

Excited-state energy eigenvalue and wave-function evaluation of the Gaussian asymmetric double-well potential problem via numerical shooting method 2

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Abstract This project aims at computation excited-state energy eigenvalues and wave-function of a particle under Gaussian asymmetric double-well potential using numerical shooting method and perturbation theory a method to deal with discrete-eigenvalue problems. We also compare the energy eigenvalue and wave-function with those obtained from other typical means popular among physics students, namely the numerical shooting method and perturbation theory. Show that the idea of program of the numerical shooting method and perturbation theory of this problem (see Sects. 2.1 and 4) The numerical shooting method is generally regarded as one of the most efficient methods that give very accurate results because it integrates the Schrödinger equation directly, though in the numerical sense. The $n = \text{even}$ case is shown in Figs. 4, 5 and 6. In this case, the wave-function has split up on asymmetric nodes under Gaussian asymmetric double-well potential. The $n = \text{odd}$ case is shown in Fig. 7. In this case, the wave-function has not split up on asymmetric nodes under Gaussian asymmetric double-well potential.

Keywords Schrödinger equation · Bound state · Numerical shooting method · Perturbation theory · Gaussian double-well · Excited-state energy

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1 Introduction

In quantum mechanics, the stationary-state Schrödinger equation for complex systems is generally too difficult to solve exactly and one must again rely on approximation methods. There exist several means to study them, e.g. time-independent perturbation theory [1], the WKB approximation [2], the variation method [1–3] and the analytical transfer matrix method [4,5] ect. The Schrödinger equation have proposed various analytical and numerical methods for the solution of this central quantum mechanics equation, approaches even to one-dimensional solutions are still a subject of debate. This is confirmed by the continuing appearance of new publications in this field [6–8]. Boyd L.Earl used the harmonic oscillator Gaussian perturbation to evaluate frequency “doubling” in the vibrational spectrum of ammonia [9]. In this project we present two of the most important types of approximation methods which are useful under different conditions.

The scheme of the paper is as follows. In Sect. 2 detailing with the perturbation theory and calculation of energy eigenvalue for Gaussian asymmetric double-well potential. In Sect. 3 the Schrödinger equation and the potential in terms of the new variable and parameter is given by

$$\frac{d^2\psi(\xi)}{d\xi^2} + \left(\varepsilon - \xi^2 - 2ae^{-b\xi^2}\right) \psi(\xi) = 0, \quad V(\xi) = \xi^2 + 2ae^{-b\xi^2}.$$

The numerical shooting method and result is given in Sect. 4. The main principle of numerical shooting method is to subdivide the domain into many tiny segment each of which possesses a constant potential. We conclusion in Sect. 5 with a discussion.

2 Time-independent perturbation theory: the non-degenerate

The approximation method we consider here is time-independent perturbation theory [1–3] sometimes known as the Rayleigh–Schrödinger perturbation theory. Consider a system whose Hamiltonian can be dissociated into separate parts, one part corresponding to the unperturbed system and the other part representing the perturbation. We can write the total Hamiltonian then as

$$\hat{H} = \hat{H}_{(0)} + gV \quad (1)$$

where $\hat{H}_{(0)}$ represents the unperturbed part of the Hamiltonian whose eigenfunction and eigenvalues are assumed to be known and V is a small perturbative potential of the order of g in smallness. Suppose the problem to be solved is of the Schrödinger form

$$\hat{H}\psi_n = E_n\psi_n, \quad (2)$$

assuming that the unperturbed problem

$$\hat{H}_{(0)}\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)} \quad (3)$$

has already been solved. In the example mentioned above, that of a hydrogen atom in an external electric field, $\hat{H}_{(0)}$ is the Hamiltonian describing the unperturbed hydrogen atom with eigenfunctions $\psi_n^{(0)}$ and gV is the perturbation corresponding to the applied field.

From our supposition that the perturbation is small, it is reasonable to assume that the energy eigenvalues for the complete problem can be written as

$$E_n = E_n^{(0)} + gE_n^{(1)} + g^2E_n^{(2)} + \dots \tag{4}$$

where $E_n^{(0)}$ is the unperturbed energy eigenvalue and $gE_n^{(1)}$ is the first-order correction to the energy, $g^2E_n^{(2)}$ is the second-order correction to the energy, etc. The wave-function can also be expand in powers of the perturbation parameter g as

$$\psi_n = \psi_n^{(0)} + g\psi_n^{(1)} + g^2\psi_n^{(2)} + \dots \tag{5}$$

By substituting Eqs. (1), (4) and (5) into Eq. (2), we obtain

$$\begin{aligned} (\hat{H}_{(0)} + gV) (\psi_n^{(0)} + g\psi_n^{(1)} + g^2\psi_n^{(2)} + \dots) &= (E_n^{(0)} + gE_n^{(1)} + g^2E_n^{(2)} + \dots) \\ &\times (\psi_n^{(0)} + g\psi_n^{(1)} + g^2\psi_n^{(2)} + \dots). \end{aligned} \tag{6}$$

The factor g reflects the order of approximation in the expansion of the eigenvalue eigenvectors, and the potential. Zeroth order corresponds to $g = 0$, the unperturbed solution. First order corresponds to g , second order to g^2 , etc. In order for the equality to hold, terms of the same order must be equal. Therefore, equating terms of equal order, which are easily grouped since the power of g in each term determines its order, yields

$$\hat{H}_{(0)}\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)} \tag{7}$$

for zeroth order,

$$\hat{H}_{(0)}g\psi_n^{(1)} + gV\psi_n^{(0)} = E_n^{(0)}g\psi_n^{(1)} + gE_n^{(1)}\psi_n^{(0)} \tag{8}$$

for first order, and

$$g^2\hat{H}_{(0)}\psi_n^{(2)} + g^2V\psi_n^{(1)} = g^2E_n^{(0)}\psi_n^{(2)} + g^2E_n^{(1)}\psi_n^{(1)} + g^2E_n^{(2)}\psi_n^{(0)} \tag{9}$$

for second order.

