

# Ground-state energy eigenvalue calculation of the quantum mechanical well $V(x) = \frac{1}{2}kx^2 + \lambda x^4$ via analytical transfer matrix method

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## Abstract

We consider a fundamental quantum mechanical bound-state problem in the form of the quartic-well potential  $V(x) = \frac{1}{2}kx^2 + \lambda x^4$ . The analytical transfer matrix method is applied. This yields a quantization condition from which we can calculate the phase contributions and ground-state energy eigenvalues numerically. We also compare the results with those obtained from other typical means popular among physics students, namely the numerical shooting method, perturbation theory and the standard WKB method.

## 1. Introduction

Bound-state problems in fundamental quantum mechanics have long been of interest to lecturers, advanced undergraduate and graduate students in physics and applied mathematics. There exist several means to study them, e.g. WKB approximation, time-independent perturbation theory [1], the numerical shooting method [2], the finite-element method [3, 4], etc. Here we analyse a one-dimensional problem using the analytical transfer matrix method (ATMM) devised by Cao *et al* [5]. This method was extensively used in planar optical wave guides [6] and tunnelling [7]. The main principle is to subdivide the domain into many tiny segments each of which possesses a constant potential. The concept of a transfer matrix arises when we connect the wavefunctions at the boundary of two different potential levels.

## 2. Single-stepped potential

For a background, we consider the single-stepped potential with a particular energy eigenvalue as shown in figure 1. It is well known that the wavefunctions are plane waves. The original

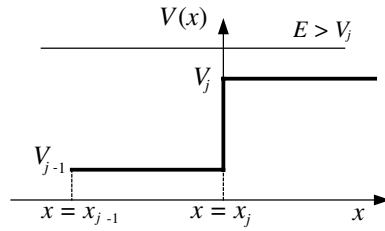


Figure 1. The single-stepped potential.

idea stems from the fact that the wavefunctions and their first derivatives can generally be written as a linear combination of the form

$$\begin{bmatrix} \psi_j(x_{j+1}) \\ \psi'_j(x_{j+1}) \end{bmatrix} = \begin{bmatrix} \alpha & \beta \\ \gamma & \eta \end{bmatrix} \begin{bmatrix} \psi_j(x_j) \\ \psi'_j(x_j) \end{bmatrix}, \quad (1)$$

where  $\alpha, \beta, \gamma, \eta$  are constants to be determined. Consider plane-wave solutions as

$$\psi_j(x_j) = A e^{i\kappa_j x_j} + B e^{-i\kappa_j x_j}, \quad (2)$$

where

$$\kappa(x)_j = \sqrt{\frac{2M}{\hbar^2}(E - V(x_j))}; \quad x_{j+1} = x_j + d. \quad (3)$$

One may solve (1) for  $\alpha, \beta, \gamma, \eta$ , and finally get

$$\begin{aligned} \alpha &= \cos(\kappa_j d), & \beta &= -\frac{1}{\kappa_j} \sin(\kappa_j d), \\ \gamma &= \kappa_j \sin(\kappa_j d), & \eta &= \cos(\kappa_j d). \end{aligned} \quad (4)$$

By substituting (4) into (1), we have

$$\begin{bmatrix} \psi_j(x_{j+1}) \\ \psi'_j(x_{j+1}) \end{bmatrix} = \begin{bmatrix} \cos(\kappa_j d) & -\frac{1}{\kappa_j} \sin(\kappa_j d) \\ \kappa_j \sin(\kappa_j d) & \cos(\kappa_j d) \end{bmatrix} \begin{bmatrix} \psi_j(x_j) \\ \psi'_j(x_j) \end{bmatrix}, \quad (5)$$

where

$$\kappa_j = \frac{\sqrt{2M(E - V_j)}}{\hbar}, \quad j = 1, 2, \dots$$

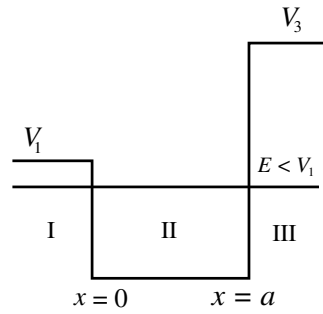
On the other hand, in the case that the energy is lower than any of the piecewise potentials, we would instead get

