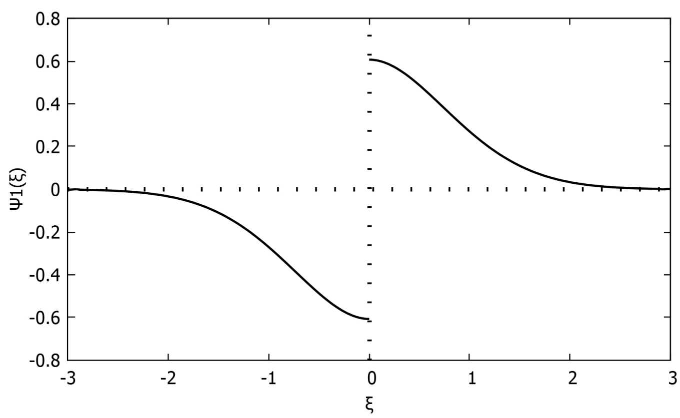

Figure 2. A plot of the inadmissible ground state ($n=0$) eigenfunction of dynamically shifted oscillator, given by Equation (40) with $\xi_0=1$ and $a_1=1$.

to the required accuracy until the eigenfunction diverges in one direction if ε is slightly smaller than the chosen value and diverges in the opposite direction if it is slightly larger [12].

Table 1 lists some of the dimensionless energy eigenvalues of the dynamically shifted oscillator obtained by numerical solution of the time-independent Schrödinger equations (17). Note that those for the harmonic oscillator, $\xi_0 = 0$, are also given for comparison. As can be seen from the table, these eigenvalues are quite different from those of the harmonic oscillator. Note also that the ground-state total energy is higher than the minimum of the potential energy in all cases, as they should be.

Figures 3-6 show the dimensionless graphs of the ground-state eigenfunctions of the dynamically shifted oscillator obtained from numerical solutions of Equations (17). These graphs show the first four eigenfunctions for $\xi_0 = 1$ and $\xi_0 = -1$ only. Plots of other eigenfunctions are given by Mohazzabi and Alexander [11]. These plots show that for $\xi_0 > 0$, the eigenfunctions of dynamically shifted oscillator are, at least qualitatively, similar to those of harmonic oscillator. But those for $\xi_0 < 0$ are quite different as they show bimodal behaviors, as can be seen in **Figure 3(b)** as well as **Figure 7**, which show the ground-state eigenfunctions, $\psi_0(\xi)$, of dynamically shifted oscillator for $\xi_0 = -2$ and $\xi_0 = -3$. This bimodal behavior emerges as the potential tends toward two separate harmonic potentials as $\xi_0 \to -\infty$.

Table 1. Dimensionless energy eigenvalues of the dynamically shifted oscillator obtained by numerically solving Equations (17).

	$\xi_0 = -1$	$\xi_0 = 0$	$\xi_0 = +1$
ε_0	0.310	0.500	1.499
ε_1	0.734	1.500	3.037
ε_2	1.500	2.500	4.328
ε_3	2.197	3.500	5.604

