

# **Excited States of the Anharmonic Oscillator Potentials: Variational Method**

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## **Abstract**

We applied variational method to calculate the first eight eigenvalues of quartic and sextic anharmonic oscillator potentials. By choosing a set of sophisticated trial wave functions, applying the orthogonal conditions between the eigenstates, and with the help of Maple software packages, we found that these eight eigenvalues accurate and agree well with those obtained from the Runge-Kutta numerical integration method.

## **I. Introduction**

A one-dimensional bound state problem, such as solving the time-independent Schrödinger equation with given potential  $V(x)$ ,

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

is a major subject regularly presented in the introductory quantum mechanics course. In most cases, the potential  $V(x)$  is the harmonic oscillator potential  $\frac{1}{2}m\omega^2x^2$ , where  $\omega$  is the angular frequency, because

its eigenvalues and eigenfunctions can be obtained analytically. On top of that the model can be applied in many different areas of physics to explain all kinds of periodic motions. But when we extend the potential to the anharmonic region such as adding a quartic ( $\alpha x^4$ ) and/or sextic ( $\beta x^6$ ) potentials, where  $\alpha$  and  $\beta$  are coupling constants, the analytic solutions are practically impossible to achieve. Usually, an approximation scheme such as a perturbation method is used to undertake the problems, and it is accomplished in an order-by-order fashion, hence tedious expansion is needed. Another alternative is the variational method, [1] an approach that can be stated in a simple fashion and easily implemented, but requires good guess of a trial wave function. However it is always taught in a rather routine manner, namely the examples used in most textbooks are familiar problems with known solutions, not to mention that several important advantages of using the method, such as attaining remarkable precision of the eigenvalues and generalization to the high excited states, are seldom demonstrated. Previously the variational method had been carried out on the same potentials and emphasis was made on different choices of trial wave functions [2]. Later more detailed investigation was carried out to illustrate that impressively accurate ground state and first excited state eigenvalues could be achieved by adding more parameters to two sets of properly selected trial wave functions [3]. In this work, we extend the experiences we gained from studying the harmonic oscillator potential and applied them to the excited states of anharmonic oscillator potentials, we demonstrated that with the properly chose wave functions and orthogonality requirements between them, we were able to achieve their accurate eigenvalues, and found that they agree well with those obtained from the numerical integration method.

## II. Theory

The variational principle used in solving time-independent Schrödinger equation states: for a given Hamiltonian  $\hat{H}$ , the energy expectation value of any trial wave function  $\psi_{\text{trial}}$  we choose will always be greater than or equal to the true total ground state energy  $E_{\text{tot}}$ :

$$E_{\text{tot}} \leq \langle \psi_{\text{trial}} | \hat{H} | \psi_{\text{trial}} \rangle. \quad (2)$$

This theorem is proved elegantly in all the known textbooks by constructing the trial wave functions as the linear combinations of all the eigenstates. In fact, this principle can be extended to the higher excited states

as long as the trial wave function is orthogonal to the previously determined ground state and lower excited states. The argument roughly goes like following: since all the eigenstates are orthogonal to each other, if the previously determined states are proved to be of lower energy, then the newly founded states can only be states with higher energies, i.e. excited states. Nevertheless we seldom find any examples in the commonly used textbooks demonstrate this particular application. Therefore, it is the purpose of this work that we implement this application by calculating the first few excited states of the  $x^4$  and  $x^6$  potentials.

First, we review the variational procedures frequently stated in the textbooks: We choose a trial wave function  $\psi_{\text{trial}}(\alpha, \beta, \gamma, \dots)$ , where  $\alpha, \beta, \gamma, \dots$  are the variational parameters. With it we then form the expectation value of the system's total energy;

$$E_{\text{tot}} = \langle \text{KE} \rangle + \langle \text{PE} \rangle. \quad (3)$$

Then by differentiating the total energy with respect to all the variational parameters and simultaneously solve those equations (which may be nonlinear), we obtain the best set of parameters. Afterward we substitute the optimized parameters back into Eq. (3), and compute the total energy. In fact, these procedures can be applied to the first excited state especially when the potential is symmetrical, i.e.  $V(x) = V(-x)$ , because the ground state wave function is certainly an even function, the orthogonality condition precludes the same parity for the first excited state wave function, thus it has to be odd in parity. Based on the known spectrum of the harmonic oscillator potential, we are aware that the wave functions of a symmetric potential can be divided into two categories according to their parities: even and odd, which are orthogonal to each other. Furthermore since coefficients of the wave functions are so well arranged that they are also orthogonal with each other, and are also orthogonal to each other within the same groups. In addition, we notice that there are more nodes in the higher excited states. In fact the number of nodes is commensurate to the order of the excited states, starting from the nodeless ground state and one node first excited state. So far the spectra of the quartic and sextic anharmonic oscillator potentials are not known analytically, but it is reasonable to assume that they have the similar property as that of the harmonic oscillator potential. Accordingly we assume the two categories of wavefunctions as following: the first four eigenstates of even parity are,

$$\psi_0 = \exp(-a_0x^2 - b_0x^4), \quad (4)$$

$$\psi_2 = (1 - c_2 x^2) \exp(-a_2 x^2 - b_2 x^4), \quad (5)$$

$$\psi_4 = (1 - c_4 x^2 + d_4 x^4) \exp(-a_4 x^2 - b_4 x^4), \quad (6)$$

$$\psi_6 = (1 - c_6 x^2 + d_6 x^4 - e_6 x^6) \exp(-a_6 x^2 - b_6 x^4). \quad (7)$$