$$\begin{bmatrix} \psi_j(x_{j+1}) \\ \psi'_j(x_{j+1}) \end{bmatrix} = \begin{bmatrix} \cosh(\kappa_j d) & -\frac{1}{\kappa_j} \sinh(\kappa_j d) \\ -\kappa_j \sinh(\kappa_j d) & \cosh(\kappa_j d) \end{bmatrix} \begin{bmatrix} \psi_j(x_j) \\ \psi'_j(x_j) \end{bmatrix}. \quad (6)$$

It is obvious that the matrix in (5) or (6) transfers the values of the wavefunction and its derivative from the position  $x_j$  to  $x_{j+1}$ . We call it the *transfer matrix*.

### 3. The multi-stepped potential well

In order to solve the Schrödinger equation in each of the three regions in figure 2, the boundary conditions due to the continuity of the wavefunction and its first derivative are applied at the boundaries of the regions I, II and III. In the case that the energy is less than both  $V_1$  and  $V_3$  [8], the solution in region I,  $x < 0$ , is given as



**Figure 2.** Asymmetric finite square-well potential without phase contribution.

$$\psi_1(x) = A e^{\alpha_1 x}, \quad \alpha_1 \equiv \sqrt{\frac{2M(V_1 - E)}{\hbar^2}}. \quad (7)$$

The solution in region III,  $x > a$ , also corresponds to a decaying wave. In region III, the wavefunction is given by

$$\psi_3(x) = C e^{-\alpha_3 x}, \quad \alpha_3 \equiv \sqrt{\frac{2M(V_3 - E)}{\hbar^2}}. \quad (8)$$

Inside the well, the wavefunction oscillates, i.e.

$$\psi_2(x) = B \sin(kx) + D \cos(kx), \quad k \equiv \sqrt{\frac{2ME}{\hbar^2}}. \quad (9)$$

At  $x = 0$ , application of the continuity of the wavefunction and its first derivative yields

$$A = D = \frac{k}{\alpha_1} B. \quad (10)$$

At  $x = a$ , by using the continuity of the wavefunction and its first derivative, we have

$$-\frac{1}{\alpha_3} = \frac{B \sin(ka) + D \cos(ka)}{kB \cos(ka) - kD \sin(ka)}. \quad (11)$$

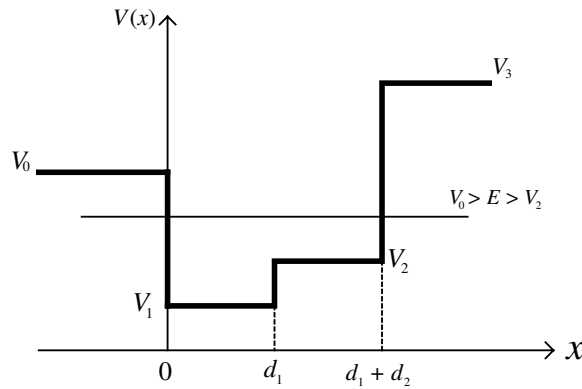
Solving (10) and (11), we finally obtain [9]

$$ka = m\pi - \tan^{-1}[\alpha_1] - \tan^{-1}[\alpha_3], \quad m = 0, 1, 2, \dots \quad (12)$$

The second and third terms on the rhs of (12) are interpreted as the phase losses due to the finite potential barriers  $V_1$  and  $V_3$ , respectively. The first term on the lhs of (12) is the phase difference between  $x = 0$  and  $x = a$ .

