Numerical Calculation of Ground-State Energies for the Gaussian Double-Well Potential Problem via Perturbation and Shooting Method

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Condensed Matter Theory Research Unit
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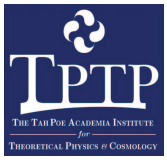
To My Family



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The candidate has passed the viva voce examination by the examination panel. This report has been accepted to the panel as partially fulfilment of the course 261493 Independent Study.

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Sawanee Tasasungkin

Title: Numerical Calculation of Ground-State Energies for the Gaussian Double-Well Potential Problem via Perturbation and Shooting Method

Candidate: Miss Sawanee Tasasungkin

Supervisor: Dr. Chanun Sricheewin

Degree: Bachelor of Science Programme in Physics

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Abstract

This project aims at computing ground-state energy eigenvalues and wave functions of a particle under Gaussian double-well potential using 1^{st}-order Brillouin-Wigner Perturbation Theory (BWPT) and Shooting Method, a method to deal with discrete-eigenvalue problems. The computing effiency relies on programming techniques and the computer itself. For accuracy, it depends on appropriate length of intervals, grid-width and initial conditions. The results from Shooting Methods are compared with the 1^{st}-order P.T. eigenvalues in order to show quantitative differences between them.

Contents

Chapter 1

Introduction

1.1 Background

In Quantum Mechanics, few problems can be solved exactly. Accordingly other approaches exist in order to solve problems approximately. One of the popular ways is Rayleigh-Schrödinger Perturbation Theory (RSPT). It is just a special case of Brillouin-Wigner Perturbation Theory (BWPT), the more accurate way for calculating the energies. However, there exists another way to calculate energy eigenvalues, the Shooting Method, where the energies are tried and the Schrödinger equation is solved numerically for the corresponding wave function.

1.2 Principles, theories, reasoning, and hypotheses

The aim of this work is to calculate ground-state energies and wave functions of a particle under anharmonic potential. Rayleigh-Schrödinger Perturbation Theory (RSPT) is a popular way to calculate the ground-state energy. It is the part of Brillouin-Wigner Perturbation Theory (BWPT). According to BWPT, the perturbed energy (E_n) is given by [8]

$$\begin{aligned} E_n &= \varepsilon_n + \lambda\langle n|\hat{H}_1|n\rangle + \lambda^2 \sum_{m_1\neq n} \frac{\langle n|\hat{H}_1|m_1\rangle\langle m_1|\hat{H}_1|n\rangle}{E_n-\varepsilon_{m_1}} + ... \\ &\quad +\lambda^{j+1} \sum_{m_1\neq n}\sum_{m_2\neq n}\sum_{m_j\neq n} \frac{\langle n|\hat{H}_1|m_1\rangle\langle m_1|\hat{H}_1|m_2\rangle ...\langle m_j|\hat{H}_1|n\rangle}{(E_n-\varepsilon_{m_1})(E_n-\varepsilon_{m_2})...(E_n-\varepsilon_{m_j})} + ... \end{aligned}$$

1.3 The purposes of this project

1) To study and understand numerical technique for calculating ground-state energies for the Gaussian double-well potential by using 2nd-order Brillouin-Wigner and Shooting Method.

2) To study and understand BWPT in a special problem.

3) To use RSPT as the basis of BWPT.

4) To compare the results of the ground-state energies between BWPT and Shooting Method.

1.4 Literature reviews

1) Brillouin-Wigner perturbation theory and the generalized eigenvalue equation
Abstract

A Brillouin-Wigner perturbation expansion is derived for the generalized eigenvalue equation $(F_0 + F_1)\Psi = \mu A\Psi$. The theory is applied through second order to calculate the ground-state energies of the helium atom and the hydrogen molecular ion. The results are compared with the corresponding Rayleigh-Schrödinger expansion. For the examples we consider, the Brillouin-Wigner results through second order are generally superior to the Rayleigh-Schrödinger ones.

2) Continued fractions and upper and lower bounds in the Brillouin-Wigner perturbation scheme
Abstract

A derivation of approximants to a continued fraction development of the energy is presented. It is based on the techniques of infinite order perturbation theory and inner projection of operators. The approximants have been introduced before; here their formal nature is clarified and conditions under which they exhibit extremal properties are presented. The oscillatory behaviour about the true eigenvalue, observed previously in the Mathieu problem, is explained.

3) Brillouin-Wigner perturbation methods for coupled oscillators
Abstract

We study the use of Brillouin-Wigner perturbation theory (BWPT) coupled with Padé approximant summation techniques to solve problems formulated as coupled (diabatic, adiabatic, "mixed") channels. Several iterative BWPT schemes are examined. BW perturbation series demonstrate better convergence properties, making them more practical and efficient than traditional Rayleigh-Schrödinger perturbation series. Obtaining proof of power-law solution.

4) Variational Solutions to Brillouin-Wigner Perturbation Differential Equations
Abstract

The usual Brillouin-Wigner (BW) perturbation theory series expansions for the energy and wave function of a perturbed system are replaced by a set of perturbation differential equations. Thus it seems probable that many of the developments of Rayleigh-Schrodinger (RS) perturbation theory which depend largely on the RS perturbation differential equations should carry over to BW theory. A variational method, analogous to the Hylleraas principle in RS6theory, is derived which can be used to obtain approximate solutions to the n-th order BW perturbation equation for systems in the lowest energy state of a given symmetry. The BW energy to (2n)-th order obtained in this manner is an upper bound to the exact BW energy to (2n)-th order if the (n-1)-th order wave function is known exactly. This is usually true for n=1 only. It is shown, however, that these variational techniques give an upper bound to the total energy even if the (n-1)-th order BW wave function is unknown. A convenient matrix method of applying the variational principles is suggested and a method of using this formulation of BW perturbation theory is discussed formally.

5) Comparison of Rayleigh-Schrödinger and Brillouin-Wigner Perturbation Theories
Abstract

Parallel derivations of Rayleigh-Schrödinger and Brillouin-Wigner Perturbation Theory are pre-

sented, using the Dirac formalism. The relative advantages and disadvantages of the two are compared with the goal of smoothing the transition between elementary qantum mechanics and advanced approximation theory.

6) Energy Splitting in Symmetric Double-Well Potentials
Abstract

We extend the analytical transfer matrix method to solve the energy splitting in an arbitrary symmetric double-well potential. Dispersion equations corresponding to the split energy levels are presented in a very explicit form. Numerical calculation shows that the proposed method can give extremely accurate results for symmetric double-well potentials.