Then here are the first four eigenstates of odd parity,

$$\psi_1 = x \exp(-a_1 x^2 - b_1 x^4), \quad (8)$$

$$\psi_3 = (x - c_3 x^3) \exp(-a_3 x^2 - b_3 x^4), \quad (9)$$

$$\psi_5 = (x - c_5 x^3 + d_5 x^5) \exp(-a_5 x^2 - b_5 x^4), \quad (10)$$

$$\psi_7 = (x - c_7 x^3 + d_7 x^5 - e_7 x^7) \exp(-a_7 x^2 - b_7 x^4). \quad (11)$$

where  $a_i, b_i$  ( $i = 0..7$ ),  $c_i$  ( $i = 2..7$ ),  $d_i$  ( $i = 4..7$ ), and  $e_i$  ( $i = 6..7$ ) are parameters to be determined from energy optimization. Owing to the orthogonally condition, that is

$$\int \psi_i^* \psi_j dx = 0 \quad \text{if } i \neq j, \quad (12)$$

thus we can see that they are not completely independent of each other. However, we have to compute them sequentially, just to obtain  $E_0$  (the ground state energy) and  $E_1$  (first excited state energy) by using the standard energy optimization scheme. Then we use the obtained values of  $a_0, b_0$  and  $a_1, b_1$  to optimize the eigenenergies of  $\psi_2$  and  $\psi_3$ . Since we know that  $\psi_2$  has to be orthogonal to  $\psi_0$  and similar condition goes to  $\psi_3$  and  $\psi_1$ , we obtained  $c_2$  and  $c_3$  as:

$$c_2 = \frac{\int_{-\infty}^{\infty} \exp[-(a_0 + a_2)x^2 - (b_0 + b_2)x^4] dx}{\int_{-\infty}^{\infty} x^2 \exp[-(a_0 + a_2)x^2 - (b_0 + b_2)x^4] dx}, \quad (13)$$

and

$$c_3 = \frac{\int_{-\infty}^{\infty} x^2 \exp[-(a_1 + a_3)x^2 - (b_1 + b_3)x^4] dx}{\int_{-\infty}^{\infty} x^4 \exp[-(a_1 + a_3)x^2 - (b_1 + b_3)x^4] dx}. \quad (14)$$

Given that the ground state and first excited wave functions are automatically orthogonal to each other, parameters  $a_0, b_0$  and  $a_1, b_1$  are computed independently. Hence, we only have to vary  $a_2, b_2$ , and  $a_3, b_3$  during the optimization of  $E_2$  (second excited state energy) and  $E_3$  (third excited state energy) separately. After that, we proceed to  $\psi_4$  and  $\psi_5$ , following the same orthogonality condition between them and the

previous determined eigenstates, we express  $c_4$ ,  $d_4$  and  $c_5$ ,  $d_5$  as the solution of the following linear simultaneous equations:

$$\begin{cases} \alpha_{11}c_4 - \alpha_{12}d_4 = \alpha_{13} \\ \alpha_{21}c_4 - \alpha_{22}d_4 = \alpha_{23} \end{cases} \quad (15)$$

$$\begin{cases} \beta_{11}c_5 - \beta_{12}d_5 = \beta_{13} \\ \beta_{21}c_5 - \beta_{22}d_5 = \beta_{23} \end{cases} \quad (16)$$

where

$$\alpha_{11} = \int_{-\infty}^{\infty} x^2 \exp[-(a_0 + a_4)x^2 - (b_0 + b_4)x^4] dx, \quad (17)$$

$$\alpha_{12} = \int_{-\infty}^{\infty} x^4 \exp[-(a_0 + a_4)x^2 - (b_0 + b_4)x^4] dx, \quad (18)$$

$$\alpha_{13} = \int_{-\infty}^{\infty} \exp[-(a_0 + a_4)x^2 - (b_0 + b_4)x^4] dx, \quad (19)$$

$$\alpha_{21} = \int_{-\infty}^{\infty} (1 - c_2x^2)x^2 \exp[-(a_2 + a_4)x^2 - (b_2 + b_4)x^4] dx, \quad (20)$$

$$\alpha_{22} = \int_{-\infty}^{\infty} (1 - c_2x^2)x^4 \exp[-(a_2 + a_4)x^2 - (b_2 + b_4)x^4] dx, \quad (21)$$