The first-order term leads to an expression for the first-order correction to the energy eigenvalues. This can be determined as follows. Dividing out the factor of g from Eq. (8) yields

$$\hat{H}_{(0)}\psi_n^{(1)} + V\psi_n^{(0)} = E_n^{(0)}\psi_n^{(1)} + E_n^{(1)}\psi_n^{(0)}. \tag{10}$$

Multiplying through on each side by the complex conjugate of $\psi_n^{(0)}$ and integrating over all space, we find that Eq. (10) becomes

$$\int \psi_n^{(0)*} \hat{H}_{(0)} \psi_n^{(1)} d^3r + \int \psi_n^{(0)*} V \psi_n^{(0)} d^3r = \int \psi_n^{(0)*} E_n^{(0)} \psi_n^{(1)} d^3r + \int \psi_n^{(0)*} E_n^1 \psi_n^{(0)} d^3r. \quad (11)$$

Making use of the hermiticity of $\hat{H}_{(0)}$ we can write the first term on the left-hand side of Eq. (11) as

$$\int \psi_n^{(0)*} \hat{H}_{(0)} \psi_n^{(1)} d^3r = \int \left(\hat{H}_{(0)} \psi_n^{(0)} \right)^* \psi_n^{(1)} d^3r = \int \psi_n^{(0)*} E_n^{(0)} \psi_n^{(1)} d^3r. \quad (12)$$

Therefore the expression for $E_n^{(1)}$, the first-order correction to the energy, is

$$E_n^{(1)} = \frac{\int \psi_n^{(0)*} V(r) \psi_n^{(0)} d^3r}{\int \psi_n^{(0)*} \psi_n^{(0)} d^3r}. \quad (13)$$

To find the second-order correction to the energy, we start with the second-order equation, Eq. (9):

$$\hat{H}_{(0)} \psi_n^{(2)} + V \psi_n^{(1)} = E_n^{(0)} \psi_n^{(2)} + E_n^{(1)} \psi_n^{(1)} + E_n^{(2)} \psi_n^{(0)}. \quad (14)$$

Multiply Eq. (14) on each side by $\psi_n^{(0)*}$ and integrate over all space to yield

$$\int \psi_n^{(0)*} V \psi_n^{(1)} d^3r = E_n^{(1)} \int \psi_n^{(0)*} \psi_n^{(1)} d^3r + E_n^{(2)} \int \psi_n^{(0)*} \psi_n^{(0)} d^3r. \quad (15)$$

By substituting

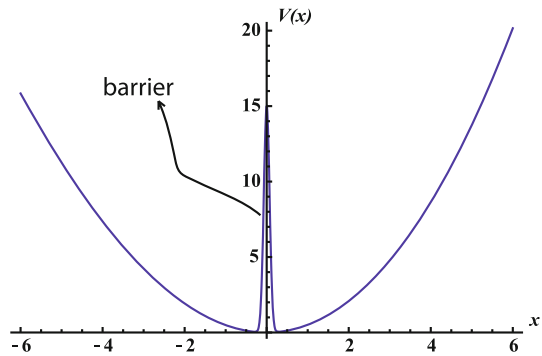
$$\begin{aligned} \psi_n^{(1)} &= \sum_m A_m \psi_m^{(0)}, \\ \psi_{n'}^{(1)} &= - \sum_{m \neq n'} \frac{V_{mn'}}{[E_m^{(0)} - E_{n'}^{(0)}]} \psi_m^{(0)} \end{aligned}$$

back into the right-hand side and left-hand side, respectively of Eq. (15), we get

$$E_n^{(2)} = \sum_{m \neq n} \frac{|V_{mn}|^2}{E_n^{(0)} - E_m^{(0)}}, \quad (16)$$

where $V_{mn} = \langle m | V | n \rangle = \int \psi_m^{(0)*} V \psi_n^{(0)} d^3r$.

Fig. 1 Potential for a particle under Gaussian asymmetric double-well. By setting $a = 15$, $b = 100$, $\lambda = 0.01$



2.1 The perturbation theory: Gaussian asymmetric double-well potential

Our potential energy of interest in this project is the Gaussian harmonic oscillator asymmetric double-well potential [9, 15] represent by

$$V(x) = \frac{1}{2}m\omega^2x^2 + \lambda x^3 + ae^{-bx^2} \tag{17}$$

where λ , a and b are positive real constant and λ are relatively small (see Fig. 1). In this case, the famous harmonic oscillator solutions for $\psi_n^{(0)}$ and $E_n^{(0)}$ are

$$\begin{aligned} \psi_n^{(0)}(\xi) &= A_n H_n(\xi) e^{-\xi^2/2}, \\ E_n^{(0)} &= \left(n + \frac{1}{2}\right) \hbar\omega, \quad n = 0, 1, 2, 3, \dots \end{aligned} \tag{18}$$

where $A_n = (2^n n!) \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}$ is the normalized factor. The polynomials $H_n(\xi)$ are, except for the normalization constants, the Hermite polynomial $H_n(\xi)$, whose properties can be found in any number of textbooks on mathematical physics. By substituting Eq. (18) back into Eqs. (13) and (16), we can now finally write the total energy eigenvalue for Gaussian asymmetric double-well potential. They are

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega + \int_{-\infty}^{\infty} \left(\psi_n^{(0)}(\xi)\right)^2 \left(\lambda x^3 + ae^{-bx^2}\right) dx. \tag{19}$$

Since $\left(\psi_n^{(0)}(\xi)\right)^2$ is an even function of x and x^3 is odd function, the contribution of the cubic term to the integral is zero. Thus the first order perturbation energy ($E_n^{(1)} = \langle n | \lambda x^3 | k \rangle = 0$) for the term λx^3 is zero. By substituting λx^3 into Eq. (16), we have the second-order perturbation energy [10]

$$E_n^{(2)} = \frac{|\langle n | \lambda x^3 | n+3 \rangle|^2}{E_n^{(0)} - E_{n+3}^{(0)}} + \frac{|\langle n | \lambda x^3 | n+1 \rangle|^2}{E_n^{(0)} - E_{n+1}^{(0)}} + \frac{|\langle n | \lambda x^3 | n-1 \rangle|^2}{E_n^{(0)} - E_{n-1}^{(0)}} + \frac{|\langle n | \lambda x^3 | n-3 \rangle|^2}{E_n^{(0)} - E_{n-3}^{(0)}}. \quad (20)$$

The required matrix elements are

$$\begin{aligned} \langle n | \lambda x^3 | n+3 \rangle &= \lambda \langle n | x^2 | n+2 \rangle \langle n+2 | x | n+3 \rangle, \\ \langle n | \lambda x^3 | n+1 \rangle &= \lambda \{ \langle n | x^2 | n+2 \rangle \langle n+2 | x | n+1 \rangle + \langle n | x^2 | n \rangle \langle n | x | n+1 \rangle \}, \\ \langle n | \lambda x^3 | n-1 \rangle &= \lambda \{ \langle n | x^2 | n-2 \rangle \langle n-2 | x | n-1 \rangle + \langle n | x^2 | n \rangle \langle n | x | n-1 \rangle \}, \\ \langle n | \lambda x^3 | n-3 \rangle &= \lambda \langle n | x^2 | n-2 \rangle \langle n-2 | x | n-3 \rangle. \end{aligned} \quad (21)$$

