

Excited States of the Anharmonic Oscillator Potentials: Variational Method

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(Submitted for publication at the Journal of Undergraduate Research in Physics)

Revised on June 12, 2008

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 ω 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 (αx^4) and/or sextic (βx^6) potentials, where α and β 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 ψ_{trial} we choose will always be greater than or equal to the true total ground state energy E_{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 ψ_2 and ψ_3 . Since we know that ψ_2 has to be orthogonal to ψ_0 and similar condition goes to ψ_3 and ψ_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 ψ_4 and ψ_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 ψ_4 and ψ_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, ψ_6 and ψ_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 σ . 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.

X^4 Eigenstates (even)			
	Variational and Numerical results		
$\psi_0, a_0=0.545673$ $b_0=0.074277$	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	
	Table 1		

X^4 Eigenstates (odd)			
	Variational and Numerical results		
$\psi_1, a_1=0.652604$ $b_1=0.0638284$	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	
	Table 2		

X^6 Eigenstates (even)			
	Variational and Numerical results		
$\psi_0, a_0=0.531079$ $b_0=0.1774098$	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	
	Table 3		

X^6 Eigenstates (odd)			
	Variational and Numerical results		
$\psi_1, a_1=0.661166$ $b_1=0.1769575$	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	
	Table 4		

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 .

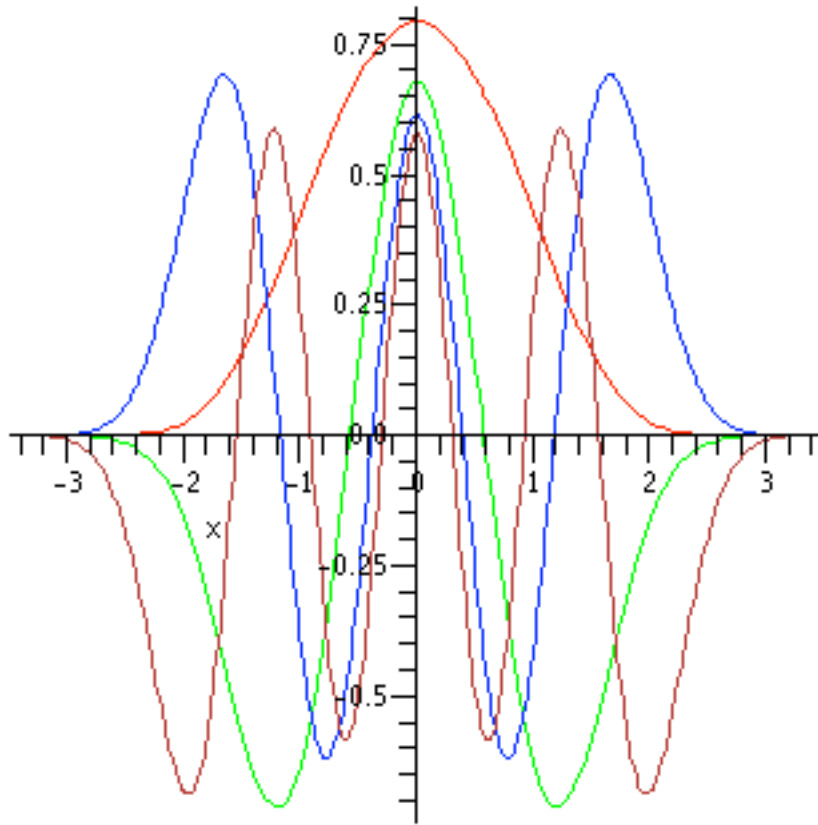


Figure 1. First four even parity eigenstates of the x^4 potential: ground state (red), second (blue), fourth (green) and sixth (brown) excited states.