$$\alpha_{23} = \int_{-\infty}^{\infty} (1 - c_2x^2) \exp[-(a_2 + a_4)x^2 - (b_2 + b_4)x^4] dx, \quad (22)$$

$$\beta_{11} = \int_{-\infty}^{\infty} x^4 \exp[-(a_1 + a_5)x^2 - (b_1 + b_5)x^4] dx, \quad (23)$$

$$\beta_{12} = \int_{-\infty}^{\infty} x^6 \exp[-(a_1 + a_5)x^2 - (b_1 + b_5)x^4] dx, \quad (24)$$

$$\beta_{13} = \int_{-\infty}^{\infty} x^2 \exp[-(a_1 + a_5)x^2 - (b_1 + b_5)x^4] dx, \quad (25)$$

$$\beta_{21} = \int_{-\infty}^{\infty} (1 - c_3x^2)x^4 \exp[-(a_3 + a_5)x^2 - (b_3 + b_5)x^4] dx, \quad (26)$$

$$\beta_{22} = \int_{-\infty}^{\infty} (1 - c_3x^2)x^6 \exp[-(a_3 + a_5)x^2 - (b_3 + b_5)x^4] dx, \quad (27)$$

and 
$$\beta_{23} = \int_{-\infty}^{\infty} (1 - c_3x^2)x^2 \exp[-(a_3 + a_5)x^2 - (b_3 + b_5)x^4] dx, \quad (28)$$

then we express them in terms of the 2x2 determinants;

$$c_4 = \frac{\begin{vmatrix} \alpha_{13} & -\alpha_{12} \\ \alpha_{23} & -\alpha_{22} \end{vmatrix}}{\begin{vmatrix} \alpha_{11} & -\alpha_{12} \\ \alpha_{12} & -\alpha_{22} \end{vmatrix}} \quad d_4 = \frac{\begin{vmatrix} \alpha_{11} & \alpha_{13} \\ \alpha_{21} & \alpha_{23} \end{vmatrix}}{\begin{vmatrix} \alpha_{11} & -\alpha_{12} \\ \alpha_{12} & -\alpha_{22} \end{vmatrix}} \quad (29)$$

and

$$c_5 = \frac{\begin{vmatrix} \beta_{13} & -\beta_{12} \\ \beta_{23} & -\beta_{22} \end{vmatrix}}{\begin{vmatrix} \beta_{11} & -\beta_{12} \\ \beta_{12} & -\beta_{22} \end{vmatrix}} \quad d_5 = \frac{\begin{vmatrix} \beta_{11} & \beta_{13} \\ \beta_{21} & \beta_{23} \end{vmatrix}}{\begin{vmatrix} \beta_{11} & -\beta_{12} \\ \beta_{12} & -\beta_{22} \end{vmatrix}} \quad (30)$$

Now we see that the optimization procedures of  $\psi_4$  and  $\psi_5$  involved only two independent parameters each;  $a_4, b_4$ , and  $a_5, b_5$ . Finally, following the same reasoning, those three coefficients,  $c_6, d_6$ , and  $e_6$ , and  $c_7, d_7$ , and  $e_7$ , in the wave functions,  $\psi_6$  and  $\psi_7$ , can be expressed in terms of the 3x3 determinants. Since those expressions are lengthy, we present them in the appendix. Also the total energies calculated from those wave functions are tedious, yet the optimizations procedures are the same as those of the previous states.

One remark regarding a mathematical trick we used often: due to the choice of our trial wave functions, we frequently encounter a special integral [4, 5],

$$\int_{-\infty}^{\infty} \exp[-2ax^2 - 2bx^4] dx = \frac{1}{4} \sqrt{\frac{a}{b}} K_{\frac{1}{4}} \left( \frac{a^2}{4b} \right) \exp \left( \frac{a^2}{4b} \right) \quad (31),$$

where  $K_{\sigma}(z)$  is the modified Bessel function of fractional order  $\sigma$ . Based on that, we derived compact expressions for the following related integrals

$$\int_{-\infty}^{\infty} x^{2n} \exp[-ax^2 - bx^4] dx, \quad (32)$$

where  $n$  is a positive integer, by differentiating repetitively the right hand side of Eq. (31) with respect to  $a$  and/or  $b$  and making use of the Bessel function recursion relations [4]. Even though the total energy equations of the excited states are lengthy and complicated, since all the integrals are analytical, the entire computation was reasonably fast because we did not have to evaluate them numerically.