7) Solution of the Schr?dinger Equation with One and Two Dimensional Double-Well Potential
Abstract

The Schrödinger equation with one and two dimensional potentials are solved in the framework of the $sl_2(R)$ Lie algebra. Eigenfunctions of the Schrödinger equation for various asymmetric double-well potentials have been determined and the eigenstates are expressed in terms of the orthogonal polynomials. The solution of the double-well potential in two dimension have been analyzed.

1.5 Regulation Researches

1) Allow 4 months to study the project in overall.
2) Study the project.
3) Study BWPT and shooting method.
4) Study numerical and Mathematica program.
5) Collect the data and study from related articles.
6) Fix the heading and the way to study.
7) Summarize and analyse.
8) Check the correctness.

1.6 Limit of the research

Study the numerical solution of double-well potential modified from single-well potential.

1.7 Instrument for the project

1) Textbooks and related documents
2) Computer
3) Mathematica program
4) Microsoft Office program
5) Math-Type program

1.8 The advantages of this study

1) Knowing more Anharmonic Oscillation in Quantum Mechanics.
2) Knowing about how to use BWPT and Shooting method to calculate the ground-state energies.

3) Enhancing the skill to use program such as Mathematica, Microsoft Office, and Math Type.
4) Trending to study in the future.
5) Being worthy for anyone wishing to study further.

Chapter 2

Perturbation Theory

2.1 Time-independent perturbation theory for a non-degenerate energy level

The eigenvalue problem we wish to solve is of the Schrödinger form:

$$\hat{H}\Psi_n = E_n\Psi_n \tag{2.1}$$

From Rayleigh-Schrödinger perturbation theory, suppose that the time-independent Hamiltonian $\hat{H}$ of a system can be expressed as

$$\hat{H} = \hat{H}_0 + \lambda\hat{H}' \tag{2.2}$$

$$\begin{aligned} \hat{H} &= \text{time} - \text{independent Hamiltonian} \\ \hat{H}_0 &= \text{unperturbed Hamiltonian} \\ \hat{H}' &= \text{a small perturbation} \end{aligned}$$

By solving the time-independent Schrödinger Equation

$$\hat{H}_0\Psi_n^{(0)} = E_n^{(0)}\Psi_n^{(0)}$$

where $\Psi_n^{(0)}$ is an unperturbed wave function which can be solved exactly,
one obtains a complete set of orthonormal eigenfunctions,$\Psi_n^{(0)}$, which may also be expressed as an eigenstate,$|\Psi_n^{(0)}\rangle$, such that

$$\langle\Psi_n^{(0)}|\Psi_m^{(0)}\rangle = \delta_{nm}$$

where δ_{nm} is a Kronecker delta defined by $\delta_{nm} = \{^{1,\ n=m}_{0,\ n\neq m}$

We can write Ψ_n and E_n as power series in λ , i.e.

$$\Psi_n = \Psi_n^{(0)} + \lambda\Psi_n^{(1)} + \lambda^2\Psi_n^{(2)} + ... \tag{2.3}$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + ... \tag{2.4}$$

By substituting Eq.'s (2.2), (2.3), (2.4) into Eq.(2.1), we obtain

$$(\hat{H^0} + \lambda\hat{H'})[\Psi_n^0 + \lambda\Psi_n^1 + \lambda^2\Psi_n^2 + ...] = (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + ...)[\Psi_n^0 + \lambda\Psi_n^1 + \lambda^2\Psi_n^2 + ...]$$

$$\begin{aligned} \hat{H^0}\Psi_n^0 + \lambda(\hat{H^0}\Psi_n^1 + \hat{H'}\Psi_n^0) &+ \lambda^2(\hat{H^0}\Psi_n^2 + \hat{H'}\Psi_n^1) + ... \\ &= E_n^0\Psi_n^0 + \lambda(E_n^0\Psi_n^1 + E_n^1\Psi_n^0) + \lambda^2(E_n^0\Psi_n^2 + E_n^1\Psi_n^1 + E_n^2\Psi_n^0) + ... \end{aligned}$$

The lowest order in λ , λ^0 , yields

$$\hat{H^0}\Psi_n^0 = E_n^0\Psi_n^0$$

The first order in λ , λ^1 , yields

$$\hat{H^0}\Psi_n^1 + \hat{H'}\Psi_n^0 = E_n^0\Psi_n^1 + E_n^1\Psi_n^0 \tag{2.5}$$

The second order in λ , λ^2 , yields

$$\hat{H^0}\Psi_n^2 + \hat{H'}\Psi_n^1 = E_n^0\Psi_n^2 + E_n^1\Psi_n^1 + E_n^2\Psi_n^0 \tag{2.6}$$

2.2 First-Order Perturbation Theory

Taking the inner product of Eq.(2.5) with Ψ_n^0 , what follows is

$$\langle\Psi_n^0|\hat{H^0}|\Psi_n^1\rangle + \langle\Psi_n^0|\hat{H'}|\Psi_n^0\rangle = E_n^0\langle\Psi_n^0|\Psi_n^1\rangle + E_n^1\langle\Psi_n^0|\Psi_n^0\rangle$$

Since $\hat{H^0}$ is Hermitian, so

$$\langle\Psi_n^0|\hat{H^0}|\Psi_n^1\rangle = \langle H^0\Psi_n^0|\Psi_n^1\rangle = \langle E_n^0\Psi_n^0|\Psi_n^1\rangle = E_n^0\langle\Psi_n^0|\Psi_n^1\rangle$$

Noting that $\langle\Psi_n^0|\Psi_n^0\rangle = 1$, we then obtain

$$E_n^1 = \langle\Psi_n^0|\hat{H'}|\Psi_n^0\rangle \tag{2.7}$$

By conclusion, the first-order correction to the energy is the expectation value of the perturbation over the unperturbed state.

