Energy eigenvalues from an analytical transfer matrix method*

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A detailed procedure based on an analytical transfer matrix method is presented to solve bound-state problems. The derivation is strict and complete. The energy eigenvalues for an arbitrary one-dimensional potential can be obtained by the method. The anharmonic oscillator potential and the rational potential are two important examples. Checked by numerical techniques, the results for the two potentials by the present method are proven to be exact and reliable.

Keywords: analytical transfer matrix method, energy eigenvalues, bound state, one-dimensional potential

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1. Introduction

Bound-state problems in quantum mechanics have long been of interest in various branches of physics since the advent of the famous Schrödinger equation. As exact analytic solutions with special or other mathematical functions to the Schrödinger equation are obtained for limited potentials, such as potentials of a free particle, linear harmonic oscillator and hydrogen atom, various approximation methods have been developed to solve the bound-state problems for other potentials, such as Wentzel–Kramers–Brillouin (WKB)[1] perturbation,[2] the quasilinearization method,[3] the variational method,[4] function analysis[5,6] and the eigenvalue moment method.[7] These methods have been widely used but accurate energy eigenvalues cannot be obtained for some problems; however, accurate knowledge of energy eigenvalues of a great number of potentials is essential.[8,9] The applicable range of these approximation methods is restricted in solving some practical problems. Highly accurate calculations for bound-state problems using the simplest possible methods are the main goal across a wide range of research areas.

In this paper, we consider the bound-state problem in the light of the analytical transfer matrix (ATM) method. The main principle of the ATM method is to divide the domain of the potential into many tiny segments, each with a constant potential.[10−12] A transfer matrix corresponds to each constant potential level. The ATM method has developed from the transfer matrix technique; however, the traditional transfer matrix method serves as a numerical method but does not act as an analytic method.[13] Since the subwaves which inherently exist in an inhomogeneous system are taken into account, the analytical quantization condition is obtained by detailed calculation from the ATM method. Moreover, the quantization condition is accurate in solving the bound-state problem and may provide applications in many areas, such as solid-state physics, nuclear physics and atomic physics.

The efficiency of the ATM method is demonstrated by its applications to bound states for the anharmonic oscillators of the potential $V(x) = x^2/2 + gx^4$ and the rational potential $V(x) = x^2 + \lambda x^2/(1 + gx^2)$, which are two important potentials which have been frequently investigated for a wide range of physics applications.[4,14−24]

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2. Theory

The energy eigenvalues of a one-dimensional finite potential well are given by the solutions of the time-independent Schrödinger equation

$$\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0, \tag{1}$$

where E is the energy eigenvalue, $V(x)$ represents the potential energy variation, $\psi(x)$ denotes the eigenfunction of a bound state, m is the effective mass, and $\hbar$ is Planck's constant h divided by 2π.

An arbitrary potential well is shown in Fig. 1. Since a continuous potential well is nothing more than a sum of the constant potentials that a stack of thin films has, we truncate the profiles of $V(x)$ at two appropriate points x_m and x_n, which are far away from the turning points x_{t1} and x_{t2}. The effect of the truncation will be negligible if the potential at the truncation point is very much larger than the energy of the relevant level. We then divide the regions (x_m, x_{t1}), (x_{t1}, x_{t2}) and (x_{t2}, x_n) into l, p and q segments respectively, each with width w. As the division becomes finer and finer, each segment has homogeneous potential energy $V(x) = V(x + w/2)$. Applying the boundary conditions at the two truncation points, the wave function $\psi(x_m)$ at the left truncation point x_m and its derivative $\psi'(x_m)$ are related to $\psi(x_n)$ and $\psi'(x_n)$ at the right truncation point x_n by the matrix equation

$$\begin{bmatrix} \psi(x_m) \\ \psi'(x_m) \end{bmatrix} = \prod_{i=1}^{l+p+q} M_i \begin{bmatrix} \psi(x_n) \\ \psi'(x_n) \end{bmatrix}, \tag{2}$$

where the prime denotes differentiation with respect to x. As is known, the wave functions in the two regions $(x < x_m)$ and $(x > x_n)$ decay exponentially with displacement along the x axis, which is given as follows:

$$\psi(x) = \begin{cases} A_m \exp[P_m(x - x_m)], & x < x_m, \\ A_n \exp[-P_n(x - x_n)], & x > x_n, \end{cases} \tag{3}$$

where A_m and A_n are the amplitude coefficients to be determined; P_m and P_n are the decaying coefficients corresponding respectively to the two truncation points x_m and x_n expressed as $P_m = \sqrt{2m[V(x_m) - E]}/\hbar$ and $P_n = \sqrt{2m[V(x_n) - E]}/\hbar$.