### III. Results and discussion

In this section, we report the numerical results obtained from using the variational method. In each of the following tables 1 - 4 we present the essential variation parameters, namely the  $a_i$  and  $b_i$ , ( $i = 0, 1 \dots 7$ ), the coefficients of the  $x^2$  and  $x^4$  terms in the trial wave functions, variational eigenvalues and compare them with those obtained from the Runge-Kutta numerical integration. As we notice that all the discrepancies are within 0.1 %, also the systematic change of  $a_i$  and  $b_i$ : that is all  $a_i$  are increasing and  $b_i$  are decreasing when

progressing from low to high excited states that are more widespread. In addition, we only list  $a_i$  and  $b_i$  in the tables, because all the other parameters in the wave functions are derivable from them.

<b><math>X^4</math> Eigenstates (even)</b>			
	<b>Variational and Numerical results</b>		
$\psi_0, a_0=0.545673$ $b_0=0.074277$	1.060450	1.060362	
$\psi_2, a_2=0.728631$ $b_2=0.057914$	7.455914	7.455698	
$\psi_4, a_4=0.844816$ $b_4=0.050574$	16.262280	16.261826	
$\psi_6, a_6=0.935001$ $b_6=0.046006$	26.529053	26.528471	
	<b>Table 1</b>		

<b><math>X^4</math> Eigenstates (odd)</b>			
	<b>Variational and Numerical results</b>		
$\psi_1, a_1=0.652604$ $b_1=0.0638284$	3.799817	3.799673	
$\psi_3, a_3=0.791054$ $b_3=0.0537548$	11.645050	11.644746	
$\psi_5, a_5=0.892066$ $b_5=0.048099$	21.238893	21.238373	
$\psi_7, a_7=0.987158$ $b_7=0.0425794$	32.100006	32.098598	
	<b>Table 2</b>		

<b><math>X^6</math> Eigenstates (even)</b>			
	<b>Variational and Numerical results</b>		
$\psi_0, a_0=0.531079$ $b_0=0.1774098$	1.145193	1.1448025	
$\psi_2, a_2=0.788120$ $b_2=0.1738413$	9.074538	9.0730846	
$\psi_4, a_4=0.996391$ $b_4=0.170359$	21.717409	21.714165	
$\psi_6, a_6=1.174986$ $b_6=0.167198$	37.618765	37.613087	
	<b>Table 3</b>		

<b><math>X^6</math> Eigenstates (odd)</b>			
	<b>Variational and Numerical results</b>		
$\psi_1, a_1=0.661166$ $b_1=0.1769575$	4.339415	4.3385987	
$\psi_3, a_3=0.897997$ $b_3=0.171806$	14.937455	14.935170	
$\psi_5, a_5=1.086226$ $b_5=0.1692858$	29.304083	29.299646	
$\psi_7, a_7=1.262520$ $b_7=0.164755$	46.602822	46.595212	
	<b>Table 4</b>		

Next we display figures 1 – 4 to show the wave functions of these two potentials, we observe that even though they share the similar feature as that of the harmonic oscillator potential, yet we can distinguish them from their ranges, namely the spread of the  $x^4$  potential wave functions are clearly wider than those of the  $x^6$ .

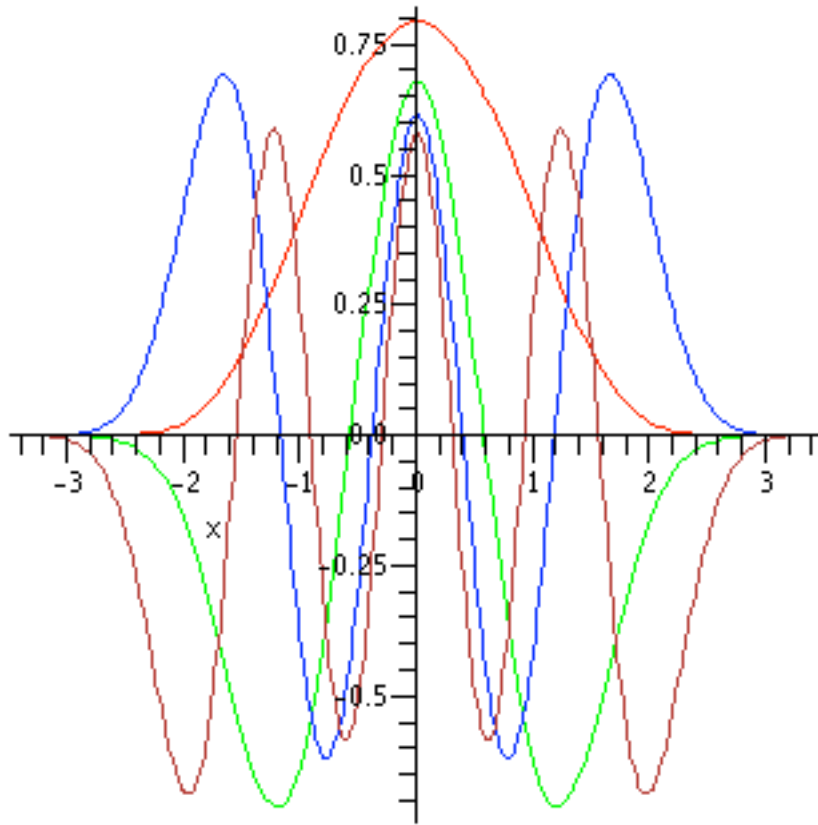


Figure 1. First four even parity eigenstates of the  $x^4$  potential: ground state (red), second (blue), fourth (green) and sixth (brown) excited states.