2.3 Second-Order Energies

Taking the inner product of the second-order equation with Ψ_n^0 yields

$$\langle\Psi_n^0|\hat{H^0}|\Psi_n^2\rangle + \langle\Psi_n^0|\hat{H'}|\Psi_n^1\rangle = E_n^0\langle\Psi_n^0|\Psi_n^2\rangle + E_n^1\langle\Psi_n^0|\Psi_n^1\rangle + E_n^2\langle\Psi_n^0|\Psi_n^0\rangle$$

By exploiting the Hermiticity of $\hat{H^0}$, we get

$$\langle\Psi_n^0|\hat{H^0}|\Psi_n^2\rangle = \langle H^0\Psi_n^0|\Psi_n^2\rangle = E_n^0\langle\Psi_n^0|\Psi_n^2\rangle$$

Taking, $\langle\Psi_n^0|\Psi_n^0\rangle = 1$, we get

$$E_n^2 = \langle\Psi_n^0|\hat{H'}|\Psi_n^1\rangle - E_n^1\langle\Psi_n^0|\Psi_n^1\rangle$$

but

$$\langle \Psi_n^0 | \Psi_n^1 \rangle = \sum_{m \neq n} c_m^{(n)} \langle \Psi_n^0 | \Psi_m^0 \rangle = 0$$

so

$$E_n^2 = \langle \Psi_n^0 | \hat{H}' | \Psi_n^1 \rangle = \sum_{m \neq n} c_m^{(n)} \langle \Psi_n^0 | \hat{H}' | \Psi_m^0 \rangle = \sum_{m \neq n} \frac{\langle \Psi_m^0 | \hat{H}' | \Psi_n^0 \rangle \langle \Psi_n^0 | \hat{H}' | \Psi_m^0 \rangle}{E_n^0 - E_m^0}$$

finally , we have

$$E_n^2 = \sum_{m \neq n} \frac{\langle \Psi_m^0 | \hat{H}' | \Psi_n^0 \rangle^2}{E_n^0 - E_m^0} \tag{2.8}$$

We can find the energy eigenvalue of Brillouin-Wigner Perturbation Theory (BWPT) by solving this equation [8],

$$\begin{aligned} E_n &= \varepsilon_n + \lambda \langle n | \hat{H}_1 | n \rangle + \lambda^2 \sum_{m_1 \neq n} \frac{\langle n | \hat{H}_1 | m_1 \rangle \langle m_1 | \hat{H}_1 | n \rangle}{E_n - \varepsilon_{m_1}} + ... \\ &\quad + \lambda^{j+1} \sum_{m_1 \neq n} \sum_{m_2 \neq n} ... \sum_{m_j \neq n} \frac{\langle n | \hat{H}_1 | m_1 \rangle \langle m_1 | \hat{H}_1 | m_2 \rangle ... \langle m_j | \hat{H}_1 | n \rangle}{(E_n - \varepsilon_{m_1})(E_n - \varepsilon_{m_2}) ... (E_n - \varepsilon_{m_j})} + ... \end{aligned}$$

Chapter 3

Gaussian Oscillator Problem

In Classical Mechanics, the total mechanical energy of a particle is called Hamiltonian, i.e.

$$H(x,p) = \frac{p^2}{2m} + V(x)$$

where

$$\begin{aligned} H &= \text{Hamiltonian} \\ p &= \text{linear momentum} \\ V &= \text{potential energy} \end{aligned}$$

In Quantum Mechanics, each quantity is changed to the operator such as in one dimension

$$\hat{p} = \frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{dx}}$$
$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{dx}^2} + V(x)$$

From time independent-Schrödinger equation in one dimension

$$\hat{H}\Psi(x) = E\Psi(x)$$

or, equivalently,

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2} + V(x)\Psi(x) = E\Psi(x) \tag{3.1}$$

Our potential energy of interest in this project is the double-well potential represented by

$$V(x) = \frac{1}{2}m\omega^2x^2 + ae^{-bx^2}$$

where

$$\begin{aligned} a, b \quad &are \quad \text{positive real constants} \\ \omega \quad &is \quad \text{the angular frequency} \end{aligned}$$

so the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2}+\left(\frac{1}{2}m\omega^2x^2+ae^{-bx^2}\right)\Psi(x)=E\Psi(x)$$

At first, we used BWPT to calculate the 2^{nd}-order energy eigenvalues. The result was not convergent, (see the calculation of using BWPT for calculating energy eigenvalues at the Appendix B). Then we turned to employ shooting method to calculate the ground-state energy eigenvalues.

Multiplying the Schrödinger equation by $-\frac{2m}{\hbar^2}$ gives

$$\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2}-\frac{m^2\omega^2x^2}{\hbar^2}\Psi(x)-\frac{2mae^{-bx^2}}{\hbar^2}\Psi(x)+\frac{2mE}{\hbar^2}\Psi(x)=0$$

$$\frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2}+\left(\frac{2mE}{\hbar^2}-\frac{m^2\omega^2x^2}{\hbar^2}-\frac{2mae^{-bx^2}}{\hbar^2}\right)\Psi(x)=0 \tag{3.2}$$

Substituting $x=\alpha\xi$ into Eq.(3.2), we obtain

$$\frac{1}{\alpha^2}\frac{\mathrm{d}^2\Psi(\xi)}{\mathrm{d}\xi^2}+\left[\frac{2mE}{\hbar^2}-\frac{m^2\omega^2}{\hbar^2}(\alpha^2\xi^2)-\frac{2mae^{-b(\alpha^2\xi^2)}}{\hbar^2}\right]\Psi(\xi)=0$$

multiplying by α^2 , we get

$$\frac{\mathrm{d}^2\Psi(\xi)}{\mathrm{d}\xi^2}+\left[\frac{2mE}{\hbar^2}\alpha^2-\frac{m^2\omega^2}{\hbar^2}(\alpha^4\xi^2)-\frac{2ma\alpha^2e^{-b(\alpha^2\xi^2)}}{\hbar^2}\right]\Psi(\xi)=0 \tag{3.3}$$

from Eq.(3.3), we set

$$\frac{m^2\omega^2\alpha^4}{\hbar^2}=1$$

so

$$\alpha^4=\frac{\hbar^2}{m^2\omega^2}$$

So that Eq.(3.3) becomes

$$\frac{\mathrm{d}^2\Psi(\xi)}{\mathrm{d}\xi^2}+\left[\frac{2E}{\hbar\omega}-\xi^2-\frac{2a}{\hbar\omega}e^{-b(\frac{\hbar}{m\omega}\xi^2)}\right]\Psi(\xi)=0 \tag{3.4}$$

By setting

$$\varepsilon=\frac{2E}{\hbar\omega}$$

and

$$m,\hbar,\omega=1$$

we arrive at

$$\frac{\mathrm{d}^2\Psi(\xi)}{\mathrm{d}\xi^2}+[\varepsilon-\xi^2-2ae^{-b\xi^2}]\Psi(\xi)=0 \tag{3.5}$$

