Energy splitting in symmetric double-well potentials

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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.

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I. INTRODUCTION

The quantum mechanical tunnelling in a smooth symmetric double-well potential is a long-standing and well-known problem. Three methods have been proposed to calculate the energy splitting: the instanton method [1,2], the WKB approximation [3,4] and numerical calculation [4–6]. The instanton method is helpful to understand the physical insight of quantum tunnelling, but the validity is restricted to the case of large separation between the two potential minima. The WKB approximation is widely used for its simple mathematical form, but the result is known to be inaccurate due to its inherent defect in connection formula. One had taken the quadratic connection formula instead of the Airy function to modify the WKB result at ground state [1,7]. Recently, some refinements were developed to improve the accuracy of WKB by changing the phase loss at the classical turning points [8,9]. The anharmonicity is also taken into consideration in the case of small separation distance [9]. To the best of knowledge of the authors, no above approximations have provided the perfect results. Without doubt using numerical methods, one can get the solution up to the desired accuracy, but a considerable deal of physical insight is lost in these processes.

In this paper, the quantization conditions to one-dimensional Schrödinger equation in symmetric double-well potential are presented by using analytical transfer matrix method (ATMM), which has been applied to arbitrary potential wells successfully [10]. Taking into account the correct phase losses at the turning points and the phase contribution of the scattered subwaves, this analysis gives the explicit quantization conditions of the split energy levels. We also calculate the energy eigenvalues of the split energy levels and compare them with that of the exact numerical method [4].

II. THEORY

In the present calculation rather than dealing with continuous variation of potential energy, we first divide the double-well potential into segments symmetrically, in every segment the potential energy can be regarded as a constant $V(x_i)$. In the limit, as the divisions become finer and finer, a continuous variation will be recovered. A symmetric double-well potential is shown in Fig. 1. If the potential at the transaction points is very much larger than energies of relevant levels, the effects of transaction could be negligible. Assuming that $x_{t1}, x_{t2}, -x_{t1}$, and $-x_{t2}$ are classical turning points, we divide the regions $(0,x_{t1})$, (x_{t1},x_{t2}), and (x_{t2},x_s) into l, m, and n layers with the corresponding width d_l, d_m, and d_n, respectively. The same treatment will be copied to the left part, i.e., $(-x_s,0)$ of the double-well potential, due to its geometrical symmetry.

In the classical allowed regions $(-x_{t2}<x<-x_{t1})$ and $(x_{t1}<x<x_{t2})$, the field has an oscillatory character, so the transfer matrix corresponding to the jth segment can be written as [10]

$$M_j=\begin{bmatrix} \cos(\kappa_j d_m) & -\frac{1}{\kappa_j}\sin(\kappa_j d_m) \\ \kappa_j \sin(\kappa_j d_m) & \cos(\kappa_j d_m) \end{bmatrix}, \quad j=l+1,l+2,\ldots,l+m, \tag{1}$$

where

$$\kappa_j=\sqrt{2m^*(E-V_j)}/\hbar, \tag{2}$$

κ_j and V_j represent the wave number and the potential energy at the jth segment, respectively, m^* is the particle mass, and E is the energy eigenvalue.

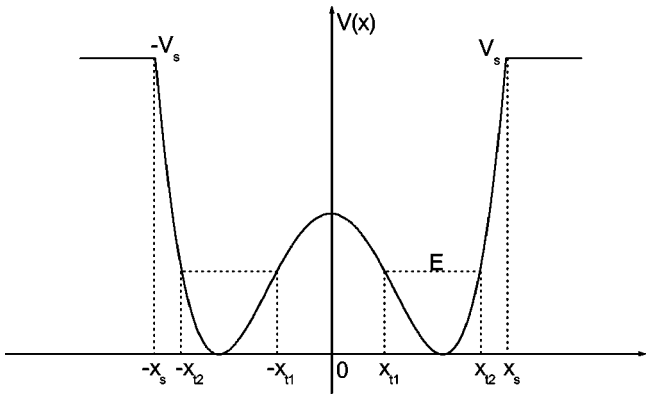

FIG. 1. One-dimensional symmetric double-well potential. E is the ground-state energy, $\pm x_s$ are the truncation points, $\pm x_{t1}$ and $\pm x_{t2}$ are the inner and outer classical turning points corresponding to E, respectively.