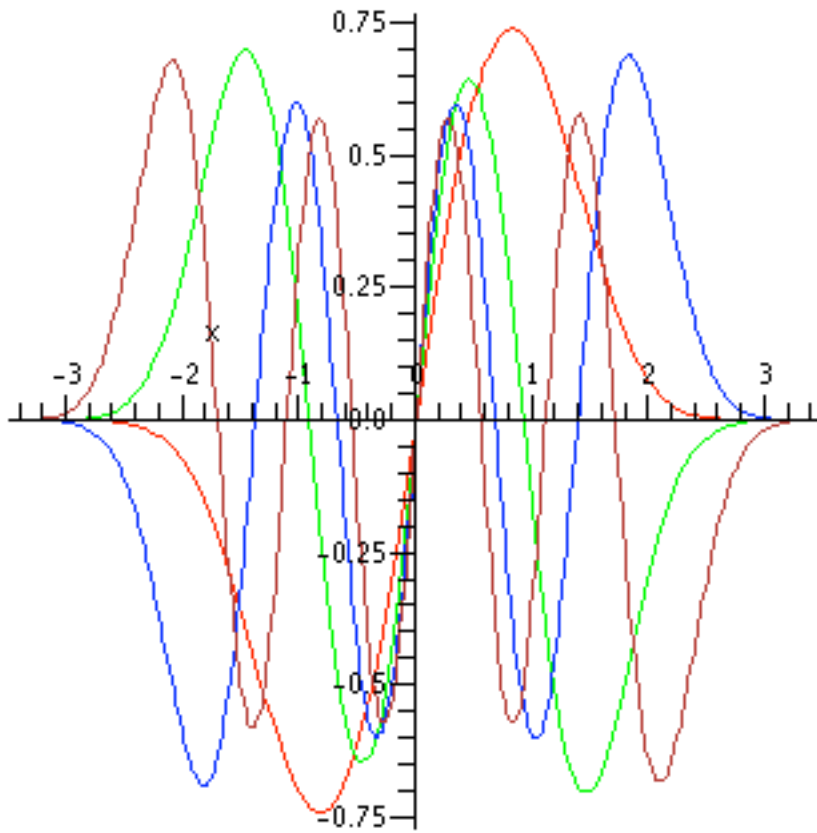


Figure 2. First four odd parity eigenstates of the  $x^4$  potential: first (red), third (green), fifth (blue) and seventh (brown) excited states.

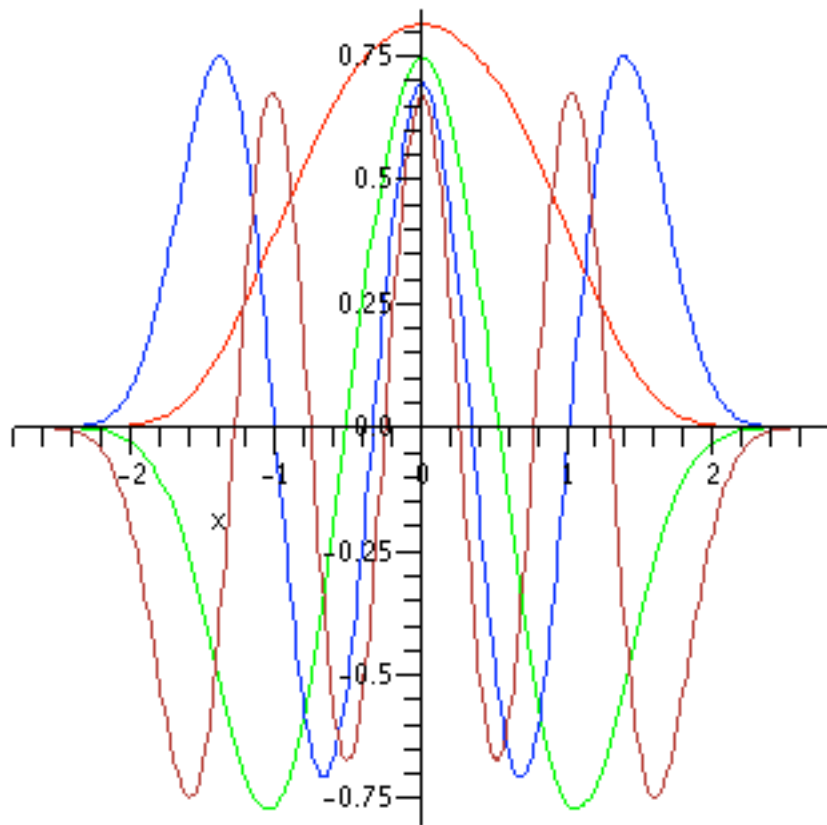


Figure 3. First four even parity eigenstates of the  $x^6$  potential: ground state (red), second (green), fourth (blue) and sixth (brown) excited states.