We can find the numerical solutions to Eq.(3.5) by deviding ξ into many small segments, each of $\Delta\xi$ in length.
The second derivative in Eq.(3.5) can be approximated in finite difference form as follows [3],

$$\frac{\mathrm{d}^2\Psi(\xi)}{\mathrm{d}\xi^2} \approx \frac{\Psi_{i+1} + \Psi_{i-1} - 2\Psi_i}{(\Delta\xi)^2} \tag{3.6}$$

substituting Eq.(3.6) into Eq.(3.5), we have

$$\Psi_{i+1} = 2\Psi_i - \Psi_{i-1} - (\Delta\xi)^2(\varepsilon - \xi^2 - 2ae^{-b\xi^2})\Psi_i, i = 2, 3, 4, ... \tag{3.7}$$

where

$$\Delta\xi = \xi_i - \xi_{i-1} \ \ or \ \ \Delta\xi = \xi_{i+1} - \xi_i$$

Chapter 4

Calculation

Let us introduce new variables for using in calculating the ground-state energy eigenvalues and wave function of the Gaussian double-well potential.

1. ξ_{min} is the initial position in the study range.
2. ξ_{max} is the final position in the study range.
3. ξ is any position in the study range.
4. N is a number of grids in the study range.
5. $\Delta\xi$ is the length of grid such that

$$\Delta\xi = \frac{\xi_{max} - \xi_{min}}{N}$$

4.1 Calculation steps

1. Input the initial position (ξ_{min}) and the final position (ξ_{max}).
2. Input the period amount.
3. Input the initial condition from Eq.(3.7)

$$\Psi_{i+1} = 2\Psi_i - \Psi_{i-1} - (\Delta\xi)^2(\varepsilon - \xi^2 - 2ae^{-b\xi^2})\Psi_i, i = 2, 3, 4, ...$$

Find the initial value for calculation. Input the initial condition by setting $\Psi_1 = 0$ for the position imprisons and set $\frac{\mathrm{d}\Psi}{\mathrm{d}\xi} = 1$ from the slope of position 1 and position 2.

$$\frac{\mathrm{d}\Psi}{\mathrm{d}\xi} \approx \frac{\Psi_2 - \Psi_1}{\Delta\xi}$$

Hence,

$$1 \approx \frac{\Psi_2 - 0}{\Delta\xi}$$

which is equivalent to

$$\Psi_2 \approx \Delta\xi$$

By inputting Ψ_1 and Ψ_2 as two initial values for calculation, we can find Ψ_3 from Eq.(3.7). In the same way, we can find Ψ_4 by substituting Ψ_2 and Ψ_3 in the equation. Keep doing this, we can findΨ_n .

4. Try 1 value of into Eq.(3.7) until $\Psi(\xi_{max})$ approaches zero at an acceptable order (such as). That value of ε is considered correct.

5. Plot wave function by the graph related to i .

6. Change wave function corresponding to any position ξ .

Chapter 5

Results (Tables)

5.1 Table displaying the ground-state energy eigenvalues of Gaussian double-well potential

b	ground-state energy via shooting method (E_0)	first excited-state energy via shooting method (E_1)	spacing between 2 lowest energy eigenvalues
500	1.48356037030	2.998600963	1.515040593
1000	1.45282024180	2.998062431	1.545242190
5000	1.45149691830	2.998039484	1.546542565

Table 5.1: **The energy eigenvalues of double-well potential from shooting method by setting $a = 6$, $n = 0$ and $N = 100$ at range 4 ($\xi_{max} = 4$). (All energies are in the $\frac{\hbar\omega}{2}$ unit.)**

b	ground-state energy via shooting method (E_0)	1^{st}-order P.T. energy eigenvalues	difference between energy eigenvalues
500	1.48356037030	1.26806	0.21550
1000	1.45282024180	1.18964	0.26318
5000	1.45149691830	1.08484	0.36665

Table 5.2: **The ground-state energy eigenvalues of double-well potential from shooting method and 1^{st}-order energy eigenvalues by setting $a = 6$, $n = 0$ and $N = 100$ at range 4 ($\xi_{max} = 4$).**
(All energies are in the $\frac{\hbar\omega}{2}$ unit.)

b	ground-state energy via shooting method (E_0)	first excited-state energy via shooting method (E_1)	spacing between 2 lowest energy eigenvalues
500	1.54682531737936	2.9970527075350	1.450227390
1000	1.54053846991773	2.9968727092930	1.456334240
5000	1.54049571048570	2.9968714873100	1.456375777

Table 5.3: **The energy eigenvalues of double-well potential from shooting method by setting $a = 6$, $n = 0$ and $N = 100$ at range 5 ($\xi_{max} = 5$).**
(All energies are in the $\frac{\hbar\omega}{2}$ unit.)

b	ground-state energy via shooting method (E_0)	1^{st}-order P.T. energy eigenvalues	difference between energy eigenvalues
500	1.54682531737936	1.26806	0.27876
1000	1.54053846991773	1.18964	0.35089
5000	1.54049571048570	1.08484	0.45565

Table 5.4: **The ground-state energy eigenvalues of double-well potential from shooting method and 1^{st}-order energy eigenvalues by setting $a = 6$, $n = 0$ and $N = 100$ at range 5 ($\xi_{max} = 5$).**
(All energies are in the $\frac{\hbar\omega}{2}$ unit.)

a	ground-state energy via shooting method (E_0)	first excited-state energy via shooting method (E_1)	spacing between 2 lowest energy eigenvalues
0.1	1.00933250270	-	-
0.2	1.01900002616	-	-
0.3	1.02860423416	-	-
0.4	1.03814551760	-	-
0.5	1.04762426650	-	-
0.6	1.05704086992	-	-
0.7	1.06639571600	-	-
0.8	1.07568919170	-	-
0.9	1.08492168320	-	-
1.0	1.09409357550	-	-
1.1	1.10320525266	2.9981426750	1.894937423
1.2	1.11225709740	2.9981520500	1.885894953
1.3	1.12124949160	2.9981614250	1.876911934
1.4	1.13018281580	2.9981707980	1.867987983
1.5	1.13905744950	2.9981801710	1.859122722
1.6	1.14787377100	2.9981895430	1.850315772
1.7	1.15663215730	2.9981989130	1.841566756
1.8	1.16533298420	2.9982082830	1.832875299
1.9	1.17397662640	2.9982176520	1.824241026
2.0	1.18256345710	2.9982270200	1.815663563
3.0	1.26538830760	2.9983206460	1.732932339
4.0	1.34293244700	2.9984141790	1.655481732
5.0	1.41554535720	2.9985076180	1.582964046
6.0	1.48356100010	2.9986009630	1.515039963