Consider now the stepped potential well shown in figure 3. We pay attention to the case of  $E > V_2$ . The wavefunction has the form of  $A_0 \exp(P_0 x)$  in the regime  $x < x_0$  and  $A_3 \exp(-P_3 x)$  in the regime  $x > d_1 + d_2$ . Between them, the wavefunction oscillates with different wavelengths whenever the particle moves from a constant potential to another step. As used previously, the wavefunction and its first derivative at the boundaries are required to satisfy the matrix equation

$$\begin{bmatrix} A_0 \\ A_0 P_0 \end{bmatrix} = \begin{bmatrix} \cos(\kappa_1 d_1) & -\frac{1}{\kappa_1} \sin(\kappa_1 d_1) \\ \kappa_1 \sin(\kappa_1 d_1) & \cos(\kappa_1 d_1) \end{bmatrix} \begin{bmatrix} \cos(\kappa_2 d_2) & -\frac{1}{\kappa_2} \sin(\kappa_2 d_2) \\ \kappa_2 \sin(\kappa_2 d_2) & \cos(\kappa_2 d_2) \end{bmatrix} \times e^{-P_3(d_1+d_2)} \begin{bmatrix} A_3 \\ -A_3 P_3 \end{bmatrix}, \quad (13)$$



**Figure 3.** The stepped potential well with phase contribution.

which is equivalent to

$$\begin{bmatrix} \psi(0) \\ \psi'(0) \end{bmatrix} = \mathbf{M}_1 \mathbf{M}_2 \begin{bmatrix} \psi(d_1 + d_2) \\ \psi'(d_1 + d_2) \end{bmatrix}, \quad (14)$$

where

$$\mathbf{M}_j = \begin{bmatrix} \cos(\kappa_j d_j) & -\frac{1}{\kappa_j} \sin(\kappa_j d_j) \\ \kappa_j \sin(\kappa_j d_j) & \cos(\kappa_j d_j) \end{bmatrix}, \quad j = 1, 2. \quad (15)$$

Substituting plane-wave solutions into (14), we finally obtain the quantization rule as [5, 10]

$$\kappa_1 d_1 + \kappa_2 d_2 + \Phi(s) = n' \pi + \tan^{-1} \left[ \frac{P_0}{\kappa_1} \right] + \tan^{-1} \left[ \frac{P_3}{\kappa_2} \right], \quad (16)$$

where

$$\kappa_j \equiv \frac{\sqrt{2M(E - V_j)}}{\hbar}, \quad j = 1, 2, \quad P_j \equiv \frac{\sqrt{2M(V_j - E)}}{\hbar}, \quad j = 0, 3,$$

$$\Phi(s) \equiv \Phi_2 - \tan^{-1} \left[ \frac{\kappa_2}{\kappa_1} \tan(\Phi_2) \right], \quad \Phi_2 = n' \pi + \tan^{-1} \left( \frac{P_3}{\kappa_2} \right) - \kappa_2 d_2,$$

$$n' = 0, 1, 2, \dots$$

The second and third terms on the rhs of (16) are half-phase losses at the potential barriers  $V_0$  and  $V_3$ , respectively. The first term on the lhs of (16) is the phase difference between  $x = 0$  and  $x = d_1$ , and the second term on the lhs of (16) is the phase difference between  $x = d_1$  and  $x = d_1 + d_2$ . We observe that by setting  $V_1 = V_2$ , we obtain  $\Phi(s) = 0$ . Accordingly, this phase contribution,  $\Phi(s)$ , may be regarded as the result of the interference of the scattered sub-waves between different potential levels  $V_1$  and  $V_2$ .

#### 4. An arbitrary potential-well function

Since a continuous potential well may be viewed as a collection of many thin bar graphs each of which possesses a constant potential, the above method can therefore be extended to study an arbitrary one-dimensional potential well of the form shown in figure 4.

In order to apply a multi-stepped potential effectively, we have set the potential in the regimes  $x < x_0$  and  $x > x_s$  as constants, as shown in figure 4.  $x_0$  and  $x_s$  are chosen in such a way that it does not substantially affect the decaying wavefunction numerically in both

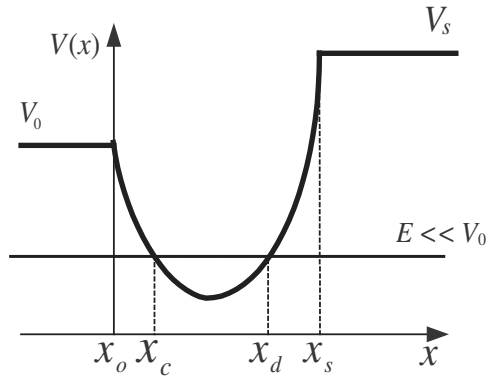


Figure 4. An arbitrary potential-well function  $V(x)$ .