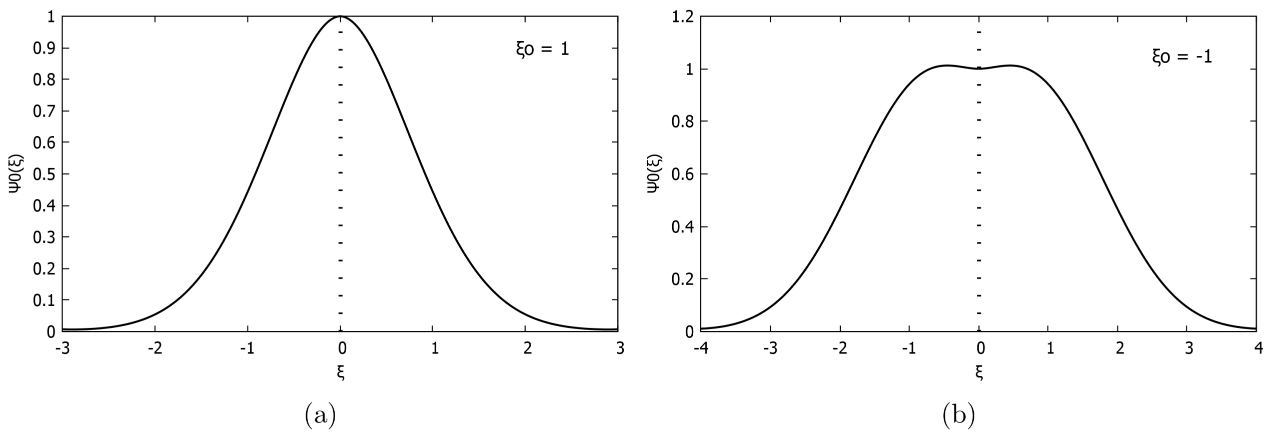

Figure 3. Ground state ($n = 0$) eigenfunctions of dynamically shifted oscillator.

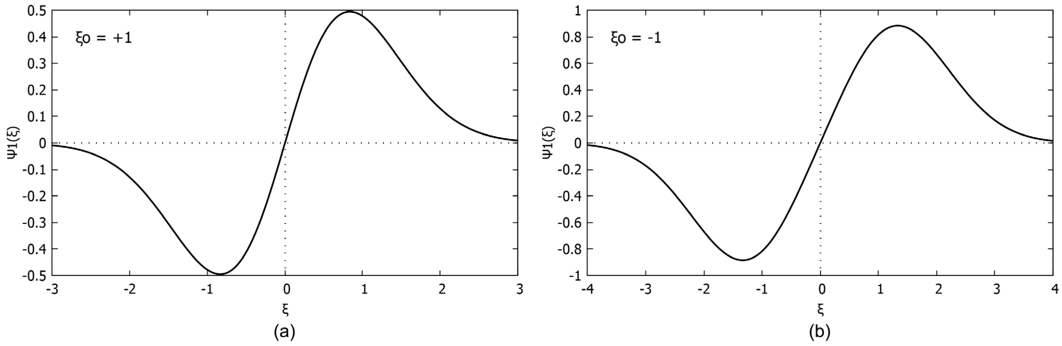

Figure 4. First excited state ($n = 1$) eigenfunctions of dynamically shifted oscillator.

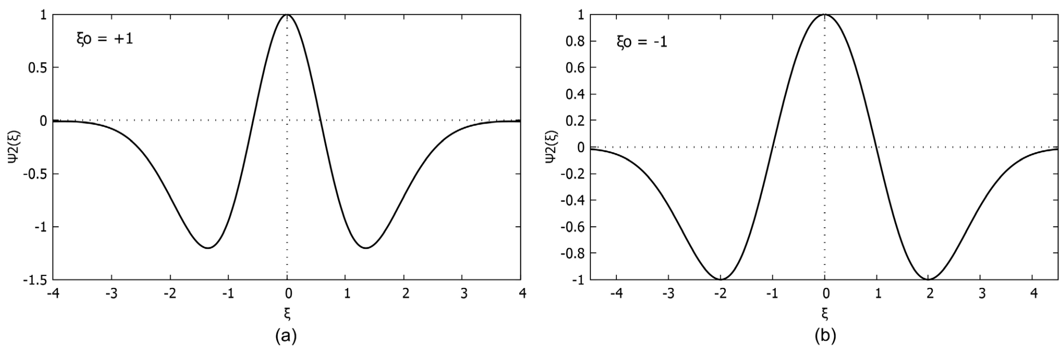

Figure 5. Second excited state ($n = 2$) eigenfunctions of dynamically shifted oscillator.