Table 5.5: **The energy eigenvalues of double-well potential from shooting method by setting $b = 500$, $n = 0$ and $N = 100$ at range 4 ($\xi_{max} = 4$). (All energies are in the $\frac{\hbar\omega}{2}$ unit.)**

a	ground-state energy via shooting method (E_0)	1^{st}-order P.T. energy eigenvalues	difference between energy eigenvalues
0.1	1.00933250270	1.00447	0.00486
0.2	1.01900002616	1.00894	0.01006
0.3	1.02860423416	1.01340	0.01520
0.4	1.03814551760	1.01787	0.02027
0.5	1.04762426650	1.02234	0.02528
0.6	1.05704086992	1.02681	0.03023
0.7	1.06639571600	1.03127	0.03512
0.8	1.07568919170	1.03574	0.03994
0.9	1.08492168320	1.04021	0.04471
1.0	1.09409357550	1.04468	0.04941
1.1	1.10320525266	1.04914	0.05406
1.2	1.11225709740	1.05361	0.05864
1.3	1.12124949160	1.05808	0.06316
1.4	1.13018281580	1.06255	0.06763
1.5	1.13905744950	1.06702	0.07203
1.6	1.14787377100	1.07148	0.07639
1.7	1.15663215730	1.07595	0.08068
1.8	1.16533298420	1.08042	0.08491
1.9	1.17397662640	1.08489	0.08908
2.0	1.18256345710	1.08935	0.09321
3.0	1.26538830760	1.13403	0.13135
4.0	1.34293244700	1.17871	0.16422
5.0	1.41554535720	1.22338	0.19216
6.0	1.48356100010	1.26806	0.21550

Table 5.6: **The ground-state energy eigenvalues of double-well potential from shooting method and 1^{st}-order energy eigenvalues by setting $b = 500$, $n = 0$ and $N = 100$ at range 4 ($\xi_{max} = 4$).**
(All energies are in the $\frac{\hbar\omega}{2}$ unit.)

a	ground-state energy via shooting method (E_0)	first excited-state energy via shooting method (E_1)	spacing between 2 lowest energy eigenvalues
0.1	1.01077303151888	-	-
0.2	1.02208216422660	-	-
0.3	1.03330267674510	-	-
0.4	1.04443523657135	-	-
0.5	1.05548050896693	-	-
0.6	1.06643915689838	-	-
0.7	1.07731184097890	-	-
0.8	1.08809921941133	-	-
0.9	1.09880194793249	-	-
1.0	1.10942067975870	-	-
1.1	1.11995606553275	-	-
1.2	1.13040875327210	2.9969077536450	1.866499000
1.3	1.14077938831840	2.9969107753368	1.856131387
1.4	1.15106861328848	2.9969137969506	1.845845183
1.5	1.16127706802637	2.9969168184870	1.835639750
1.6	1.17140538955700	2.9969198399454	1.825514450
1.7	1.18145421204093	2.9969228613270	1.815468649
1.8	1.19142416673056	2.9969258826316	1.805501716
1.9	1.20131588192760	2.9969289038580	1.795613022
2.0	1.21112998294193	2.9969319250076	1.785801943
3.0	1.30513756608160	2.9969621322430	1.691824566
4.0	1.39204798753092	2.9969923317410	1.604944344
5.0	1.47243214769530	2.9970225235040	1.524590376
6.0	1.54682531737936	2.9970527075350	1.450227390

Table 5.7: **The energy eigenvalues of double-well potential from shooting method by setting $b = 500$, $n = 0$ and $N = 100$ at range 5 ($\xi_{max} = 5$).**
(All energies are in the $\frac{\hbar\omega}{2}$ unit.)

a	ground-state energy via shooting method (E_0)	1^{st}-order P.T. energy eigenvalues	difference between energy eigenvalues
0.1	1.01077303151888	1.00447	0.00630
0.2	1.02208216422660	1.00894	0.01314
0.3	1.03330267674510	1.01340	0.01990
0.4	1.04443523657135	1.01787	0.02656
0.5	1.05548050896693	1.02234	0.03314
0.6	1.06643915689838	1.02681	0.03962
0.7	1.07731184097890	1.03127	0.04604
0.8	1.08809921941133	1.03574	0.05235
0.9	1.09880194793249	1.04021	0.05859
1.0	1.10942067975870	1.04468	0.06474
1.1	1.11995606553275	1.04914	0.07081
1.2	1.13040875327210	1.05361	0.07679
1.3	1.14077938831840	1.05808	0.08269
1.4	1.15106861328848	1.06255	0.08851
1.5	1.16127706802637	1.06702	0.09425
1.6	1.17140538955700	1.07148	0.09992
1.7	1.18145421204093	1.07595	0.10550
1.8	1.19142416673056	1.08042	0.11100
1.9	1.20131588192760	1.08489	0.11642
2.0	1.21112998294193	1.08935	0.12177
3.0	1.30513756608160	1.13403	0.17110
4.0	1.39204798753092	1.17871	0.21333
5.0	1.47243214769530	1.22338	0.24905
6.0	1.54682531737936	1.26806	0.27876

Table 5.8: **The ground-state energy eigenvalues of double-well potential from shooting method and 1^{st}-order energy eigenvalues by setting $b = 500$, $n = 0$ and $N = 100$ at range 5 ($\xi_{max} = 5$).**
(All energies are in the $\frac{\hbar\omega}{2}$ unit.)

Chapter 6

Results (Graphs)

6.1 Comparing the wave function of Gaussian double-well potential from shooting method by setting $a = 6$, $n = 0$, $N = 100$, varying b at range 4 ($\xi_{max} = 4$) and range 5 ($\xi_{max} = 5$).