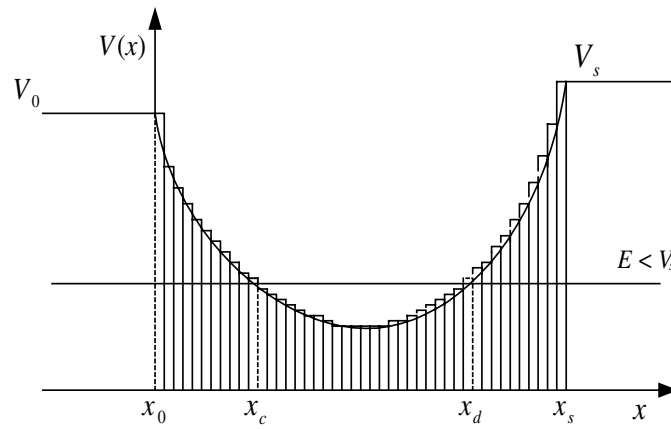


Figure 5. A graph of an arbitrary single potential well is equivalent to an assembly of tiny bars.

regimes. Accordingly, they are selected so that  $x_0 \ll x_c$  and  $x_s \gg x_d$ . By this, it will not numerically affect the energy eigenvalues that we are about to compute. According to the classically allowed or forbidden regions, the multi-stepped potentials corresponding to the  $i$ th,  $j$ th and  $k$ th section layers are shown in figure 5.

The transfer matrices can be written as

$$\mathbf{M}_i = \begin{bmatrix} \cosh(\alpha_i d) & -\frac{1}{\alpha_i} \sinh(\alpha_i d) \\ -\alpha_i \sinh(\alpha_i d) & \cosh(\alpha_i d) \end{bmatrix}, \quad i = 1, 2, \dots, l, \quad (17)$$

$$\mathbf{M}_j = \begin{bmatrix} \cos(\kappa_j d) & -\frac{1}{\kappa_j} \sin(\kappa_j d) \\ \kappa_j \sin(\kappa_j d) & \cos(\kappa_j d) \end{bmatrix}, \quad j = l+1, l+2, \dots, l+m \quad (18)$$

and

$$\mathbf{M}_k = \begin{bmatrix} \cosh(\alpha_k d) & -\frac{1}{\alpha_k} \sinh(\alpha_k d) \\ -\alpha_k \sinh(\alpha_k d) & \cosh(\alpha_k d) \end{bmatrix}, \quad k = l+m+1, \dots, l+m+n, \quad (19)$$

where

$$\alpha_i = \frac{\sqrt{2M[V(x_i) - E]}}{\hbar}, \quad \kappa_j = \frac{\sqrt{2M[E - V(x_j)]}}{\hbar}, \quad \alpha_k = \frac{\sqrt{2M[V(x_k) - E]}}{\hbar}. \quad (20)$$

Applying the boundary conditions at  $x = x_0$  and  $x = x_s$  yields

$$\begin{bmatrix} \psi(x_0) \\ \psi'(x_0) \end{bmatrix} = \left[ \prod_{i=1}^l \mathbf{M}_i \right] \left[ \prod_{j=l+1}^{l+m} \mathbf{M}_j \right] \left[ \prod_{k=l+m+1}^{l+m+n} \mathbf{M}_k \right] \begin{bmatrix} \psi(x_s) \\ \psi'(x_s) \end{bmatrix}, \quad (21)$$

where the prime denotes differentiation with respect to  $x$ . As known, the wavefunction in the region  $x < x_0$  is  $A_0 e^{P_0(x-x_0)}$  and the wavefunction in the region  $x > x_s$  is  $A_s e^{-P_s(x-x_s)}$ , where

$$P_0 = \frac{\sqrt{2M[V_0 - E]}}{\hbar}, \quad P_s = \frac{\sqrt{2M[V_s - E]}}{\hbar}. \quad (22)$$