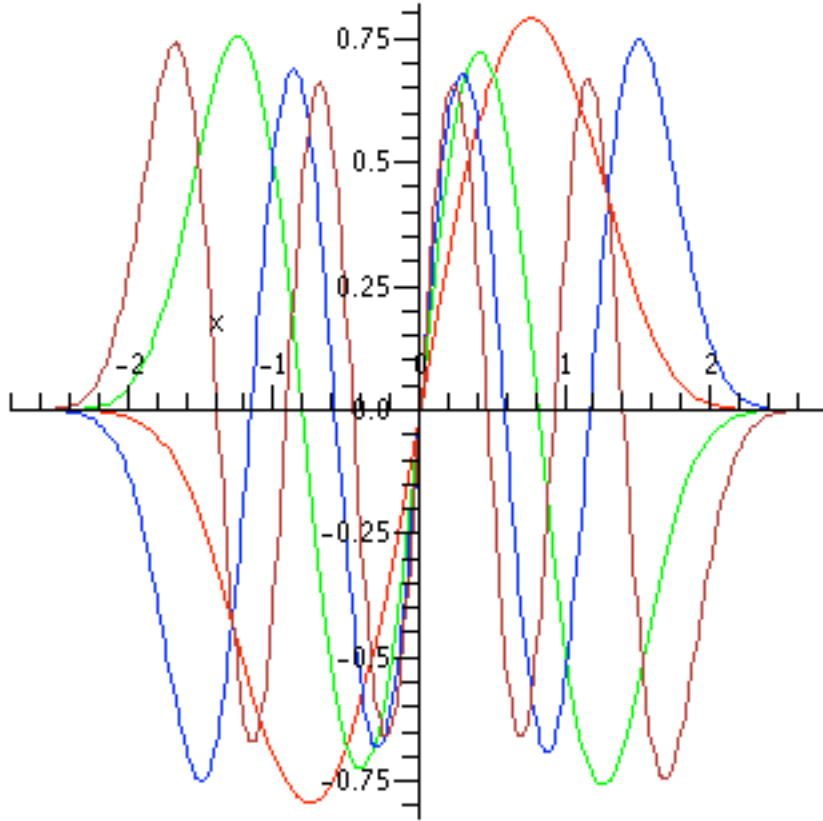


Figure 4. First four odd parity eigenstates of the  $x^6$  potential: first (red), third (green), fifth (blue) and seventh (brown) excited states.

To conclude, two remarks regarding our numerical computation are in order: first, when carrying out the numerical calculation, for convenience we set  $2m$ , the Planck's constant  $\hbar$ , and coupling constants of the potential in Eq. (1),  $\alpha$  and  $\beta$ , equal to one. In fact, that is equivalent to transforming Eq. (1) to a dimensionless differential equation by using a simple scale transformation: i.e. when  $V(x) = \alpha x^4$ , we convert it to

$$-\frac{d^2\psi}{dz^2} + z^4\psi = \varepsilon\psi \quad (33),$$

by substituting  $z = \left(\frac{\hbar^2}{2m\alpha}\right)^{1/6} x$  and  $\varepsilon = \left(\frac{2m}{\hbar^2}\right)^{2/3} \frac{E}{\alpha^{1/3}}$ , or when  $V(x) = \beta x^6$ , then we convert Eq. (1) to

$$-\frac{d^2\psi}{dz^2} + z^6\psi = \epsilon\psi \quad (34),$$

by substituting  $z = \left(\frac{\hbar^2}{2m\beta}\right)^{1/8} x$  and  $\epsilon = \left(\frac{2m}{\hbar^2}\right)^{3/4} \frac{E}{\beta^{1/4}}$ . Second, we used the Maple 10 to perform all the

analytical and numerical calculations, our worksheets are available for the interested readers, please send request to the attached addresses.

## V. Conclusion

In this work, we applied the variational method to the quartic and sextic anharmonic oscillator potentials: first we choose a set of trial wave functions from studying the spectrum of harmonic oscillator potential and require them to be orthogonal to each other, then we demonstrated not only could we achieve accurate ground and first excited state energies, but also those of the higher excited states agree well the numerical integration scheme. Nevertheless the procedures have to be performed consecutively. Also, while carrying out this project, we used Maple 10 packages intensively and found that it is a useful tool in manipulating lengthy equations and optimizing variational parameters in complex trial wave functions.