(All energies are in the $\frac{\hbar\omega}{2}$ unit)

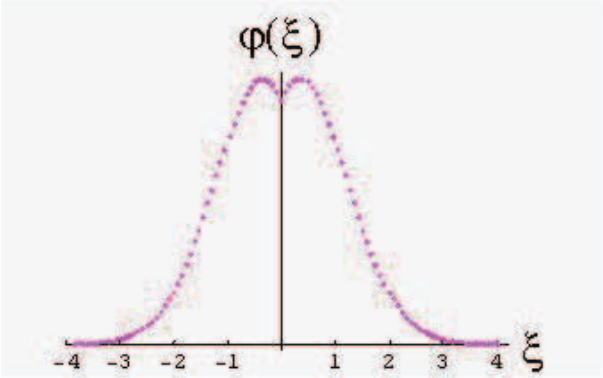

Figure 6.1: Ground-state energy via shooting method (E_0), $b = 500$ at range 4 ($\xi_{max} = 4.$)

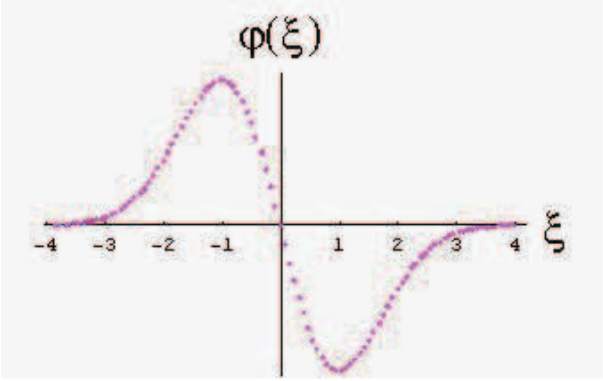

Figure 6.2: First excited-state energy via shooting method (E_1), $b = 500$ at range 4 ($\xi_{max} = 4.$)

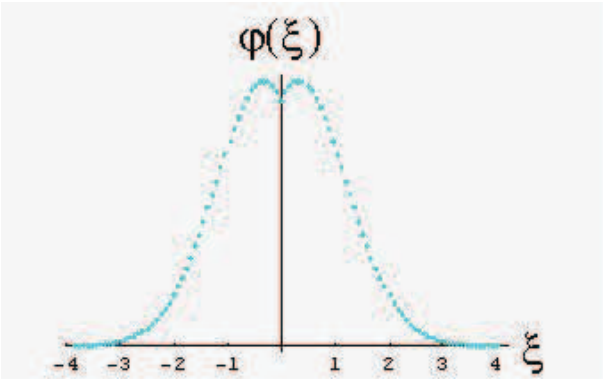

Figure 6.3: Ground-state energy via shooting method (E_0), $b = 1000$ at range 4 ($\xi_{max} = 4.$)

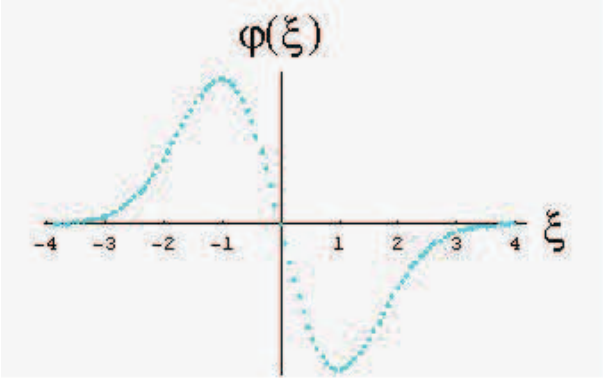

Figure 6.4: First excited-state energy via shooting method (E_1), $b = 1000$ at range 4 ($\xi_{max} = 4.$)

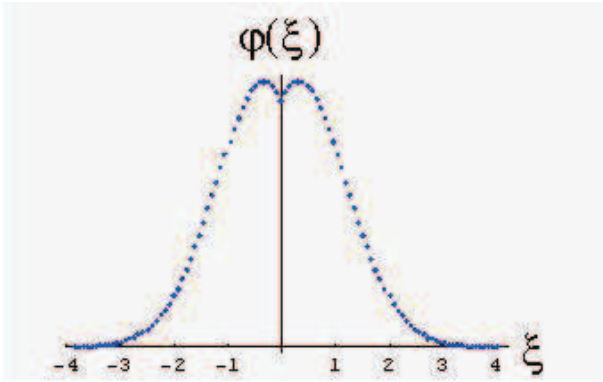

Figure 6.5: Ground-state energy via shooting method (E_0), $b = 5000$ at range 4 ($\xi_{max} = 4.$)

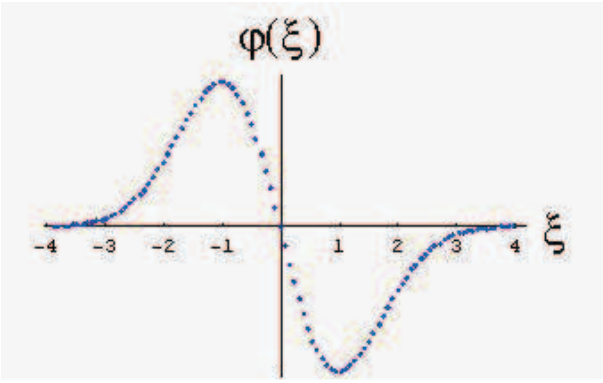

Figure 6.6: First excited-state energy via shooting method (E_1), $b = 5000$ at range 4 ($\xi_{max} = 4.$)

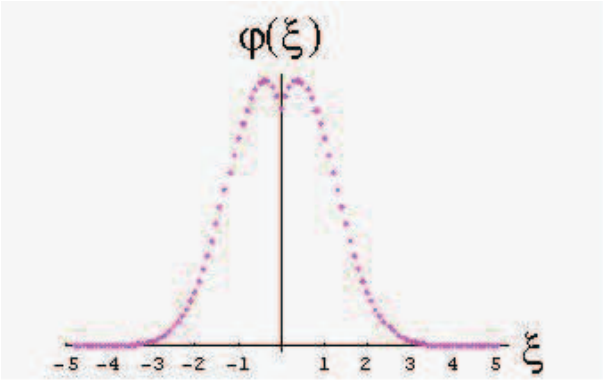

Figure 6.7: Ground-state energy via shooting method (E_0), $b = 500$ at range 5 ($\xi_{max} = 5.$)