Here,  $A_0, A_s$  are the amplitude coefficients to be determined. From (21) the solution for  $j = l + m$  by using similar algebra manipulation as developed in the reference is given by [6]

$$\kappa_j d + \left[ \Phi_{j+1} + \tan^{-1} \left[ \frac{\kappa_{j+1}}{\kappa_j} \tan \Phi_{j+1} \right] \right] = n_j \pi + [\Phi_{j+1} - \Phi_j], \quad (23)$$

substituting the definition  $\Phi_j = \tan^{-1} \left( \frac{P_j}{\kappa_j} \right)$  and  $j = l + m$  into (23), we get

$$\kappa_{l+m} d = \pi n_{l+m} - \tan^{-1} \left( \frac{P_{l+m}}{\kappa_{l+m}} \right) + \tan^{-1} \left( \frac{\kappa_{l+m+1}}{\kappa_{l+m}} \tan \Phi_{l+m+1} \right). \quad (24)$$

It follows that

$$\kappa_{l+m} d = n_{l+m} \pi + \tan^{-1} \left[ \frac{P_{l+m+1}}{\kappa_{l+m}} \right] - \Phi_{l+m}. \quad (25)$$

Summing all indices  $j$ , we have

$$\sum_{j=l+1}^{l+m} \kappa_j d + \sum_{j=l+1}^{l+m-1} \left[ \Phi_{j+1} - \tan^{-1} \left( \frac{\kappa_{j+1}}{\kappa_j} \tan \Phi_{j+1} \right) \right] = n_0 \pi + \tan^{-1} \left( \frac{P_{l+m+1}}{\kappa_{l+m}} \right) - \Phi_{l+1}. \quad (26)$$

Substituting the definition  $\Phi_{l+1} = \tan^{-1} \left( \frac{P_{l+1}}{\kappa_{l+1}} \right)$  and  $P_l + P_{l+1} = 0$  [6] into (26), we get

$$\sum_{j=l+1}^{l+m} \kappa_j d + \Phi(s) = n_0 \pi + \tan^{-1} \left[ \frac{P_l}{\kappa_{l+1}} \right] + \tan^{-1} \left[ \frac{P_{l+m+1}}{\kappa_{l+m}} \right], \quad n_0 = 0, 1, \dots, \quad (27)$$

where

$$\Phi(s) = \sum_{j=l+1}^{l+m-1} \left[ \Phi_{j+1} - \tan^{-1} \left[ \frac{\kappa_{j+1}}{\kappa_j} \tan \Phi_{j+1} \right] \right] \quad (28)$$

and

$$\Phi_j = \tan^{-1} \left( \frac{P_j}{\kappa_j} \right), \quad P_j = \kappa_j \tan \left[ \tan^{-1} \left( \frac{P_{j+1}}{\kappa_j} \right) - \kappa_j d \right].$$

As usual, the phase contribution,  $\Phi(s)$ , looks almost the same as in the case of a multi-stepped potential well in section 3, but this time it is more complicated due to many more constant-potential layers.  $P_l$  and  $P_{l+m+1}$  are the equivalent exponential decaying coefficients corresponding to the regions  $x < x_c$  and  $x > x_d$ , respectively,  $P_i$  is the momentum that transfers energy at a stack of thin films interval  $i = 1, 2, \dots, l$  and  $P_k$  is the momentum that transfers energy at a stack of thin films interval  $k = l + m + 1, l + m + 2, \dots, l + m + n$ . We now investigate the half-phase losses at the turning point, i.e. the two terms  $\tan^{-1} \left[ \frac{P_l}{\kappa_l} \right]$  and  $\tan^{-1} \left[ \frac{P_{l+m+1}}{\kappa_{l+m}} \right]$  in (27). It is obviously clear that as  $l, m$  and  $n \rightarrow \infty, d \rightarrow 0$ , we have  $\kappa_{l+1} = 0$  at  $x_{l+1}$  and  $\kappa_{l+m} = 0$  at  $x_{l+m}$ . For bound states  $P_l, P_{l+m+1}$  are finite and positive, resulting in the value  $\frac{\pi}{2}$  of the half-phase losses at each turning point. We thus obtain a quantization condition as the width of the section layers  $d$  tends to zero, i.e.