## VI. Acknowledgements

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## VII. Appendix

After we applied the orthogonality conditions, the coefficients,  $c_6$ ,  $d_6$ ,  $e_6$ ,  $c_7$ ,  $d_7$ , and  $e_7$  in  $\psi_6$  and  $\psi_7$  are shown to be determined by the following linear simultaneous equations:

$$\begin{cases} \gamma_{11}c_6 - \gamma_{12}d_6 + \gamma_{13}e_6 = \gamma_{14} \\ \gamma_{21}c_6 - \gamma_{22}d_6 + \gamma_{23}e_6 = \gamma_{24} \\ \gamma_{31}c_6 - \gamma_{32}d_6 + \gamma_{33}e_6 = \gamma_{34} \end{cases} \quad (A1)$$

and

$$\begin{cases} \delta_{11}c_6 - \delta_{12}d_6 + \delta_{13}e_6 = \delta_{14} \\ \delta_{21}c_6 - \delta_{22}d_6 + \delta_{23}e_6 = \delta_{24} \\ \delta_{31}c_6 - \delta_{32}d_6 + \delta_{33}e_6 = \delta_{34} \end{cases} \quad (A2)$$

where

$$\gamma_{11} = \int_{-\infty}^{\infty} x^2 \exp[-(a_0 + a_6)x^2 - (b_0 + b_6)x^4] dx \quad (A3)$$

$$\gamma_{12} = \int_{-\infty}^{\infty} x^4 \exp[-(a_0 + a_6)x^2 - (b_0 + b_6)x^4] dx \quad (A4)$$

$$\gamma_{13} = \int_{-\infty}^{\infty} x^6 \exp[-(a_0 + a_6)x^2 - (b_0 + b_6)x^4] dx \quad (A5)$$

$$\gamma_{14} = \int_{-\infty}^{\infty} \exp[-(a_0 + a_6)x^2 - (b_0 + b_6)x^4] dx \quad (A6)$$

$$\gamma_{21} = \int_{-\infty}^{\infty} (1 - c_2x^2)x^2 \exp[-(a_2 + a_6)x^2 - (b_2 + b_6)x^4] dx \quad (A7)$$

$$\gamma_{22} = \int_{-\infty}^{\infty} (1 - c_2x^2)x^4 \exp[-(a_2 + a_6)x^2 - (b_2 + b_6)x^4] dx \quad (A8)$$

$$\gamma_{23} = \int_{-\infty}^{\infty} (1 - c_2x^2)x^6 \exp[-(a_2 + a_6)x^2 - (b_2 + b_6)x^4] dx \quad (A9)$$

$$\gamma_{24} = \int_{-\infty}^{\infty} (1 - c_2x^2) \exp[-(a_2 + a_6)x^2 - (b_2 + b_6)x^4] dx \quad (A10)$$

$$\gamma_{31} = \int_{-\infty}^{\infty} (1 - c_4x^2 + d_4x^4)x^2 \exp[-(a_4 + a_6)x^2 - (b_4 + b_6)x^4] dx \quad (A11)$$

$$\gamma_{32} = \int_{-\infty}^{\infty} (1 - c_4x^2 + d_4x^4)x^4 \exp[-(a_4 + a_6)x^2 - (b_4 + b_6)x^4] dx \quad (A11)$$

$$\gamma_{33} = \int_{-\infty}^{\infty} (1 - c_4x^2 + d_4x^4)x^6 \exp[-(a_4 + a_6)x^2 - (b_4 + b_6)x^4] dx \quad (A12)$$

$$\gamma_{34} = \int_{-\infty}^{\infty} (1 - c_4x^2 + d_4x^4) \exp[-(a_4 + a_6)x^2 - (b_4 + b_6)x^4] dx \quad (A13)$$

$$\delta_{11} = \int_{-\infty}^{\infty} x^4 \exp[-(a_1 + a_7)x^2 - (b_1 + b_7)x^4] dx \quad (A14)$$

$$\delta_{12} = \int_{-\infty}^{\infty} x^6 \exp[-(a_1 + a_7)x^2 - (b_1 + b_7)x^4] dx \quad (A15)$$

$$\delta_{13} = \int_{-\infty}^{\infty} x^8 \exp[-(a_1 + a_7)x^2 - (b_1 + b_7)x^4] dx \quad (A16)$$

$$\delta_{14} = \int_{-\infty}^{\infty} x^2 \exp[-(a_1 + a_7)x^2 - (b_1 + b_7)x^4] dx \quad (A17)$$

$$\delta_{21} = \int_{-\infty}^{\infty} (1 - c_3 x^2) x^4 \exp[-(a_3 + a_7)x^2 - (b_3 + b_7)x^4] dx \quad (\text{A18})$$

$$\delta_{22} = \int_{-\infty}^{\infty} (1 - c_3 x^2) x^6 \exp[-(a_3 + a_7)x^2 - (b_3 + b_7)x^4] dx \quad (\text{A19})$$

$$\delta_{23} = \int_{-\infty}^{\infty} (1 - c_3 x^2) x^8 \exp[-(a_3 + a_7)x^2 - (b_3 + b_7)x^4] dx \quad (\text{A20})$$