In the classically allowed region (x_{t1}, x_{t2}), the transfer matrices can be written as

$$M_i = \begin{bmatrix} \cos(k_i w) & -\dfrac{1}{k_i}\sin(k_i w) \\ k_i \sin(k_i w) & \cos(k_i w) \end{bmatrix},$$

$$i = l+1, l+2, \ldots, l+p, \tag{4}$$

where $k_i = \sqrt{2m[E - V(x_i)]}/\hbar$.

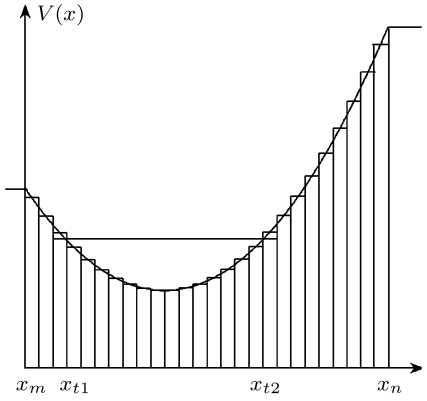


Fig. 1. Energy variation of an arbitrary potential.

In the classically forbidden regions (x_m, x_{t1}) and (x_{t2}, x_n), the transfer matrices can be written as

$$M_i = \begin{bmatrix} \cosh(\alpha_i w) & -\dfrac{1}{\alpha_i}\sinh(\alpha_i w) \\ -\alpha_i \sinh(\alpha_i w) & \cosh(\alpha_i w) \end{bmatrix}, \tag{5}$$

where $\alpha_i = \sqrt{2m[V(x_i) - E]}/\hbar$ and i varies from 1 to l and from $l + p + 1$ to $l + p + q$.

After multiplying Eq. (2) by $[-\psi'(x_m) \;\; \psi(x_m)]$, we obtain the following equation:

$$\begin{bmatrix} -\psi'(x_m) & \psi(x_m) \end{bmatrix} \prod_{i=1}^{l+p+q} M_i \begin{bmatrix} \psi(x_n) \\ \psi'(x_n) \end{bmatrix} = 0. \tag{6}$$

Substituting Eq. (3) into Eq. (6), we have

$$\begin{bmatrix} -P_m & 1 \end{bmatrix} \prod_{i=1}^{l+p+q} M_i \begin{bmatrix} 1 \\ -P_n \end{bmatrix} = 0. \tag{7}$$

Equation (7) can be reduced by simple algebraic manipulations to

$$\begin{bmatrix} -P_{t1} & 1 \end{bmatrix} \prod_{i=l+1}^{l+p} M_i \begin{bmatrix} 1 \\ -P_{t2} \end{bmatrix} = 0, \tag{8}$$

where

$$\begin{aligned} &P_{t2} = P_{l+p+1}, \\ &P_i = \alpha_i \frac{\sinh(\alpha_i w) + \dfrac{P_{i+1}}{\alpha_i}\cosh(\alpha_i w)}{\cosh(\alpha_i w) + \dfrac{P_{i+1}}{\alpha_i}\sinh(\alpha_i w)}, \\ &i = l+p+1, l+p+2, \ldots, l+p+q, \\ &P_{l+p+q+1} = P_n, \end{aligned} \tag{9}$$

and

$$\begin{aligned} &P_{t1} = P_l, \\ &P_i = \alpha_i \frac{\sinh(\alpha_i w) + \dfrac{P_{i-1}}{\alpha_i}\cosh(\alpha_i w)}{\cosh(\alpha_i w) + \dfrac{P_{i-1}}{\alpha_i}\sinh(\alpha_i w)}, \\ &i = 1, 2, \ldots, l, \\ &P_0 = P_m. \end{aligned} \tag{10}$$

In the classically allowed region (x_{t1}, x_{t2}), with a treatment analogous to that in Eq. (7), equation (8) can be written as

$$P_l + P_{l+1} = 0, \tag{11}$$

where P_{l+1} can be obtained by the following recursion formula:

$$\begin{aligned} &P_i = k_i \tan\left[\tan^{-1}\left(\frac{P_{i+1}}{k_i}\right) - k_i w\right], \\ &i = l+1, l+2, \ldots, l+p. \end{aligned} \tag{12}$$