Thus, we use the lowering and raising operators \hat{a} and \hat{a}^\dagger into Eq. (21) thus into Eq. (20), we can now finally write the second-order correction to the eigenenergies

$$E_n^{(2)} = -\frac{15\lambda^2}{4\hbar\omega\alpha^3} \left(n^2 + n + \frac{11}{30} \right). \quad (22)$$

Then

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega + \int_{-\infty}^{\infty} \left(\psi_n^{(0)}(\xi) \right)^2 \left(a e^{-b x^2} \right) dx - \frac{15\lambda^2}{4\hbar\omega\alpha^3} \left(n^2 + n + \frac{11}{30} \right). \quad (23)$$

Logic of calculate energy eigenvalues by the perturbation theory of Gaussian asymmetric double-well potential

- Input values a, b, n, λ in mathematica programm.
- Input the wave-function to the harmonic oscillator in mathematica programm.
- Calculate energy eigenvalue.

For example, numerical evaluation of energy of Gaussian asymmetric double-well potential. Consider the following program:

- In[1]:= Clear[a, b, n, λ]
- In[2]:= a = 8; b = 100; n = 2; λ = 0.01;
- In[3]:= $\psi[n_, x_] := \frac{\text{HermiteH}[n, x] \text{Exp}[-\frac{x^2}{2}]}{\sqrt{2^n n! \sqrt{\pi}}}$;
- In[4]:= SetPrecision[N[($\int_{-\infty}^{\infty} (\lambda x^3 + a \text{Exp}[-b x^2]) \text{Abs}[\psi[n, x]]^2 dx$) + (2 n + 1) - ($\lambda^2 (\frac{15}{4}) (n^2 + n + \frac{11}{30})$)], 15]
- Out[4]:= 5.38786294511245

3 Gaussian asymmetric double-well potential

By substituting Eq. (17) into Schrödinger equation and multiplying by $-\frac{2m}{\hbar^2}$, we get

$$\frac{d^2\psi(x)}{dx^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2x^2}{\hbar^2} - \frac{2m\lambda}{\hbar^2}x^3 - \frac{2ma}{\hbar^2}e^{-bx^2} \right) \psi(x) = 0. \tag{24}$$

Substituting $x = \alpha\xi$ and multiplying by α^2 into Eq. (24), we obtain

$$\frac{d^2\psi(\xi)}{d\xi^2} + \left(\frac{2mE}{\hbar^2}\alpha^2 - \frac{m^2\omega^2\xi^2}{\hbar^2}\alpha^4 - \frac{2m\lambda}{\hbar^2}\xi^3\alpha^5 - \frac{2ma}{\hbar^2}\alpha^2e^{-b\alpha^2\xi^2} \right) \psi(\xi) = 0. \tag{25}$$

From Eq. (25), we set $\varepsilon = \frac{2E}{\hbar\omega}$, $m, \hbar, \omega = 1$, $\alpha^4 = \frac{\hbar^2}{m^2\omega^2}$, so that Eq. (25) become

$$\frac{d^2\psi(\xi)}{d\xi^2} + \left(\varepsilon - \xi^2 - 2\lambda\xi^3 - 2ae^{-b\xi^2} \right) \psi(\xi) = 0. \tag{26}$$

Also, the potential in terms of the new variable and parameter is given by

$$V(\xi) = \xi^2 + 2\lambda\xi^3 + 2ae^{-b\xi^2}. \tag{27}$$

We can find the numerical solution to Eq. (26) by dividing ξ into many small segments, each of $\Delta\xi$ in length. The second derivative in Eq. (26) can be approximated in finite difference [11–14] form as follows,

$$\frac{d^2\psi(\xi)}{d\xi^2} \approx \frac{\psi_{i+1} + \psi_{i-1} - 2\psi_i}{(\Delta\xi)^2}. \tag{28}$$

By substituting Eq. (28) back into Eq. (26), we obtain in case of case Gaussian asymmetric double-well potential

$$\psi_{i+1} = 2\psi_i - \psi_{i-1} - (\Delta\xi)^2 \left(\varepsilon - \xi^2 - 2\lambda\xi^3 - 2ae^{-b\xi^2} \right) \psi_i; \quad i = 2, 3, 4, \dots, \tag{29}$$

where $\xi_{i+1} = \Delta\xi + \xi_i$ or $\xi_i = \Delta\xi + \xi_{i-1}$. The special potential given by Gaussian symmetric and asymmetric double-wells potential has been used in evaluate Eq. (29) in mathematica program (see Sect. 4).

4 Numerical shooting method and result

We define the new variables for using in evaluating the excited-state energy eigenvalues and wave-function of the Gaussian symmetric and asymmetric double-wells potential.

Table 1 Comparison of **energy spectrum** of the potential $V(x) = \frac{1}{2}m\omega^2x^2 + \lambda x^3 + ae^{-bx^2}$ (the Gaussian asymmetric double-well potential) obtained from numerical shooting method (NSM), perturbation theory (PT)

b	State	Energy via NSM	Energy via PT	%Difference
100	$n = 0$	2.030752497940	1.795892252168	12.274996
	$n = 1$	3.011425504799	3.006993982695	0.147265
	$n = 2$	5.703883913835	5.387862945125	5.698308
	$n = 3$	7.008022840507	7.006952552143	0.015274
	$n = 4$	9.513471357524	9.279455352879	2.490469
250	$n = 0$	1.759494695253	1.504818022478	15.603693
	$n = 1$	2.998868630499	3.001124274989	0.075188
	$n = 2$	5.470492753899	5.248090508809	4.149844
	$n = 3$	6.986339025945	6.998356197197	0.171862
	$n = 4$	9.325937503576	9.178744998467	1.590868
500	$n = 0$	1.678894931262	1.357276141287	21.185815
	$n = 1$	2.996074668133	2.999825900482	0.125127
	$n = 2$	5.408920830023	5.275608056092	2.495436
	$n = 3$	6.981444921847	6.997360942442	0.227716
	$n = 4$	9.278393393755	9.241676504791	0.396509

Setting $a = 8$, $N = 100$ and $\lambda = 0.01$ at rang $5(\xi_{max} = 5)$, $\xi_{min} = -5$. All energies are in the $\hbar\omega/2$ unit

1. ξ_{min} is the begin position in the study range.
2. ξ_{max} is the ultimate position in the study range.
3. ξ is any position in the study range.
4. nn is a number of tiny bars in the study range.
5. $\Delta\xi$ is the length of tiny bars so that

$$\Delta\xi = \frac{\xi_{max} - \xi_{min}}{nn}. \quad (30)$$

4.1 Logic of the numerical shooting method calculation of energy for the Gaussian asymmetric double-well potential

- Input values ξ_{min} , ξ_{max} , a , b , λ in mathematica program.
- Input the period amount.
- Input Eq. (29) into mathematica program.
- The next task is to calculate wave-function in Eq. (29) (ψ_{i+1}) so that it approaches zero as closely as desired. Normally, we assign a small value as the standard to make sure wave-function in Eq. (29) get close enough to zero. For example, if $|\psi_{i+1}| \leq 10^{-6}$, we stop the calculation and accept the final energy as the numerical solution (see also the flowchart Fig. 3 and see Tables 1, 2, 3 and 4).
- Plot wave-function by the graph related to i .