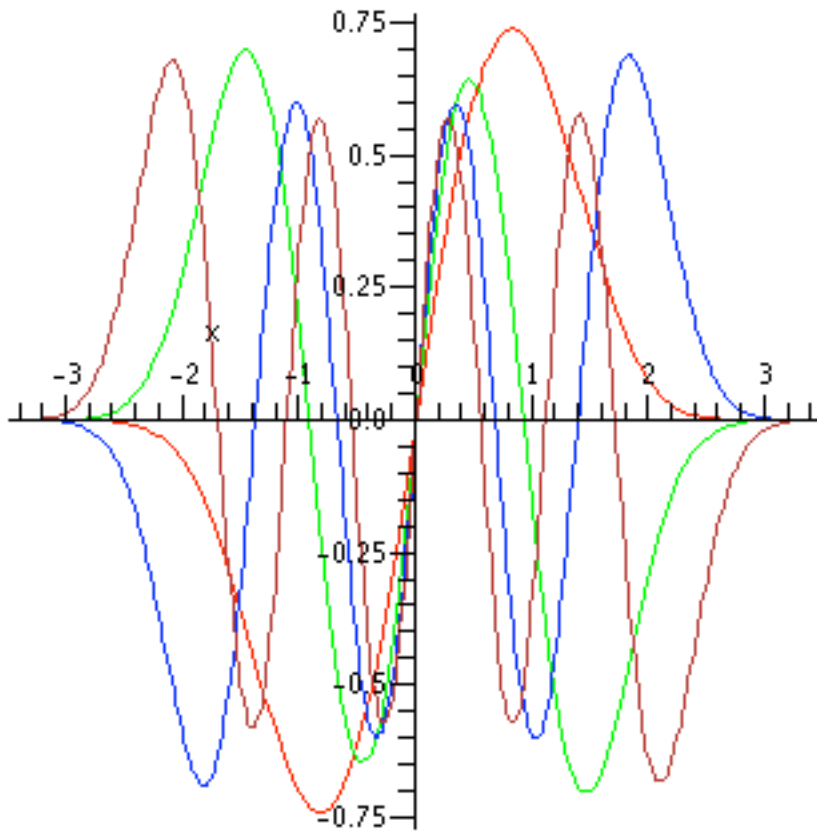


Figure 2. First four odd parity eigenstates of the x^4 potential: first (red), third (green), fifth (blue) and seventh (brown) excited states.