$$\int_{x_c}^{x_d} \kappa(x) dx + \Phi(s) = (n_0 + 1)\pi, \quad n_0 = 0, 1, 2, \dots \quad (29)$$

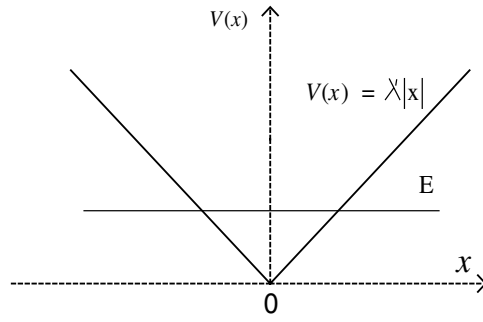


Figure 6. Graph of the potential  $V(x) = \lambda|x|$ .

## 5. An illustrative example

For an example, consider the case of the even linear potential in the form  $V(x) = \lambda|x|$  as shown in figure 6.

### 5.1. Exact solution

We have, from the Schrödinger equation,

$$\frac{d^2\psi(x)}{dx^2} + \frac{2M}{\hbar^2}(E - \lambda|x|)\psi(x) = 0. \quad (30)$$

We define the new variable  $z$  so that

$$x \equiv \alpha z. \quad (31)$$

Equation (30) is hence transformed to

$$\frac{d^2\psi(z)}{dz^2} + \left[ \frac{2M\alpha^2}{\hbar^2}E - \frac{2M\alpha^3}{\hbar^2}\lambda'|z| \right] \psi(z) = 0. \quad (32)$$

The constant  $\alpha$  will be chosen to make  $\frac{2M\alpha^3}{\hbar^2}\lambda' = 1$ , therefore

$$\alpha = \left( \frac{\hbar^2}{2M\lambda'} \right)^{\frac{1}{3}}. \quad (33)$$

We also set  $\frac{2M\alpha^2}{\hbar^2}E = \varepsilon$ . Together with (33) we get

$$E_{\text{exact}} = \varepsilon \left( \frac{\hbar^2\lambda'^2}{2M} \right)^{\frac{1}{3}}. \quad (34)$$

Substituting (34) into (32) and considering the domain  $z \geq 0$  only, due to the symmetry of the potential, (32) reads

$$\frac{d^2\psi(z)}{dz^2} - (z - \varepsilon)\psi(z) = 0. \quad (35)$$

Applying the bound-state B.C.,  $\psi(z \rightarrow \infty) = 0$ , the solution becomes the Airy function of the first kind, i.e.

$$\psi(z) = c_1 \text{Ai}(z - \varepsilon). \quad (36)$$

**Table 1.** Ground-state energies obtained from the ATMM and standard WKB, displayed together with exact solutions.

$\lambda'$	ATMM $(\hbar^2/2M)^{\frac{1}{3}}$	WKB $(\hbar^2/2M)^{\frac{1}{3}}$	Exact $(\hbar^2/2M)^{\frac{1}{3}}$	% error of ATMM	% error of WKB
0.5	0.635 273 44	0.702 695 92	0.641 799 35	1.02	9.49
1.0	1.022 718 75	1.115 460 24	1.018 792 97	0.39	9.49
1.5	1.351 386 71	1.461 666 40	1.334 996 45	1.23	9.49
2.0	1.624 902 34	1.770 682 75	1.617 233 03	0.47	9.49
2.5	1.920 780 27	2.054 695 32	1.876 632 69	2.35	9.49
3.0	2.177 617 18	2.320 250 79	2.119 174 77	2.76	9.49
3.5	2.421 503 90	2.571 379 18	2.348 540 05	3.11	9.49
4.0	2.654 824 18	2.810 783 67	2.567 197 42	3.41	9.49
4.5	2.879 233 39	3.040 388 65	2.776 904 53	3.69	9.49
5.0	3.095 825 19	3.261 625 52	2.978 968 72	3.92	9.49