Table 2 Comparison of energy spectrum of the potential $V(x) = \frac{1}{2}m\omega^2x^2 + \lambda x^3 + ae^{-bx^2}$ (the Gaussian asymmetric double-well potential) obtained from numerical shooting method (NSM), perturbation theory (PT)

b	State	Energy via NSM	Energy via PT	%Difference
100	$n = 0$	2.415588567393	2.492418285315	3.130791
	$n = 1$	3.024729152256	3.013890280053	0.358985
	$n = 2$	6.127407500865	5.720332084586	6.871782
	$n = 3$	7.036757569574	7.017093847767	0.279834
	$n = 4$	9.903111104965	9.530661599149	3.833013
250	$n = 0$	2.117094923749	1.946654104647	8.388354
	$n = 1$	3.002145910869	3.002884578106	0.024602
	$n = 2$	5.798074677121	5.467258766517	5.873167
	$n = 3$	6.996338500455	7.000975682244	0.066258
	$n = 4$	9.601989218593	9.341829684625	2.746643
500	$n = 0$	2.016313919871	1.670013077413	18.788395
	$n = 1$	2.996930367460	3.000450125903	0.117377
	$n = 2$	5.700336425099	5.331354167672	6.689496
	$n = 3$	6.986995293759	6.997360942442	0.148246
	$n = 4$	9.518838220835	9.241676504791	2.954735

Setting $a = 15$, $N = 100$ and $\lambda = 0.01$ at rang $5(\xi_{max} = 5)$, $\xi_{min} = -5$. All energies are in the $\hbar\omega/2$ unit

For example, numerical evaluation of energy eigenvalue of the numerical shooting method for the Gaussian asymmetric double-well potential [16, 17].

- $\text{In}[1] := \xi_{min} = -5; \xi_{max} = 5; nn = 100; \xi_{max} = 5 \Delta\xi = N \left(\frac{\xi_{max} - \xi_{min}}{nn} \right) \psi_1 = 0; N[\psi_2 = \Delta\xi]; \xi_1 = -5; \xi_2 = \xi_1 + \Delta\xi; \lambda = 0.01; a = 15; b = 100;$
- $\text{In}[2] := \varepsilon = 6.12740750086522874260515404980405318459$
- $\text{Out}[2] = 6.12740750086522874260515404980405318459$
- $\text{In}[3] := N[\text{Table}[\psi_{i+1} = 2\psi_i - \psi_{i-1} - (\Delta\xi)^2(\varepsilon - (\xi_{i+1} = \xi_i + \Delta\xi)^2 - (2\lambda(\xi_{i+1} = \xi_i + \Delta\xi)^3) - 2ae^{-b(\xi_{i+1} = \xi_i + \Delta\xi)^2})\psi_i, \{i, 2, 99\}]]$
- $\text{Out}[3] = \{0.214701, 0.359215, 0.550736, 0.809998, 1.16264, 1.64053, 2.28298, 3.13785, 4.26233, 5.72338, 7.59738, 9.96897, 12.9287, 16.5691, 20.9794, 26.2381, 32.4039, 39.5051, 47.5278, 56.4035, 65.9976, 76.0992, 86.4146, 96.5659, 106.095, 114.478, 121.144, 125.504, 126.994, 125.112, 119.472, 109.847, 96.2133, 78.7839, 58.0281, 34.6718, 9.6783, -15.7937, -40.4527, -62.9548, -81.9958, -96.4088, -105.257, -107.917, -104.135, -94.0697, -78.7945, -67.3952, -72.0849, -80.3204, -84.108, -82.8212, -76.5932, -65.8654, -51.3417, -33.9272, -14.6545, 5.39537, 25.1697, 43.7129, 60.2223, 74.0859, 84.9026, 92.4847, 96.8431, 98.1616, 96.7602, 93.0557, 87.5204, 80.6441, 72.9014, 64.7256, 56.4909, 48.502, 40.9904, 34.1168, 27.9772, 22.6127, 18.0198, 14.1619, 10.9792, 8.3983, 6.33968, 4.72357, 3.47429,$

Table 3 Comparison of energy spectrum of the potential $V(x) = \frac{1}{2}m\omega^2x^2 + \lambda x^3 + ae^{-bx^2}$ (the Gaussian asymmetric double-well potential) obtained from numerical shooting method (NSM), perturbation theory (PT)

λ	State	Energy via NSM	Energy via PT	%Difference
0.02	$n = 0$	2.012662086855	1.669600577413	18.633191
	$n = 1$	2.995727978026	2.997787625903	0.068729
	$n = 2$	5.663388038380	5.324191667672	6.174178
	$n = 3$	6.992050375342	6.983448442442	0.123100
	$n = 4$	9.403167030215	9.218764004791	1.980493
0.03	$n = 0$	2.006522642657	1.668913077413	18.371132
	$n = 1$	2.993649715885	2.993350125903	0.010008
	$n = 2$	5.602334684017	5.312254167672	5.315464
	$n = 3$	6.997520158626	6.960260942442	0.533885
	$n = 4$	9.222265911102	9.180576504791	0.453076
0.04	$n = 0$	1.997810541999	1.667950577413	17.996806
	$n = 1$	2.990573277036	2.987137625903	0.114949
	$n = 2$	5.517408945459	5.295541667672	4.103732
	$n = 3$	6.998661517352	6.927798442442	1.017675
	$n = 4$	8.984492237866	9.127114004791	1.574921
0.05	$n = 0$	1.986394409736	1.666713077413	17.501885
	$n = 1$	2.986301459524	2.979150125903	0.239758
	$n = 2$	5.407960247924	5.274054167672	2.507132
	$n = 3$	6.987326605618	6.886060942442	1.459855
	$n = 4$	8.693816953897	9.058376504791	4.107206