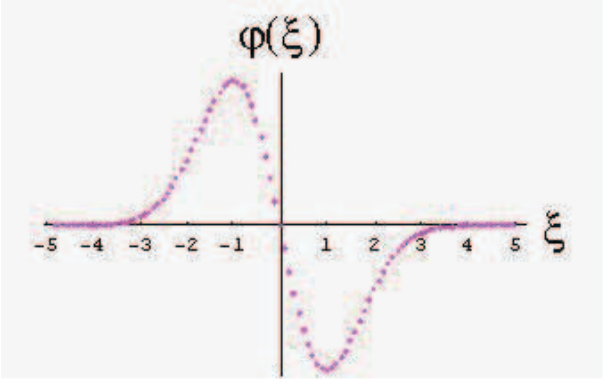

Figure 6.8: First excited-state energy via shooting method (E_1), $b = 500$ at range 5 ($\xi_{max} = 5.$)

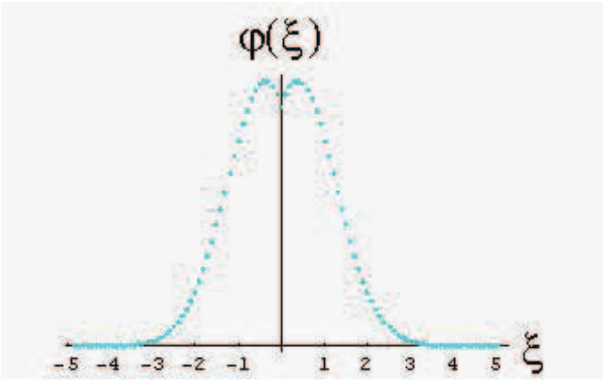

Figure 6.9: Ground-state energy via shooting method (E_0), $b = 1000$ at range 5 ($\xi_{max} = 5.$)

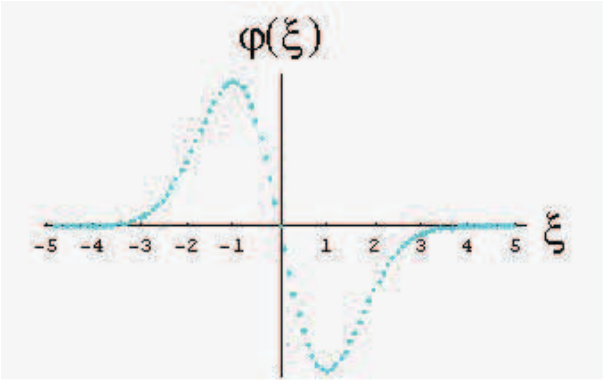

Figure 6.10: First excited-state energy via shooting method (E_1), $b = 1000$ at range 5 ($\xi_{max} = 5.$)

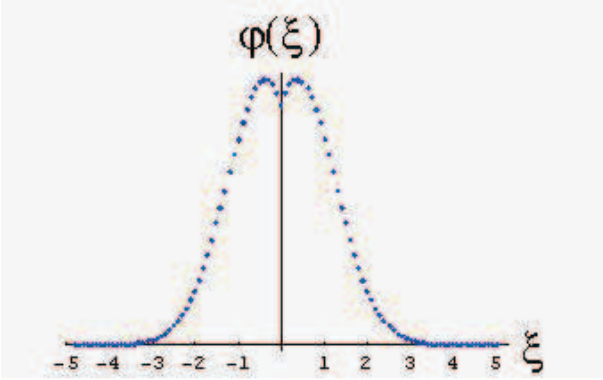

Figure 6.11: Ground-state energy via shooting method (E_0), $b = 5000$ at range 5 ($\xi_{max} = 5.$)

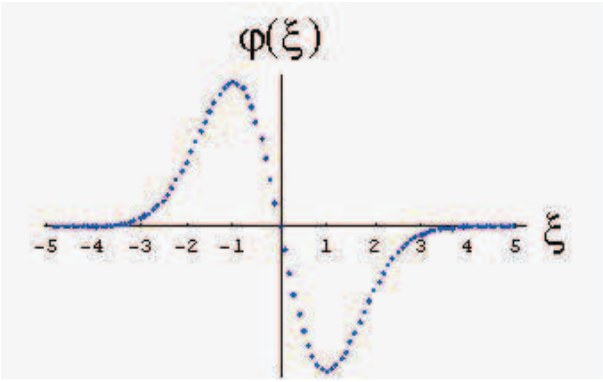

Figure 6.12: First excited-state energy via shooting method (E_1), $b = 5000$ at range 5 ($\xi_{max} = 5.$)

Chapter 7

Analysis and Conclusion

7.1 Analysis

7.1.1 In case of using BWPT to calculate the energy-eigenvalues

The result when we use 2^{nd}-order BWPT and Mathematica program to calculate the energy-eigenvalues was not accomplished, the P.T. series becomes divergent, (see the calculation of using BWPT for calculating energy eigenvalues at the Appendix B).

7.1.2 In case of using Shooting Method to calculate the energy-eigenvalues

The energy eigenvalues at range 4 ($\xi_{max} = 4$) and at range 5 ($\xi_{max} = 5$) are in harmony.

By setting $a = 6$, and varying $b = 500$, 1000, 5000, we obtain the followings :

1. The ground-state energy eigenvalues in case of small b is larger than those in case of large b 's.
2. The spacing between ground-state energy eigenvalues (E_0) and first excited-state (E_1) in case of small b is smaller than those in case of large b 's.
3. The difference between energy eigenvalues and 1^{st}-order P.T. energy eigenvalues in case of small b is smaller than those in case of large b 's.

By setting $b = 500$, and varying $a = 0.1$, 0.2, 0.3,, 6 we see that

1. The ground-state energy eigenvalues in case of small b is smaller than those in case of large b 's.
2. The spacing between ground-state energy eigenvalues (E_0) and first excited-state (E_1) in case of small b is larger than those in case of large b 's.
3. The difference between energy eigenvalues and 1^{st}-order P.T. energy eigenvalues in case of small b is smaller than those in case of large b 's.

7.2 Conclusions

1. We may not use 2^{nd}-order BWPT to calculate the ground-state energies since the BWPT series is divergent. (see the calculation of using BWPT for calculating energy eigenvalues at the Appendix B).

2. Similarly, we cannot use BWPT to calculate higher-order energy eigenvalues.

3. We can, however, calculate energy eigenvalues by using 1^{st}-order BWPT which is equivalent to the 1^{st}-order RSPT since it is of non-series form.

4. Unlike BWPT, the shooting method is applicable. We can, in principle, calculate higher excited-state energies via this method.