Because of the evanescent character in the classical forbidden regions $(x<-x_{t2})$, $(-x_{t1}<x<0)$, $(0<x<x_{t1})$, and $(x>x_{t2})$, the transfer matrices corresponding to the ith and kth segments become

$$M_i=\begin{bmatrix} \cosh(\alpha_i d_l) & -\frac{1}{\alpha_i}\sinh(\alpha_i d_l) \\ -\alpha_i\sinh(\alpha_i d_l) & \cosh(\alpha_i d_l) \end{bmatrix},$$
$$i=1,2,\ldots,l \tag{3}$$

and

$$M_k=\begin{bmatrix} \cosh(\alpha_k d_n) & -\frac{1}{\alpha_k}\sinh(\alpha_k d_n) \\ -\alpha_k\sinh(\alpha_k d_n) & \cosh(\alpha_k d_n) \end{bmatrix},$$
$$k=l+m+1,l+m+2,\ldots,l+m+n, \tag{4}$$

where

$$\alpha_j=\sqrt{2m^*(V_i-E)}/\hbar,$$
$$\alpha_k=\sqrt{2m^*(V_k-E)}/\hbar. \tag{5}$$

Applying the boundary conditions at $x=x_s$ and $x=-x_s$, we can get the matrix equation according to the geometrical symmetry,

$$\begin{bmatrix} \psi(x_{-s}) \\ \psi'(x_{-s}) \end{bmatrix}=\left[\prod_{k=l+m+n}^{l+m+1} M_k\right]\left[\prod_{k=l+m}^{l+1} M_j\right]\left[\prod_{i=l}^{1} M_i\right]\left[\prod_{i=1}^{l} M_i\right]\times\left[\prod_{j=l+1}^{l+m} M_j\right]\left[\prod_{k=l+m+1}^{l+m+n} M_k\right]\begin{bmatrix} \psi(x_s) \\ \psi'(x_s) \end{bmatrix}. \tag{6}$$

The prime of the wave function ψ denotes differentiation with respect to x. Since we have regarded the potential energies as constants V_s and V_{-s}, respectively, in the transaction regions $(x<-x_s)$ and $(x>x_s)$, the wave functions decay exponentially with displacement along the x axis:

$$\psi(x)=\begin{cases} A_{-s}\exp[P_{-s}(x+x_s)], & x<-x_s \\ A_s\exp[-P_s(x-x_s)], & x>x_s, \end{cases} \tag{7}$$

where $P_{-s}=P_s=\sqrt{2m^*(V_s-E)}/\hbar$ according to the system symmetry.

By using Eq. (7), Eq. (6) can be changed into

$$[-P_s\ 1]\left[\prod_{k=l+m+n}^{l+m+1} M_k\right]\left[\prod_{k=l+m}^{l+1} M_j\right]\left[\prod_{i=l}^{1} M_i\right]\left[\prod_{i=1}^{l} M_i\right]\times\left[\prod_{j=l+1}^{l+m} M_j\right]\left[\prod_{k=l+m+1}^{l+m+n} M_k\right]\begin{bmatrix} 1 \\ -P_s \end{bmatrix}=0. \tag{8}$$

After direct algebraic manipulations, Eq. (8) can be written as

$$[-P_{l+1}\ 1]\left[\prod_{i=l}^{1} M_i\right]\left[\prod_{i=1}^{l} M_i\right]\begin{bmatrix} 1 \\ -P_{l+1} \end{bmatrix}=0, \tag{9}$$

$$P_k=\alpha_k\frac{\sinh(\alpha_k d_n)+\frac{P_{k+1}}{\alpha_k}\cosh(\alpha_k d_n)}{\cosh(\alpha_k d_n)+\frac{P_{k+1}}{\alpha_k}\sinh(\alpha_k d_n)}, \tag{10}$$
$$k=l+m+1,l+m+2,\ldots,l+m+n,$$
$$P_{l+m+n+1}=P_s,$$
$$P_j=\kappa_j\tan\left[\tan^{-1}\left(\frac{P_{j+1}}{\kappa_j}\right)-\kappa_j d_m\right],\quad j=l+1,l+2,\ldots,l+m. \tag{11}$$

We can obtain the equation from Eq. (11) by using the similar method developed in Ref. [11],

$$\sum_{j=l+1}^{l+m}\kappa_j d_m+\Phi(s)=N\pi+\tan^{-1}\left(\frac{P_{l+m+1}}{\kappa_{l+m}}\right)-\tan^{-1}\left(\frac{P_{l+1}}{\kappa_{l+1}}\right), \tag{12}$$

where

$$\Phi(s)=\sum_{j=l+1}^{l+m-1}\left[\Phi_j-\tan^{-1}\left(\frac{\kappa_{j+1}}{\kappa_j}\tan\Phi_{j+1}\right)\right],$$
$$\Phi_j=\tan^{-1}\left(\frac{P_j}{\kappa_j}\right). \tag{13}$$

$\Phi(s)$ is the phase contribution devoted by the scattered subwaves [10]. P_{l+m+1} is the equivalent exponentially decaying coefficient of the regions $(x<-x_{t2})$ and $(x>x_{t2})$. The expression of P_{l+1} is also determined by the rest of the matrices corresponding to the region of the central barrier $(-x_{t1}<x<x_{t1})$.