Setting $a = 15$, $N = 100$ and $b = 500$ at rang $5(\xi_{max} = 5)$, $\xi_{min} = -5$. All energies are in the $\hbar\omega/2$ unit

2.52294, 1.80901, 1.28084, 0.895514, 0.6182, 0.421216, 0.283004, 0.187062, 0.120947, 0.0753685, 0.0433854, 0.0196996, $1.27722 * 10^{-7}$ }

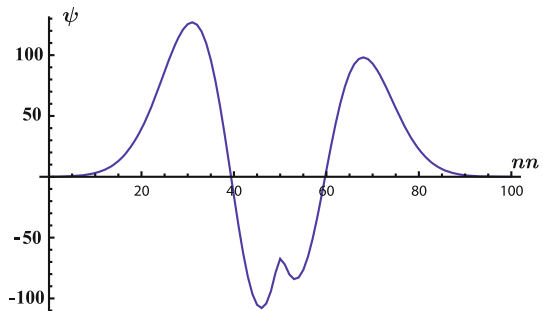
- In[4]:= SetPrecision[1/2 (6.12740750086668393412807543827944267713 + 6.12740750086377355108223266132866369206), 15]
- Out[4]= 6.12740750086523
- In[5]:= {0, 0.1, 0.21470075249913478[∘], 0.3592151359669389[∘], 0.5507359541249702[∘], 0.8099978040663655[∘], 1.162643592083485[∘], 1.6405346087920323[∘], 2.2829849041988446[∘], 3.1378480532215245[∘], 4.262333698699565[∘], 5.723382270449154[∘], 7.597381601120093[∘], 9.96897390883968[∘], 12.928683090757184[∘], 16.569099396323054[∘], 20.979400976333142[∘], 26.238078587028188[∘], 32.4038675777825[∘], 39.505082506428295[∘], 47.52779002639605[∘], 56.40353226232009[∘], 65.9976030929712[∘], 76.09915094245416[∘], 86.41459257731142[∘], 96.56592641902226[∘], 106.09548433042632[∘], 114.47841794639844[∘], 121.14375458399813[∘], 125.504176831302[∘], 126.99380712386751[∘],

Table 4 Comparison of **energy spectrum** of the potential $V(x) = \frac{1}{2}m\omega^2x^2 + \lambda x^3 + ae^{-bx^2}$ (the Gaussian asymmetric double-well potential) obtained from numerical shooting method (NSM), perturbation theory (PT)

λ	State	Energy via NSM	Energy via PT	%Difference
0.06	$n = 0$	1.972080221774	1.665200577413	16.874124
	$n = 1$	2.980523143789	2.969387625903	0.374309
	$n = 2$	5.271534494613	5.247791667672	0.451413
	$n = 3$	6.947570219636	6.835048442442	1.632807
	$n = 4$	8.353151379526	8.974364004791	7.170245
0.07	$n = 0$	1.954581824163	1.663413077413	16.095586
	$n = 1$	2.972731590932	2.957850125903	0.501855
	$n = 2$	5.102194552193	5.216754167672	2.220374
	$n = 3$	6.842390605435	6.774760942442	0.9933012
	$n = 4$	7.978600680828	8.875076504791	10.638341
0.08	$n = 0$	1.933463447654	1.661350577413	15.139190
	$n = 1$	2.962030096806	2.944537625903	0.592306
	$n = 2$	4.886537969718	5.180941667672	5.848608
	$n = 3$	6.589930755645	6.705198442442	1.733984
	$n = 4$	7.630777323246	8.760514004791	13.784596
0.09	$n = 0$	1.908011031137	1.659013077413	13.961103
	$n = 1$	2.946560055744	2.929450125903	0.582366
	$n = 2$	4.593166601029	5.140354167672	11.243364
	$n = 3$	6.119489237294	6.626360942442	7.953517
	$n = 4$	7.380085182189	8.630676504791	15.621884

Setting $a = 15$, $N = 100$ and $b = 500$ at rang $5(\xi_{max} = 5)$, $\xi_{min} = -5$. All energies are in the $\hbar\omega/2$ unit

Fig. 2 The wave-function of Gaussian asymmetric double-well potential in case of second excited-state energy via numerical shooting method (ϵ_2), $a = 15$, $b = 100$, $\lambda = 0.01$ at range $5(\xi_{max} = 5)$



125.11227568564995°, 119.47231205642201°, 109.84714934139572°,
 96.21330439653738°, 78.78393358970975°, 58.02807860223384°,
 34.67178376451662°, 9.678298565468655°, -15.793684376271925°,
 -40.452702023765305°, -62.95478665558926°, -81.99583903216717°,
 -96.4088269141907°, -105.25736001994633°, -107.91685771911497°,
 -104.13513906360902°, -94.06965077062246°, -78.79449271531726°