Applying the even-state B.C.,  $\psi'(z = 0) = 0$ , any even-state energy may be obtained from the relation

$$\frac{dAi}{dy}(y = -\varepsilon) = 0. \quad (37)$$

For the ground state, we take the smallest value of  $\varepsilon$  that satisfies (37). The numerical answer, to the fifth digit, is

$$\varepsilon = 1.018\,79. \quad (38)$$

Substituting (38) into (34) gives

$$E_{\text{exact}} = 1.018\,79 \left( \frac{\hbar^2 \lambda'^2}{2M} \right)^{\frac{1}{3}}. \quad (39)$$

## 5.2. WKB approach

In this case, the WKB quantization rule reads

$$2 \int_0^{\frac{E}{\lambda'}} \sqrt{2M(E - \lambda'x)} \, dx = \left(N + \frac{1}{2}\right) \pi \hbar, \quad (40)$$

whose solution reads

$$E_{\text{WKB}} = \left( \frac{3\lambda'}{4} \left(N + \frac{1}{2}\right) \pi \right)^{\frac{2}{3}} \left( \frac{\hbar^2}{2M} \right)^{\frac{1}{3}}. \quad (41)$$

The percentage error of the WKB method for this potential for ground state can be calculated easily. It is independent of  $\lambda'$ , i.e.

$$\% \text{Error}_{\text{WKB}} = \frac{\left| \varepsilon \lambda'^{\frac{2}{3}} - \left( \frac{3\pi}{4} \right)^{\frac{2}{3}} \lambda'^{\frac{2}{3}} \right|}{\varepsilon \lambda'^{\frac{2}{3}}} \times 100 = \left| 1 - \frac{\left( \frac{3\pi}{8} \right)^{2/3}}{\varepsilon} \right| \times 100 = 9.488\,73.$$

## 6. Numerical results of the quartic-well problem

We now pay attention to the particular problem of calculating the ground-state energy of the potential well

$$V(x) = \frac{1}{2} M \omega^2 x^2 + \lambda x^4, \quad (42)$$





**Table 2.** Comparison of the ground-state energy obtained from the ATMM, standard WKB, first-order perturbation and numerical shooting methods.

$\beta \equiv \frac{2\hbar\lambda}{m^2\omega^3}$	ATMM ( $\hbar\omega/2$ )	WKB ( $\hbar\omega/2$ )	First-order perturbation [15] ( $\hbar\omega/2$ )	NSM [15] ( $\hbar\omega/2$ )
0.1	1.066 406 25	1.035 156 25	1.075 000 00	1.064 518 96
0.2	1.121 312 50	1.066 562 50	1.150 000 00	1.117 404 50
0.3	1.169 062 50	1.095 156 25	1.225 000 00	1.163 049 19
0.4	1.212 343 75	1.121 718 75	1.300 000 00	1.203 710 79
0.5	1.251 562 50	1.146 875 50	1.375 000 00	1.240 659 19
0.6	1.287 812 50	1.169 343 75	1.450 000 00	1.274 698 29
0.7	1.321 718 75	1.191 068 75	1.525 000 00	1.306 377 09
0.8	1.353 906 25	1.212 031 25	1.600 000 00	1.336 090 65
0.9	1.383 593 75	1.231 875 50	1.675 000 00	1.364 135 29
1.0	1.411 835 95	1.251 562 50	1.750 000 00	1.390 739 67

Due to this, the phase integral in the quantization condition (29) may be written in reduced units as

$$\int_{x_c}^{x_d} \kappa(x) dx = \int_{\xi_c}^{\xi_d} \sqrt{\varepsilon - \xi^2 - \beta\xi^4} d\xi, \quad (45)$$

where  $\xi_c = \left(\frac{M\omega}{\hbar}\right)^{\frac{1}{2}} x_c$ ,  $\xi_d = \left(\frac{M\omega}{\hbar}\right)^{\frac{1}{2}} x_d$ . The ATMM gives a quantization rule similar to that obtained from the WKB method (cf [11–13]), the only difference is that for ATMM the phase contribution can be calculated [14] with a slight complication, whereas the WKB result may be equivalent to the ATMM case by setting the phase contribution equal to  $\frac{\pi}{2}$ . We obtain the numerical values ground-state energy as displayed in table 2.