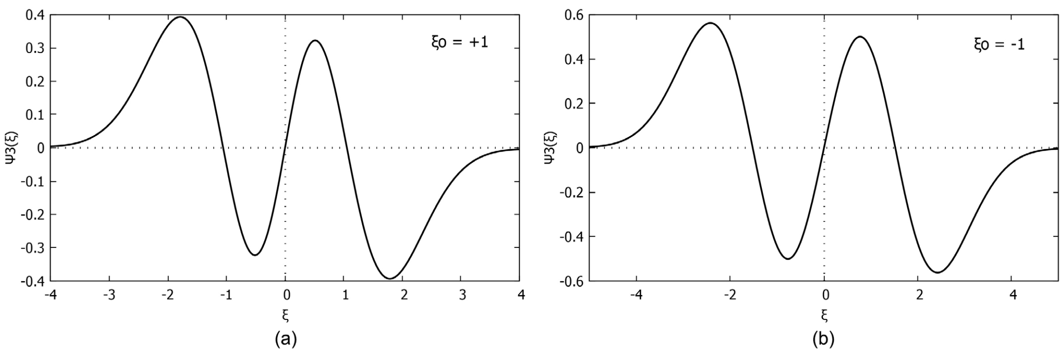

Figure 6. Third excited state ($n = 3$) eigenfunctions of dynamically shifted oscillator.

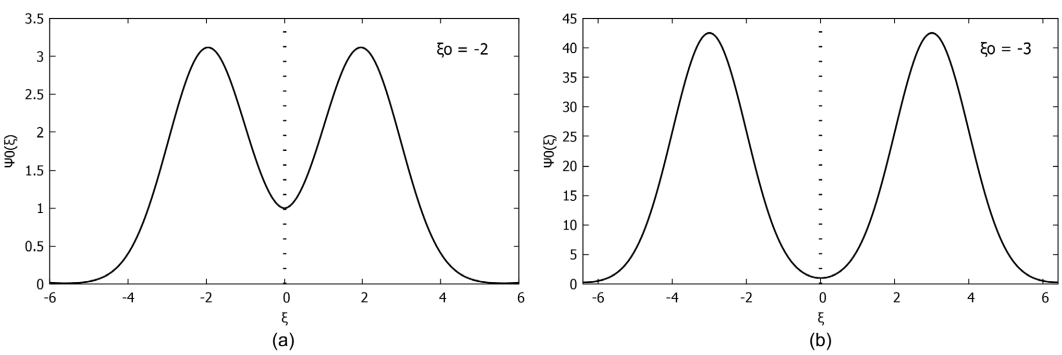

Figure 7. Ground state eigenfunctions of dynamically shifted oscillator for $\xi_0 = -2$ and $\xi_0 = -3$ with corresponding eigenvalues $\varepsilon_0 = 0.476$ and $\varepsilon_0 = 0.500$, respectively.

3. Discussion and Conclusion

The time-independent Schrödinger equation for dynamically shifted oscillator lends itself to the standard method of power series solution which is commonly used in quantum mechanics. However, in this article we have shown that this method results in incorrect eigenvalues and eigenfunctions for this system. More specifically, the method yields the same eigenvalues as those for harmonic oscillator, and eigenfunctions some of which are even quantum mechanically inadmissible.

We have also numerically calculated the correct eigenvalues and eigenfunctions of dynamically shifted oscillator. The results show that the functional form of the eigenfunctions corresponding to positive dynamic shift ($\xi_0 > 0$) are qualitatively similar to the eigenfunctions of a harmonic oscillator. But those corresponding to negative dynamic shift ($\xi_0 < 0$) are quite different and show bimodal behavior.

In conclusion, in applying the standard method of series solution to solving time-independent Schrödinger equation, caution should be exercised as the method might result in incorrect eigenvalues and eigenfunctions. Therefore, the analytical result obtained by this method for a new potential should always be checked against numerical solution.

Acknowledgements

This work was supported in part by a URAP grant from the University of Wisconsin-Parkside.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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