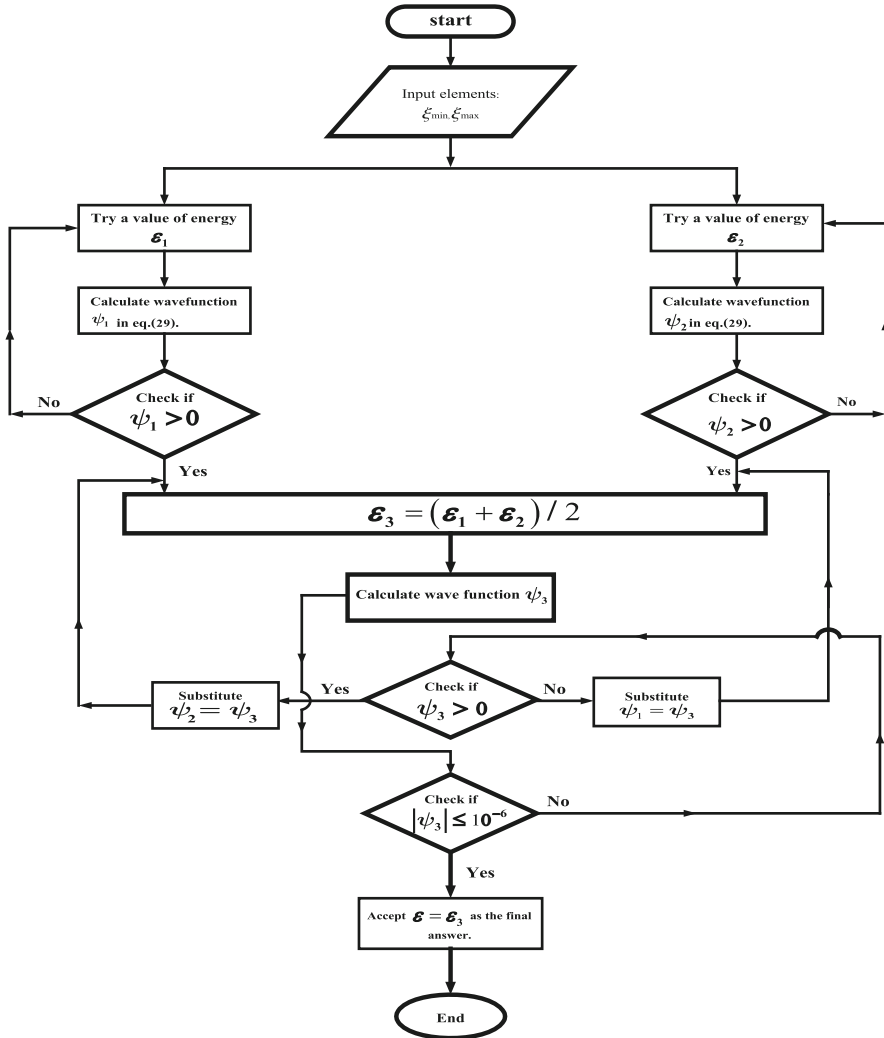


Fig. 3 The flowchart schematic energy eigenvalue and wave-function evaluation procedures

-67.39520087772728° , -72.08489070965042° , -80.32043324064043° ,
 -84.10800822169212° , -82.82120811462845° , -76.59319192977884° ,
 -65.86539656741367° , -51.34172076807657° , -33.92722499313133° ,
 -14.65447827691688° , 5.395370143474243° , 25.16965502445812° ,
 43.7129455634949° , 60.22233940732602° , 74.08588434103551° ,
 84.9026269069607° , 92.48465792192599° , 96.84314774480457° ,
 98.16158831549289° , 96.76019949880242° , 93.0556978037494° ,
 87.52041133012293° , 80.64414805339048° , 72.90140574330432° ,
 64.7255798740233° , 56.490900652542294° , 48.50200910249418° ,
 40.99043188635519° , 34.11676929085374° , 27.97717419106913° ,

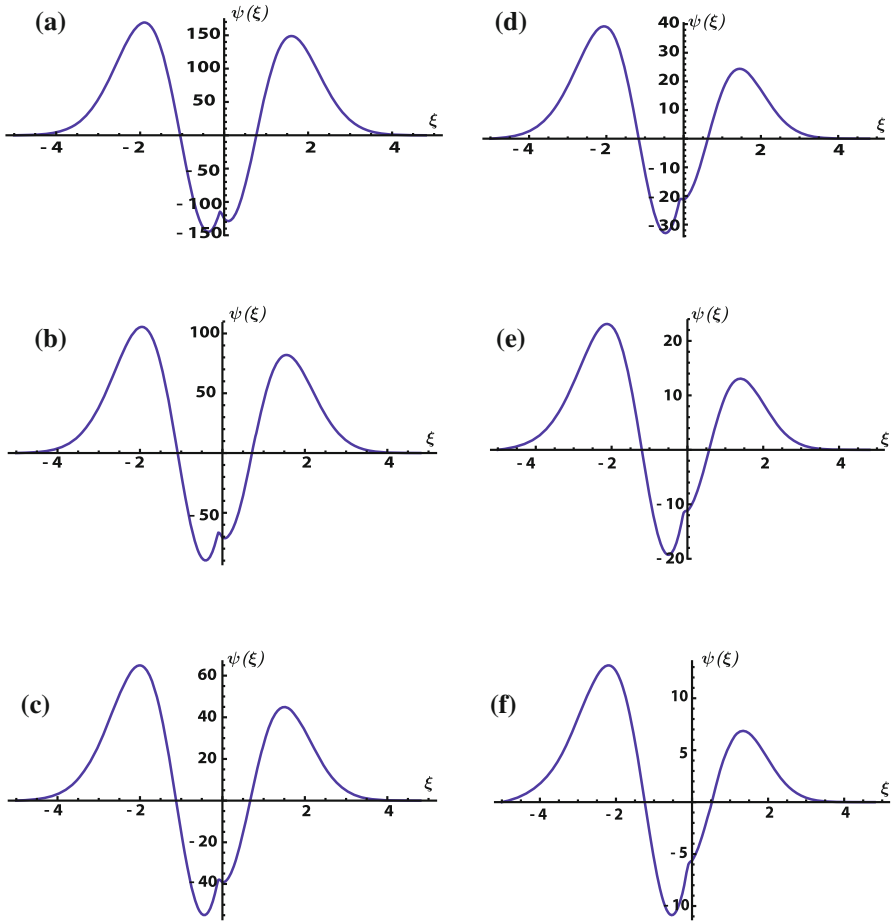


Fig. 4 Plot of several functions involving wave-functions of the Gaussian asymmetric double-well potential via numerical shooting method. **a** wave-function $a = 15, b = 500, \lambda = 0.01, e = 5.7003364$. **b** wave-function $a = 15, b = 500, \lambda = 0.02, e = 5.6633880$. **c** wave-function $a = 15, b = 500, \lambda = 0.03, e = 5.6023346$. **d** wave-function $a = 15, b = 500, \lambda = 0.04, e = 5.5174089$. **e** wave-function $a = 15, b = 500, \lambda = 0.05, e = 5.4079602$ **f** wave-function $a = 15, b = 500, \lambda = 0.06, e = 5.2715344$

22.61265103110893[∘], 18.019805504091874[∘], 14.16188197707348[∘],
 10.979190255705477[∘], 8.398304457965299[∘], 6.339681709946219[∘],
 4.723574609432114[∘], 3.4742867327686353[∘], 2.5229416131309383[∘],
 1.809006119223058[∘], 1.2808369662058587[∘], 0.8955143406078796[∘],
 0.6181998115621612[∘], 0.42121634517981693[∘], 0.2830040686830447[∘],
 0.1870620510684105[∘], 0.1209472505274131[∘], 0.0753684616125766[∘],
 0.04338542905582301[∘], 0.019699613593310288[∘], 1.2772152127235592[∘] * - 7}

- Out[5]={0, 0.1, 0.214701, 0.359215, 0.550736, 0.809998, 1.16264, 1.64053, 2.28298, 3.13785, 4.26233, 5.72338, 7.59738, 9.96897, 12.9287, 16.5691, 20.9794, 26.2381, 32.4039, 39.5051, 47.5278, 56.4035, 65.9976, 76.0992,