Appendix A

One dimensional double-well potential

A.1 Introduction

The importance of the double-well potentials in Quantum Mechanics, Condensed Matter Physics, Statistical Physics or Field Theory can hardly be overestimated. The Schrödinger equation has no exact, analytical solution with double-well potentials. It can be solved by using approximate methods or numerical methods. On the other hand, in Quantum Mechanics there exist potentials for which it is possible to find a number of eigenvalues and associated eigenfunctions exactly and in a closed form. These systems are said to be Quasi-Exactly Solvable (QES) and this property is ultimately connected with the existence of a hidden dynamical algebra.

A.2 Double-well potential

A double-well consists of two wells identical to Fig. A.1 (a), separated by a distance somewhat larger than the width of each well (Fig. A.1 (b)). Consider first the lowest,even energy state in the single-well. We see that to match slopes at the edges of the well the wave function on the inside must match the falling, exponential curves on both sides outside the well. This determines the rate at which the exponential falls, and which thus determines the binding energy. If we look at the double-well, the wave function must be symmetric about the midpoint between the two wells. However, this does not prevent the wave function inside the well on the right, for example, from dropping quite a bit more on the far right side, and still connecting to a fairly flat curve between the wells, as shown in Fig. A.1 (b). Thus a double-well can bind a particle much more strongly than a single-well, not because two wells are somewhat stronger than one well,but rather because one can maintain an almost constant wave function between the two potentials. This means that the bound particle has a high probability of being anywhere between the two wells.

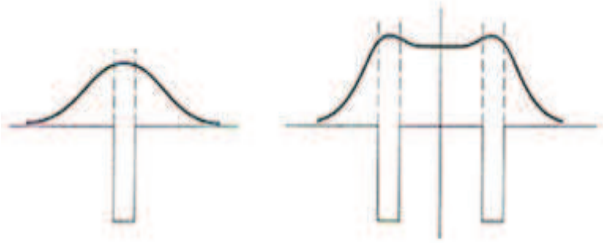

Figure A.1: (a) Wave function for the lowest bound state in a single square well potential.

(b) Wave function for the lowest bound state in a double well. Note that the wave functions at the inner edges of the wells do not have to fall off as rapidly to satisfy the continuity condition for $u(x)$ and $\frac{\mathrm{d}u(x)}{\mathrm{d}x}$, allowing for a large wave function between the wells and a steeper drop-off at the outer edges.

For the first-excited state (*odd* under reflection), the wave function must go through zero at the midpoint, so that it matches on to a flatter falling curve at the outer edges of the wells. This implies a smaller binding, as expected. When the wells are very far apart, then, roughly speaking, a particle bound on the right side does not know that there is a well on the left. If the wave functions for the two case are $u_R(x)$ and $u_L(x)$, then the symmetric wave function is

$$u_{even}(x) = \frac{1}{N_e}\left(u_R(x) + u_L(x)\right)$$

while the antisymmetric wave function, corresponding to the first excited state, is

$$u_{odd}(x) = \frac{1}{N_0}\left(u_R(x) - u_L(x)\right)$$

The normalization factors differ slightly because of the nonvanishing overlap of the $u_R(x)$ and $u_L(x)$. If the wells were so far apart that there was no overlap, then the normalization constants would each be $1\sqrt{2}$. Because of the small overlap, the eigenvalues are not quite the same. Thus the $u_R(x)$ and the $u_L(x)$ do not represent stationary states. For example, the wave function of aparticle localized on the right will be approximately given by

$$u(x) \approx C\left(u_{even}(x) + u_{odd}(x)\right)$$

If we start with a particle " on the right " at time t = 0, then at a later time the wave function will be

$$\begin{aligned} u(x,t) &= C\left(u_{even}(x)e^{-iE_e t/\hbar} + u_{odd}(x)e^{-iE_0 t/\hbar}\right) \\ &= Ce^{-iE_e t/\hbar}(u_{even}(x) + u_{odd}(x)e^{-i(E_0-E_e)t/\hbar}) \\ &\equiv Ce^{-iE_e t/\hbar}(u_{even}(x) + u_{odd}(x)e^{-i\Delta E t/\hbar}) \end{aligned}$$

Now after a time t such that $e^{-i\Delta Et/\hbar}$ = -1 that is, after a time

$$t = \frac{\hbar\pi}{\Delta E} = \frac{\hbar\pi}{E_0 - E_e}$$

That wave function becomes one that is approximately localized on the left side. The particle thus oscillates between the two wells with a period $2t$ that is, with an angular frequency

$$\omega = \frac{\Delta E}{\hbar}$$

Appendix B

The calculation of using BWPT for calculating energy eigenvalues

Appendix C

Example of Mathematica program

Example of writing ground-state energy eigenvalues calculation and wave function program by using shooting method and perturbation theory.

Example 1 The ground-state energy eigenvalues of double-well potential from shooting method by setting $a = 6$, $b = 500$, $n = 0$ and $N = 100$ at range 4 ($\xi_{max} = 4$).
(All energies are in the $\frac{\hbar\omega}{2}$ unit.)

Example 2 The ground-state energy eigenvalues of double-well potential from shooting method by setting $a = 6$, $b = 1000$, $n = 0$ and $N = 100$ at range 4 ($\xi_{max} = 4$).
(All energies are in the $\frac{\hbar\omega}{2}$ unit.)

Example 3 The ground-state energy eigenvalues of double-well potential from shooting method by setting $a = 6$, $b = 5000$, $n = 0$ and $N = 100$ at range 4 ($\xi_{max} = 4$).
(All energies are in the $\frac{\hbar\omega}{2}$ unit.)

Example 4 The ground-state energy eigenvalues of double-well potential from shooting method by setting $a = 6$, $b = 500$, $n = 0$ and $N = 100$ at range 5 ($\xi_{max} = 5$).
(All energies are in the $\frac{\hbar\omega}{2}$ unit.)

Example 5 The ground-state energy eigenvalues of double-well potential from shooting method by setting $a = 6$, $b = 1000$, $n = 0$ and $N = 100$ at range 5 ($\xi_{max} = 5$).
(All energies are in the $\frac{\hbar\omega}{2}$ unit.)

Example 6 The ground-state energy eigenvalues of double-well potential from shooting method by setting $a = 6$, $b = 5000$, $n = 0$ and $N = 100$ at range 5 ($\xi_{max} = 5$).
(All energies are in the $\frac{\hbar\omega}{2}$ unit.)

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