In order to obtain a clear equation for the split energy eigenvalues, by employing the same manipulations as previous process to the further investigation, Eq. (9) can be changed into

$$[-P_2\ 1]\begin{bmatrix} \cosh(2\alpha_1 d_l) & -\frac{1}{\alpha_1}\sinh(2\alpha_1 d_l) \\ -\alpha_1\sinh(2\alpha_1 d_l) & \cosh(2\alpha_1 d_l) \end{bmatrix}\begin{bmatrix} 1 \\ -P_2 \end{bmatrix}=0. \tag{14}$$

P_2 is defined by

$$P_i=\alpha_i\frac{\sinh(\alpha_i d_l)+\frac{P_{i+1}}{\alpha_i}\cosh(\alpha_i d_l)}{\cosh(\alpha_i d_l)+\frac{P_{i+1}}{\alpha_i}\sinh(\alpha_i d_l)},\quad i=2,3,\ldots,l, \tag{15}$$

then we have the following equation from Eq. (14):

$$\tanh(2\alpha_1 d_l)=-\frac{2\alpha_1 P_1}{\alpha_1^2+P_1^2}, \tag{16}$$

which has two solutions

$$\tanh(\alpha_1 d_l) = -\frac{P_2}{\alpha_1}, \tag{17}$$

$$\coth(\alpha_1 d_l) = -\frac{P_2}{\alpha_1}. \tag{18}$$

Combining Eqs. (17) and (15), finally we have the expression for P_{l+1}

$$P_{i+1} = -\alpha_i \tanh\Phi_i, \quad i = 2,3,\ldots,l, \tag{19}$$

$$\tanh\Phi_i = \frac{\tanh(\alpha_i d_l) + \frac{\alpha_{i-1}}{\alpha_i}\tanh\Phi_{i-1}}{1 + \frac{\alpha_{i-1}}{\alpha_i}\tanh(\alpha_{i-1} d_l)\tanh(\alpha_i d_l)},$$

$$\tanh\Phi_1 = \tanh(\alpha_1 d_l).$$

Thus, Eq. (12) can be changed into

$$\sum_{j=l+1}^{l+m} \kappa_j d_m + \Phi(s) = N\pi + \tan^{-1}\left(\frac{P_{l+m+1}}{\kappa_{l+m}}\right) + \tan^{-1}\left(\frac{\alpha_l}{\kappa_{l+1}}\tanh\Phi_l\right). \tag{20}$$

According to the conclusion developed in Ref. [10], the second and the third terms on the right-hand side of Eq. (20) represent the half-phase losses at the outer turning points $\pm x_{t2}$ and inner turning points $\pm x_{t1}$, respectively.

Likewise, by performing a similar deducting in the case of the second solution, it is obtained as

$$\sum_{j=l+1}^{l+m} \kappa_j d_m + \Phi(s) = N\pi + \tan^{-1}\left(\frac{P_{l+m+1}}{\kappa_{l+m}}\right) + \tan^{-1}\left(\frac{\alpha_l}{\kappa_{l+1}}\coth\Phi_l\right), \tag{21}$$

where

$$P_{i+1} = -\alpha_i \coth\Phi_i, \quad i = 2,3,\ldots,l, \tag{22}$$

$$\coth\Phi_i = \frac{\tanh(\alpha_i d_l) + \frac{\alpha_{i-1}}{\alpha_i}\coth\Phi_{i-1}}{1 + \frac{\alpha_{i-1}}{\alpha_i}\coth(\alpha_{i-1} d_l)\tanh(\alpha_i d_l)},$$

$$\coth\Phi_1 = \coth(\alpha_1 d_l).$$

In order to simplify the above equations, letting $l,m,n \to \infty$ and $d_l, d_m, d_n \to 0$, then $\kappa_{l+m} \to 0$ and $\tan^{-1}(P_{l+m+1}/\kappa_{l+m}) \to \pi/2$, we may consequently write Eqs. (20) and (21) as

$$\int_{x_{t1}}^{x_{t2}} \kappa(x)dx + \Phi(s) = \left(N + \frac{1}{2}\right)\pi + \tan^{-1}\left(\frac{\alpha_l}{\kappa_{l+1}}\tanh\Phi_l\right), \tag{23}$$

TABLE I. Eigenvalues of the two split states from the ground state in the double-well potential.