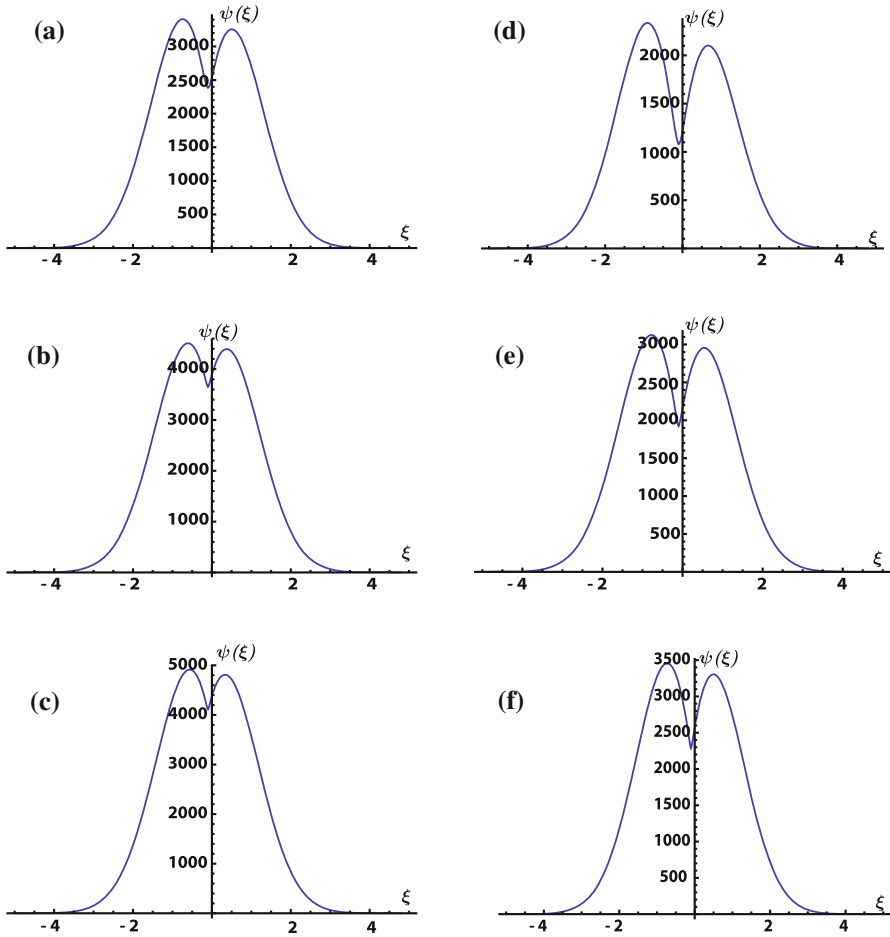


Fig. 5 The wave-function for ground-state energy via numerical shooting method ($a = 8, a = 15$). **a** wave-function $a = 8, b = 100, \lambda = 0.01, e = 2.0307525$. **b** wave-function $a = 8, b = 250, \lambda = 0.01, e = 1.7594946$. **c** wave-function $a = 8, b = 500, \lambda = 0.01, e = 1.6788949$. **d** wave-function $a = 15, b = 100, \lambda = 0.01, e = 2.4155885$. **e** wave-function $a = 15, b = 250, \lambda = 0.01, e = 2.1170949$. **f** wave-function $a = 15, b = 500, \lambda = 0.01, e = 2.0163139$

86.4146, 96.5659, 106.095, 114.478, 121.144, 125.504, 126.994, 125.112, 119.472, 109.847, 96.2133, 78.7839, 58.0281, 34.6718, 9.6783, -15.7937, -40.4527, -62.9548, -81.9958, -96.4088, -105.257, -107.917, -104.135, -94.0697, -78.7945, -67.3952, -72.0849, -80.3204, -84.108, -82.8212, -76.5932, -65.8654, -51.3417, -33.9272, -14.6545, 5.39537, 25.1697, 43.7129, 60.2223, 74.0859, 84.9026, 92.4847, 96.8431, 98.1616, 96.7602, 93.0557, 87.5204, 80.6441, 72.9014, 64.7256, 56.4909, 48.502, 40.9904, 34.1168, 27.9772, 22.6127, 18.0198, 14.1619, 10.9792, 8.3983, 6.33968, 4.72357, 3.47429, 2.52294, 1.80901, 1.28084, 0.895514, 0.6182, 0.421216, 0.283004, 0.187062, 0.120947, 0.0753685, 0.0433854, 0.0196996, 1.27722×10^{-7} }