### 6.1. Logic of the ATMM calculation

- (i) Input  $\varepsilon$ .
- (ii) Calculate  $x_c, x_d, P_s$ .
- (iii) Calculate  $P_k$ , varying from segment to segment in the regime  $x_d < x < x_s$ , according to

$$P_k = \alpha_k \frac{\sinh(\alpha_k d) + \frac{P_{k+1}}{\alpha_k} \cosh(\alpha_k d)}{\cosh(\alpha_k d) + \frac{P_{k+1}}{\alpha_k} \sinh(\alpha_k d)}.$$

- (iv) At  $x_d$ ,  $P_k$  becomes  $P_j$ .
- (v) Calculate  $P_j$ , varying from segment to segment, in the regime  $x_c \leq x \leq x_d$ , according to

$$P_j = \kappa_j \tan \left[ \tan^{-1} \left( \frac{P_{j+1}}{\kappa_j} \right) - \kappa_j d \right].$$

- (vi) At the same time, calculate  $\Phi(s)$  via (28).
- (vii) Calculate phase integral  $= \int_{x_c}^{x_d} \kappa(x) dx$ .
- (viii) According to (29), for the ground state,

$$\frac{\int_{x_c}^{x_d} \kappa(x) dx + \Phi(s)}{\pi} - 1 \equiv n = 0.$$

This expression will hold only if the energy is a correct one. Due to this, we define

$$n_0 \equiv \frac{\int_{x_c}^{x_d} \kappa(x) dx + \Phi(s)}{\pi} - 1.$$

The next task is to calculate  $n_0$  so that it approaches zero as closely as desired. Normally, we assign a small value as the standard to make sure  $n_0$  gets close enough to zero. For example, if  $|n_0| \leq 10^{-6}$ , we stop the calculation and accept the final energy as the numerical solution (see also the flowchart).

### 6.2. Logic of the WKB calculation

For the WKB calculation, we normally start with the WKB quantization rule

$$\int_{x_c}^{x_d} \kappa(x) dx = (N + 1/2)\pi.$$

However, this phase integral cannot be evaluated analytically (except in a few cases where  $V(x)$  is simple enough) in general. A numerical technique is therefore needed in many cases to calculate the energy. In practice, we borrow the technique of calculation from the ATMM, provided that we must set  $\Phi(s) = \frac{\pi}{2}$ . Therefore, the evaluation is much simpler than in the ATMM case.

## 7. Conclusion

The NSM [15] 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. We therefore regard it as the standard to compare with. From table 2, we see that the ATMM we have adopted from Cao *et al* [5] gives outstandingly better results for the ground state than those obtained from first-order perturbation theory and the typical WKB method for every value of  $\lambda(\beta)$  under this quartic single-well potential. In our viewpoint, the complication of the ATMM computation lies in the evaluation of phase contribution, especially when the potential is not of very simple form so that we cannot obtain an analytical expression from the quantization rule (29) but a numerical one instead, in which we employ the binary searching method to work them out. In fact, the ATMM is claimed by Cao *et al* [5] to give the *exact* formalism of the quantization rule without any approximation. One slight disagreement is emphasized here that the truncation of the bound potential at  $x_0, x_s$  in fact indicates a kind of approximation, although this estimation seems to be a precise one that does not considerably affect the energy calculation especially when we choose  $x_s$  far away enough from the rhs turning point. Since the ATMM works pretty well, it might become another useful technique for the ground-state energy calculation such as the variational method or some other efficient means.

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