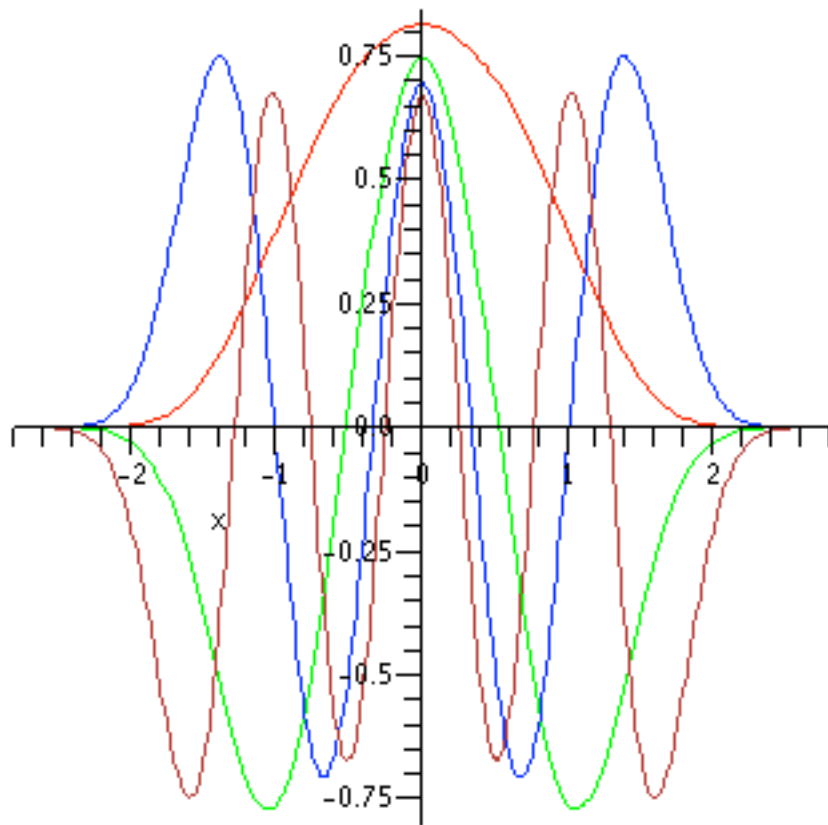


Figure 3. First four even parity eigenstates of the x^6 potential: ground state (red), second (green), fourth (blue) and sixth (brown) excited states.

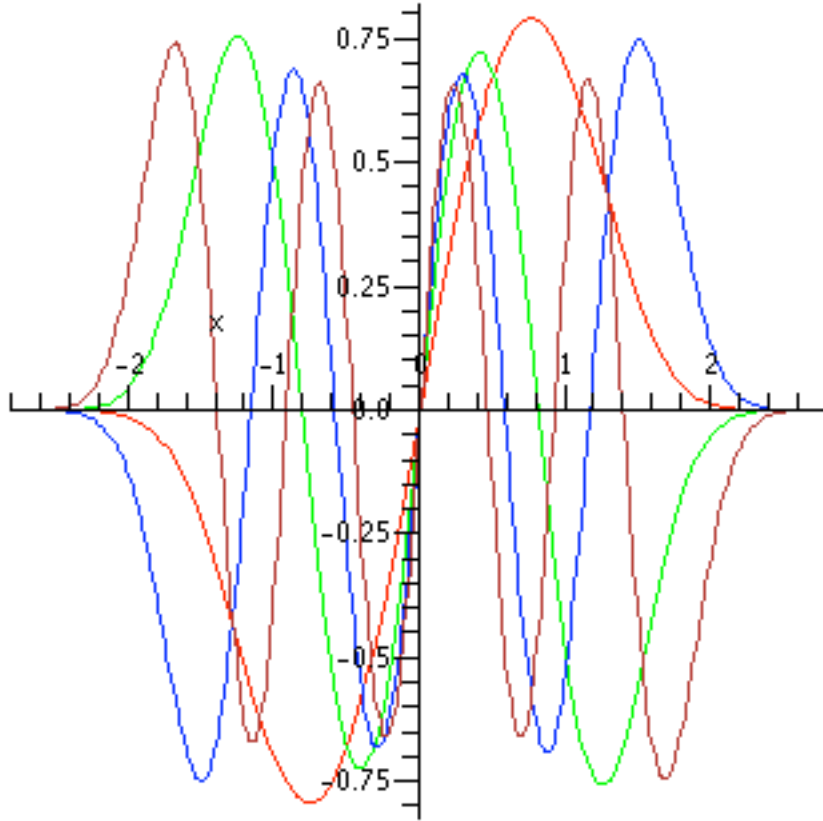


Figure 4. First four odd parity eigenstates of the x^6 potential: first (red), third (green), fifth (blue) and seventh (brown) excited states.

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), α and β , 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

We are grateful to the Department of Physics of the University of Nebraska at Omaha (UNO) for providing us with a superb study atmosphere. This work started from taking the Quantum Mechanics II course offered by Dr. Wai-Ning Mei, whose encouragement and supervision through out the entire project are deeply treasured. We would also like to express our appreciations to Drs. Glen Sowell, Dan Wilkins, Renat Sabirianov and Robert Graham of the Physics Department for their constant guidance and support to the Physics Student Society of the UNO Department of Physics.

VII. Appendix

After we applied the orthogonality conditions, the coefficients, c_6 , d_6 , e_6 , c_7 , d_7 , and e_7 in ψ_6 and ψ_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 ψ_6 and ψ_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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