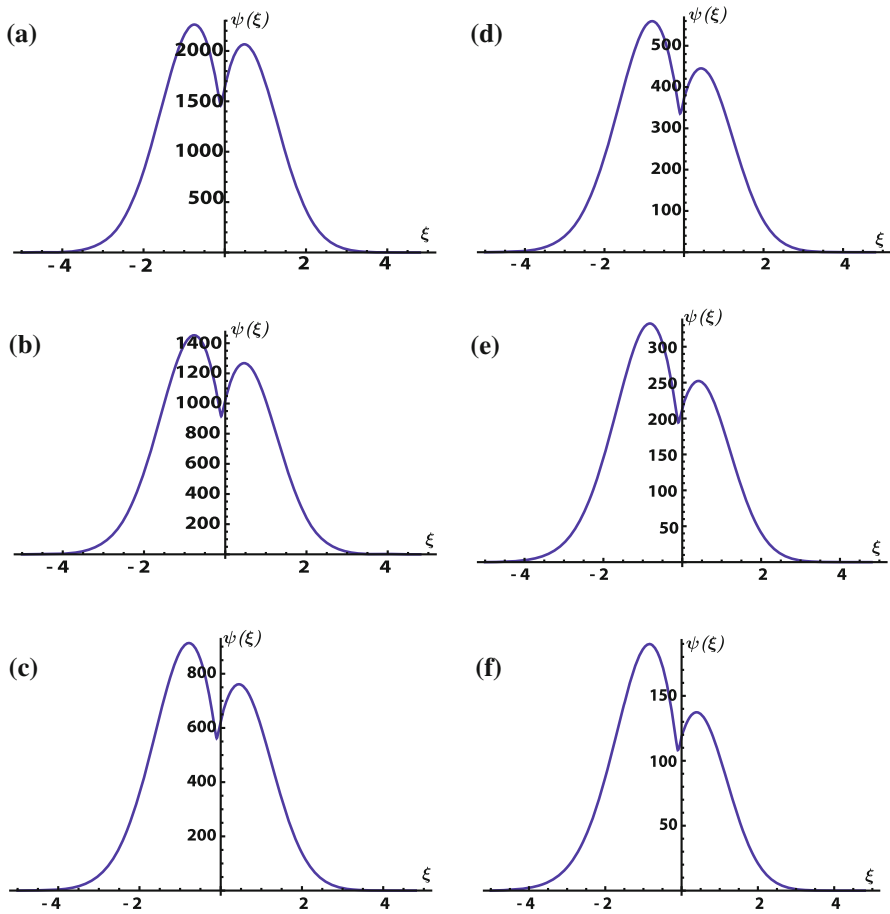


Fig. 6 The wave-function for ground-state energy via numerical shooting method ($\lambda = 0.02 - \lambda = 0.07$). **a** wave-function $a = 15, b = 500, e = 2.0126620, n = 0, \lambda = 0.02$ **b** wave-function $a = 15, b = 500, e = 2.0065226, n = 0, \lambda = 0.03$ **c** wave-function $a = 15, b = 500, e = 1.9978105, n = 0, \lambda = 0.04$ **d** wave-function $a = 15, b = 500, e = 1.9863944, n = 0, \lambda = 0.05$ **e** wave-function $a = 15, b = 500, e = 1.9720802, n = 0, \lambda = 0.06$ **f** wave-function $a = 15, b = 500, e = 1.9545818, n = 0, \lambda = 0.07$

- In[6]:= `ListPlot[%, PlotJoined -> True]`
- Out[6]= graph see Fig. 2

5 Conclusion

The numerical shooting method [12] is generally regarded as one of the most efficient methods that give very accurate results because it integrates the Schrödinger equation directly, though in the numerical sense (Fig. 3).

case 2: The Gaussian asymmetric double-well potential.

The energy eigenvalue at range 5 ($\xi_{max} = 5$) are in harmony. From Tables 1, 2, 3 and 4 the excited-state energy eigenvalue in case of the numerical shooting method a little

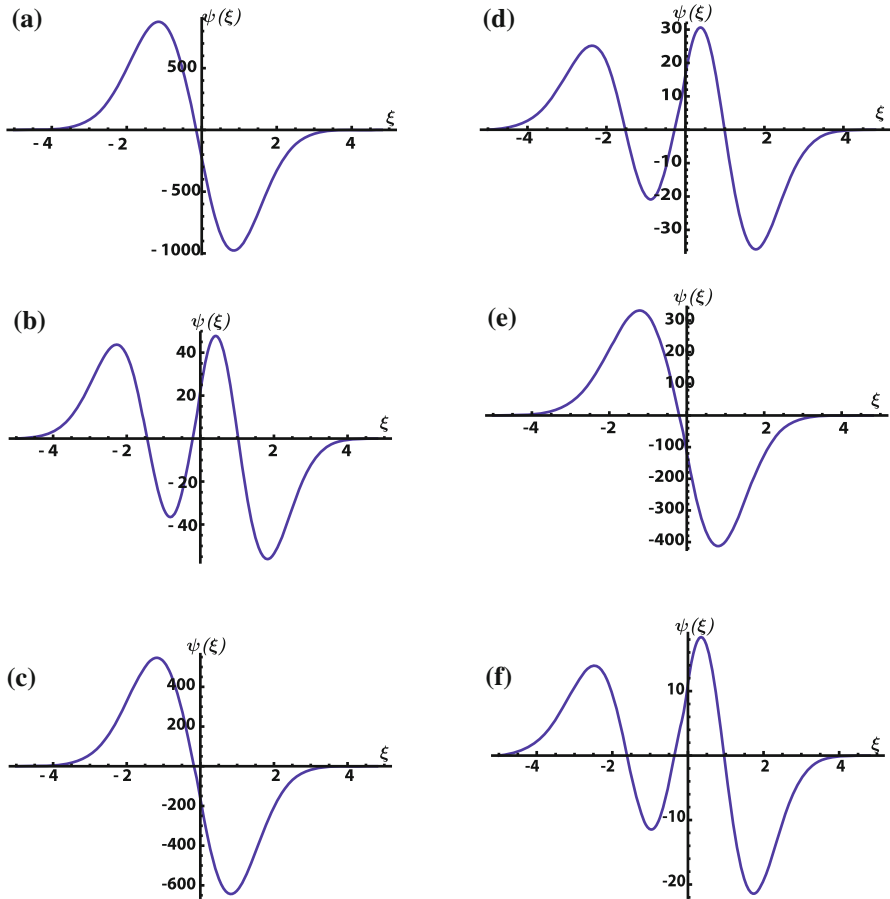


Fig. 7 Plot of several functions involving wave-functions of the Gaussian symmetric double-well potential via numerical shooting method. **a–f** is plot of the wave-functions for excited-state ($n = 1, n = 3$) of potential. **a** wave-functions $a = 15, b = 500, e = 2.9957279, n = 1, \lambda = 0.02$. **b** wave-functions $a = 15, b = 500, e = 6.9920503, n = 3, \lambda = 0.02$. **c** wave-functions $a = 15, b = 500, e = 2.9936497, n = 1, \lambda = 0.03$. **d** wave-functions $a = 15, b = 500, e = 6.9975201, n = 3, \lambda = 0.03$. **e** wave-functions $a = 15, b = 500, e = 2.9905732, n = 1, \lambda = 0.04$. **f** wave-functions $a = 15, b = 500, e = 6.9986615, n = 3, \lambda = 0.04$

is different from the perturbation theory. From Tables 1, 2, 3 and 4 the ground-state energy eigenvalue in case of the numerical shooting method a increase is different from the perturbation theory. From Tables 1, 2, 3 and 4, if the value of b has increase, the energy eigenvalue (ε) has lessen. From Tables 3 and 4, if the value of λ has increase the energy eigenvalue (ε) has little. Figure 4 shows sketches of the numerical shooting method wave-functions for second excited-state energy of a Gaussian asymmetric double-well potential. The wave-function of a particle whose energy ε is less than the Gaussian asymmetric double-well potential barrier height (a). Note that wave-function decays exponentially within region barrier show Fig. 1. The $n =$ even case is shown in Figs. 4, 5 and 6. In this case, the wave-function has split up

asymmetric nodes. The $n = \text{odd}$ case is shown in fig. 4–18 of the Ref. [18] (see Fig. 7). In this case, the wave function similar to in case of a typical harmonic oscillator and the wave-function has not split up asymmetric nodes (see Fig 7). If height b or a affect the wave-function has split up increase typical asymmetric nodes. From Fig. 5, if the value of a has increase, the wave-function for ground-state energy has split up asymmetric increase nodes (Setting $b = 500$, $\lambda = 0.01$ every-case). From Fig. 5, if the value of a has increase, the wave-function ($\psi(\xi)$) for ground-state energy lessen. From Fig. 6, if the value of λ has increase, the wave-function ($\psi(\xi)$) for ground-state energy lessen.

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