To obtain an appropriate form that can give a clear physical insight, we transform Eq. (12) into

$$\begin{aligned} &\tan^{-1}\left(\frac{P_i}{k_i}\right) = n_i\pi + \tan^{-1}\left(\frac{P_{i+1}}{k_i}\right) - k_i w, \\ &n_i = 0, 1, 2, \ldots\ . \end{aligned} \tag{13}$$

Rearranging Eq. (13) yields

$$\begin{aligned} &k_i w + \left[\tan^{-1}\left(\frac{P_{i+1}}{k_{i+1}}\right) - \tan^{-1}\left(\frac{P_{i+1}}{k_i}\right)\right] \\ &= n_i\pi + \tan^{-1}\left(\frac{P_{i+1}}{k_{i+1}}\right) - \tan^{-1}\left(\frac{P_i}{k_i}\right). \end{aligned} \tag{14}$$

The solution for $i = l+1$ is

$$\begin{aligned} k_{l+1} w \;=\; & n_{l+1}\pi + \tan^{-1}\left(\frac{P_{l+2}}{k_{l+1}}\right) \\ & - \tan^{-1}\left(\frac{P_{l+1}}{k_{l+1}}\right). \end{aligned} \tag{15}$$

Summing the solutions corresponding to the values of index i from $l+1$ to $l+p$, we have

$$\begin{aligned} &\sum_{i=l+1}^{l+p} k_i w + \sum_{i=l+1}^{l+p-1}\left[\tan^{-1}\left(\frac{P_{i+1}}{k_{i+1}}\right)\right. \\ &\left. - \tan^{-1}\left(\frac{P_{i+1}}{k_i}\right)\right] \\ &= n\pi + \tan^{-1}\left(\frac{P_{l+p+1}}{k_{l+p}}\right) - \tan^{-1}\left(\frac{P_{l+1}}{k_{l+1}}\right), \\ &n = 0, 1, 2, \ldots\ . \end{aligned} \tag{16}$$

With Eq. (11), we obtain

$$-\tan^{-1}\left(\frac{P_{l+1}}{k_{l+1}}\right) = \tan^{-1}\left(\frac{P_l}{k_{l+1}}\right). \tag{17}$$

Substituting Eq. (17) into Eq. (16) and letting $p \to \infty$ $(w \to 0)$, we obtain

$$\begin{aligned} &\int_{x_{t1}}^{x_{t2}} k(x)\mathrm{d}x + \Phi(s) \\ &= n\pi + \tan^{-1}\left(\frac{P_{l+p+1}}{k_{l+p}}\right) + \tan^{-1}\left(\frac{P_l}{k_{l+1}}\right), \\ &n = 0, 1, 2, \ldots\ , \end{aligned} \tag{18}$$

where

$$\Phi(s) = \sum_{i=l+1}^{l+p-1}\left[\tan^{-1}\left(\frac{P_{i+1}}{k_{i+1}}\right) - \tan^{-1}\left(\frac{P_{i+1}}{k_i}\right)\right], \tag{19}$$

which is the phase contribution from the scattered subwaves and which describes the interaction between the two neighbouring layers of the potential.

Now we come to investigate the two terms $\tan^{-1}(P_l/k_{l+1})$ and $\tan^{-1}(P_{l+p+1}/k_{l+p})$ in Eq. (18), which are the half-phase losses at the turning points. As l, p and $q \to \infty$ $(w \to 0)$, we have

$$\begin{aligned} &k_{l+1} \\ &= \sqrt{2m[E - V(x_{l+1})]}/\hbar \to \sqrt{2m[E - V(x_{t1})}/\hbar \\ &= 0, \end{aligned} \tag{20}$$

and

$$\begin{aligned} &k_{l+p} \\ &= \sqrt{2m[E - V(x_{l+p})]}/\hbar \to \sqrt{2m[E - V(x_{t2})}/\hbar \\ &= 0. \end{aligned} \tag{21}$$

Meanwhile, P_l and P_{l+p+1} are positive and finite for bound states so that the half-phase losses at the turning points become

$$\tan^{-1}\left(\frac{P_l}{k_{l+1}}\right) = \tan^{-1}\left(\frac{P_{l+p+1}}{k_{l+p}}\right) = \pi/2. \tag{22}$$

The above derivation does not involve the conventional short wave limit or long wave limit. As the width w of each segment tends to zero, we have the quantization condition

$$\int_{x_{t1}}^{x_{t2}} k(x)\mathrm{d}x + \Phi(s) = (n+1)\pi, \quad n = 0, 1, 2, \ldots\ , \tag{23}$$

where $k(x) = \sqrt{2m[E - V(x)]}/\hbar$, and n is the quantum number.