$$\delta_{24} = \int_{-\infty}^{\infty} (1 - c_3 x^2) x^2 \exp[-(a_3 + a_7)x^2 - (b_3 + b_7)x^4] dx \quad (\text{A21})$$

$$\delta_{31} = \int_{-\infty}^{\infty} (1 - c_5 x^2 + d_5 x^4) x^4 \exp[-(a_5 + a_7)x^2 - (b_5 + b_7)x^4] dx \quad (\text{A22})$$

$$\delta_{32} = \int_{-\infty}^{\infty} (1 - c_5 x^2 + d_5 x^4) x^6 \exp[-(a_5 + a_7)x^2 - (b_5 + b_7)x^4] dx \quad (\text{A23})$$

$$\delta_{33} = \int_{-\infty}^{\infty} (1 - c_5 x^2 + d_5 x^4) x^8 \exp[-(a_5 + a_7)x^2 - (b_5 + b_7)x^4] dx \quad (\text{A24})$$

$$\delta_{34} = \int_{-\infty}^{\infty} (1 - c_5 x^2 + d_5 x^4) x^2 \exp[-(a_5 + a_7)x^2 - (b_5 + b_7)x^4] dx \quad (\text{A25})$$

then we can express them in terms of the 3x3 determinants:

$$c_6 = \frac{\begin{vmatrix} \gamma_{14} & -\gamma_{12} & \gamma_{13} \\ \gamma_{24} & -\gamma_{22} & \gamma_{23} \\ \gamma_{34} & -\gamma_{32} & \gamma_{33} \end{vmatrix}}{\begin{vmatrix} \gamma_{11} & -\gamma_{12} & \gamma_{13} \\ \gamma_{21} & -\gamma_{22} & \gamma_{23} \\ \gamma_{31} & -\gamma_{32} & \gamma_{33} \end{vmatrix}}, \quad d_6 = \frac{\begin{vmatrix} \gamma_{11} & \gamma_{14} & \gamma_{13} \\ \gamma_{21} & \gamma_{24} & \gamma_{23} \\ \gamma_{31} & \gamma_{34} & \gamma_{33} \end{vmatrix}}{\begin{vmatrix} \gamma_{11} & -\gamma_{12} & \gamma_{13} \\ \gamma_{21} & -\gamma_{22} & \gamma_{23} \\ \gamma_{31} & -\gamma_{32} & \gamma_{33} \end{vmatrix}}, \quad \text{and } e_6 = \frac{\begin{vmatrix} \gamma_{11} & -\gamma_{12} & \gamma_{14} \\ \gamma_{21} & -\gamma_{22} & \gamma_{24} \\ \gamma_{31} & -\gamma_{32} & \gamma_{34} \end{vmatrix}}{\begin{vmatrix} \gamma_{11} & -\gamma_{12} & \gamma_{13} \\ \gamma_{21} & -\gamma_{22} & \gamma_{23} \\ \gamma_{31} & -\gamma_{32} & \gamma_{33} \end{vmatrix}} \quad (\text{A26})$$

and

$$c_7 = \frac{\begin{vmatrix} \delta_{14} & -\delta_{12} & \delta_{13} \\ \delta_{24} & -\delta_{22} & \delta_{23} \\ \delta_{34} & -\delta_{32} & \delta_{33} \end{vmatrix}}{\begin{vmatrix} \delta_{11} & -\delta_{12} & \delta_{13} \\ \delta_{21} & -\delta_{22} & \delta_{23} \\ \delta_{31} & -\delta_{32} & \delta_{33} \end{vmatrix}}, \quad d_7 = \frac{\begin{vmatrix} \delta_{11} & \delta_{14} & \delta_{13} \\ \delta_{21} & \delta_{24} & \delta_{23} \\ \delta_{31} & \delta_{34} & \delta_{33} \end{vmatrix}}{\begin{vmatrix} \delta_{11} & -\delta_{12} & \delta_{13} \\ \delta_{21} & -\delta_{22} & \delta_{23} \\ \delta_{31} & -\delta_{32} & \delta_{33} \end{vmatrix}}, \quad \text{and } e_7 = \frac{\begin{vmatrix} \delta_{11} & -\delta_{12} & \delta_{14} \\ \delta_{21} & -\delta_{22} & \delta_{24} \\ \delta_{31} & -\delta_{32} & \delta_{34} \end{vmatrix}}{\begin{vmatrix} \delta_{11} & -\delta_{12} & \delta_{13} \\ \delta_{21} & -\delta_{22} & \delta_{23} \\ \delta_{31} & -\delta_{32} & \delta_{33} \end{vmatrix}} \quad (\text{A27})$$

Now we notice that all the coefficients in  $\psi_6$  and  $\psi_7$  are dependent on the parameters in the previous eigenstates and only  $a_6$ ,  $b_6$ ,  $a_7$ , and  $b_7$  have to be calculated from the variational procedures.

## VIII. References

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