Considering the differential formula

$$\mathrm{d}[\arctan(P/k)]/\mathrm{d}x = (k\mathrm{d}P - P\mathrm{d}k)/(P^2 + k^2),$$

and defining that $\Delta\Phi_i = \arctan(P_{i+1}/k_{i+1}) - \arctan(P_{i+1}/k_i) = (k_i\Delta P - P_i\Delta k)/(P_i^2 + k_i^2)$, where $\Delta P = P_{i+1} - P_{i+1} = 0$, and $\Delta k = k_{i+1} - k_i$, we can rewrite Eq. (19) as

$$\begin{aligned}\Phi(s) &= \lim_{w\to 0}\sum_{i=l+1}^{l+p-1}\Delta\Phi_i \\ &= -\lim_{w\to 0}\sum_{i=l+1}^{l+p-1}\frac{P_i\Delta k}{P_i^2+k_i^2} \\ &= -\int_{x_{t1}}^{x_{t2}}\frac{P\,\mathrm{d}k}{P^2+k^2} \\ &= -\int_{x_{t1}}^{x_{t2}}P\frac{\mathrm{d}k/\mathrm{d}x}{P^2+k^2}\,\mathrm{d}x, \end{aligned} \tag{24}$$

where $P = -\psi'(x)/\psi(x)$.

Substituting $P = -\psi'(x)/\psi(x)$ into the Schrödinger equation (1) yields $P' = P^2 + k^2$. The phase contribution can then be expressed as $\Phi(s) = \int_{x_{t1}}^{x_{t2}} -(P/P')k'\,\mathrm{d}x$ and the quantization condition (23) can be rewritten as

$$\int_{x_{t1}}^{x_{t2}}\left(k - \frac{P}{P'}k'\right)\mathrm{d}x = (n+1)\pi,\ n = 0, 1, 2, \ldots\ . \tag{25}$$

According to the quantization condition (25), we can calculate the exact energy eigenvalue of any quantum number for the one-dimensional potential.

3. Anharmonic oscillator

We first consider an anharmonic oscillator. The potential is given by

$$V(x) = \frac{1}{2}x^2 + gx^4, \tag{26}$$

where g is a constant.[14–17] The potential has a single minimum and is symmetric with respect to $x = 0$. The potential becomes infinite as $|x| \to \infty$ and the number of bound states for the potential is infinite. The mass and the frequency of the oscillator are both set to be 1 for convenience.

The results obtained by the ATM method are presented in Table 1. In order to illustrate the performance of our simple method, we take different values of g in Table 1, where E_0^{PT} and E_1^{PT} are respectively the ground state energy and the energy of the first excited state from the proper time version of the renormalization flow equation.[19] The ATM method produces good results of the ground state and the first excited state for small values of coupling constant g, as well as for large coupling constant g. The results are in excellent agreement with the exact eigenvalues obtained by high precision conventional methods.[19] However, the eigenvalues from the functional renormalization group are larger than the exact values, especially for large values of coupling constant g.

Table 1. Energy eigenvalues of the lowest four bound states for the anharmonic oscillator potential.

g	E_0^{PT}	E_0^{ATM}	E_0^{ex}	E_1^{PT}	E_1^{ATM}	E_1^{ex}	E_2^{ATM}	E_3^{ATM}
0.1	0.5593	0.5591	0.5591	1.7721	1.7695	1.7695	3.1386	4.6289
0.2	0.6028	0.6024	0.6024	1.9556	1.9505	1.9505	3.5363	5.2913
0.3	0.6386	0.6380	0.6380	2.1016	2.0946	2.0946	3.8448	5.7966
0.4	0.6696	0.6688	0.6688	2.2255	2.2169	2.2169	4.1028	6.2156
0.5	0.6971	0.6962	0.6962	2.3343	2.3244	2.3244	4.3275	6.5784
0.6	0.7221	0.7210	0.7210	2.4321	2.4210	2.4210	4.5281	6.9011
0.7	0.7451	0.7439	0.7439	2.5214	2.5092	2.5092	4.7103	7.1933
0.8	0.7651	0.7651	0.7651	2.6038	2.5907	2.5907	4.8779	7.4614
0.9	0.7864	0.7850	0.7850	2.6806	2.6666	2.6666	5.0336	7.7101
1.0	0.8052	0.8038	0.8038	2.7527	2.7379	2.7379	5.1793	7.9424
10.0	1.5092	1.5050	1.5050	5.3617	5.3216	5.3216	10.3471	16.0901
50.0	2.5068	2.4997	2.4997	8.9855	8.9151	8.9151	17.4370	27.1926
100.0	3.1401	3.1314	3.1314	11.2758	11.1873	11.1873	21.9069	34.1825
500.0	5.3325	5.3199	5.3199	19.1901	19.0434	19.0434	37.3407	58.3016
1000.0	6.7081	6.6942	6.6942	24.1525	23.9722	23.9722	47.0173	73.4191

The turning points for the anharmonic oscillators are $x_{t1} = -\sqrt{(-1/2 + \sqrt{1/4 + 4gE})/2g}$ and $x_{t2} =$

$\sqrt{(-1/2+\sqrt{1/4+4gE})/2g}$ respectively. In our calculation we divide the potential between the two turning points into 10000 layers. We truncate the potential profile at the right truncation point 10 times the separation between the two turning points from the right turning point, and at the left truncation point also 10 times the separation $x_{t2}-x_{t1}$ from the left turning point x_{t1}. As the width of the segment tends to zero and the number of segments tends to infinity, we can solve the bound-state problem in any desired accuracy. In Table 1 we demonstrate our results to four decimal places. Besides the eigenvalues of the ground state and first excited state, those of the second and third excited states are also presented in Table 1. The results are accurate and meaningful for research on anharmonic oscillators.

4. Rational potential

Next, we consider the rational potential, which may be written as

$$V(x) = x^2 + \lambda x^2/(1+gx^2),$$
$$-\infty < \lambda < \infty, \quad g > 0. \tag{27}$$

This potential is of interest and has been studied by several methods.[17,20–24] The mass is set to be 0.5 in our calculation. The energy eigenvalues of the lowest four bound states are shown in Table 2. Those with superscripts are cited from the relevant references, obtained by the corresponding methods, to test the accuracy of eigenvalues calculated from the ATM method. The results with superscript a only give energy eigenvalues of the ground state for $g = 0.1$, $g = 0.2$ and $g = 1$, obtained by using the power-series expansions.[23] Those with superscript b give the eigenvalues only for $g = 1$, obtained from numerical calculations.[17] Those with superscript c give the energy of the lowest two odd states for $g = 1$, $g = 10$ and $g = 100$, obtained by the variational method.[4] The ATM method gives accurate results not only for the ground states, but also for the excited states. The value of g varies from 0.1 to 1000 in Table 2. After examining our results with superscripts, obtained by different methods, we come to the conclusion that the eigenvalues without superscripts, obtained by the ATM method, are also reliable. This provides a basis for discussion in many fields ranging from quantum mechanics to atomic physics.

Table 2. Energy eigenvalues of the bound states for the rational potential with $\lambda = 1$.

g	$E_0^{\rm ATM}$	$E_1^{\rm ATM}$	$E_2^{\rm ATM}$	$E_3^{\rm ATM}$
0.1	1.38053[a]	4.07988	6.66792	9.16657
0.2	1.35295[a]	3.95556	6.38921	8.71429
0.3	1.32982	3.85778	6.18825	8.41606
0.4	1.31007	3.77890	6.03752	8.20677
0.5	1.29295	3.71390	5.92063	8.05238
0.6	1.27794	3.65939	5.82747	7.93392
0.7	1.26464	3.61298	5.75153	7.84019
0.8	1.25275	3.57296	5.68846	7.76415
0.9	1.24205	3.53808	5.63526	7.70120
1	1.23235[a,b]	3.50739[b,c]	5.58978[b]	7.64820[b,c]
10	1.05930	3.08809[c]	5.08285	7.09037[c]
50	1.01569	3.01937	5.01809	7.01944
100	1.00841	3.00983[c]	5.00927	7.00984[c]
500	1.00185	3.00199	5.00193	7.00199
1000	1.00095	3.00100	5.00097	7.00100

[a] Amore P and Fernández F M.[21]
[b] Ishikawa H.[15]
[c] Saad N, Hall R L and Ciftci H.[4]

5. Conclusion

The ATM method provides a good way of solving the Schrödinger equation. As the phase contribution of the subwave in an inhomogeneous potential is considered, the exact quantization condition is obtained by detailed derivation using the ATM method. The quantization condition is presented in a closed form and works well in solving bound-state problems. Due to its effectiveness and simplicity, the ATM method can be applied to various one-dimensional quantum problems and other fields of physics as well.

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