λ	Exact	Present
0.02	1.39352758504	1.39352759203
	1.39352758715	1.39352759414
0.04	1.37112223656	1.37112224729
	1.37130846161	1.37130847236
0.10	1.23450716279	1.23450717706
	1.34694086892	1.34694088632
0.15	1.06249924796	1.06249926237
	1.42108689054	1.42108691499
0.20	0.94175034208	0.94175034299
	1.53553020408	1.53553022368

$$\int_{x_{t1}}^{x_{t2}} \kappa(x)dx + \Phi(s) = \left(N + \frac{1}{2}\right)\pi + \tan^{-1}\left(\frac{\alpha_l}{\kappa_{l+1}}\coth\Phi_l\right). \tag{24}$$

Thus we obtain the two quantization conditions for the split energy levels in a symmetric double-well potential. It is clear that for any certain quantum number N, there will be two different energy eigenvalues corresponding to Eqs. (23) and (24). The difference of the two energy eigenvalues is just the energy splitting. If the two potential wells are infinitely separated, which means that the quantum tunnelling is negligible, the quantization condition in either well can be written as $\int_{x_{t1}}^{x_{t2}} \kappa(x)dx + \Phi(s) = (N + \frac{1}{2} + \frac{1}{2})\pi$ [10]. In order for the tunnelling not to vanish, the half-phase losses at the inner turning points $\pm x_{t1}$ are substituted by $\tan^{-1}[(\alpha_l/\kappa_{l+1})\tanh\Phi_l]$ and $\tan^{-1}[(\alpha_l/\kappa_{l+1})\coth\Phi_l]$, which correspond to the symmetric and antisymmetric energy levels. So, these two split energy levels are derived from the corresponding level of the original single potential well.

We would like to point out that the above derivation is general, it does not involve any approximations such as the conventional short-wave limit or long-wave limit. It is exact.

III. NUMERICAL COMPARISON

In order to illustrate the accuracy of our method, we apply it to a typical example of a symmetric double-well potential, which has the potential form as

$$V(x) = \lambda x^4 - kx^2. \tag{25}$$

Here we set the particle mass $m = \frac{1}{2}$, $\hbar = 1$, and $k = 1$. We calculate the energy eigenvalues via the quantization conditions for the case of ground state and compare them with the exact values obtained by the nonperturbative method [4]. Table I shows the details.

It is clear that our numerical results are in excellent agreement with the exact results. The absolute errors ($|E^{calculate} - E^{exact}|$) are only about 10^{-8}. Since we just divided the whole potential profile ($-x_s < x < x_s$) into 10^4 layers in current calculations, more accurate results can be expected

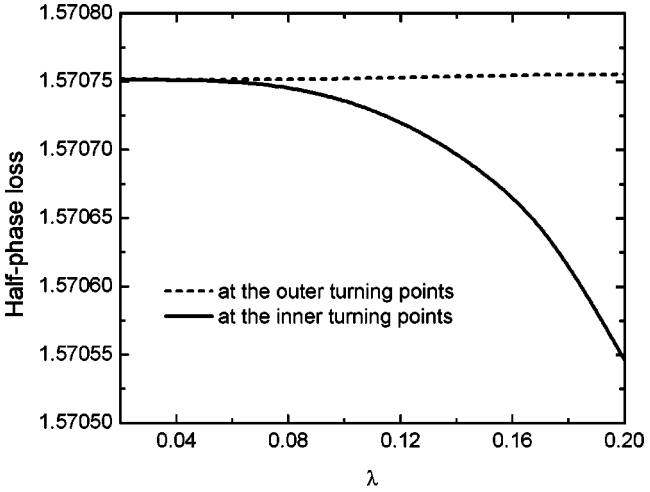

FIG. 2. Half-phase loss at the turning points to the ground state as a function of λ. The whole potential profile $(-x_s<x<x_s)$ is divided into 10^9 layers. The dashed line represents the half-phase loss at the outer turning points and the solid line represents the half phase loss at the inner turning points.

through finer divisions. Compared with other numerical methods such as the Numerov method [5] and the symplectic scheme-shooting method (SSSM) [6], whose results have the absolute errors about 10^{-6}, our method not only presents the explicit split of energy levels but also achieves the better accuracy. Moreover, it is noticed during our calculation that, when the separation between the two potential minima is too small, for instance, in the case of $\lambda=0.2$, the antisymmetric energy level will be higher than the height of the central barrier. Hereby we can only calculate the symmetric energy eigenvalue. However, if we utilize the quantization conditions for any arbitrary potential wells $\int_{-x_{t2}}^{x_{t2}}\kappa(x)dx+\Phi(s)=(N+1)\pi$ [10] to calculate the antisymmetric energy eigenvalue, energy splitting can still be obtained.

Finally, we will discuss the half-phase losses at the turning points $\pm x_{t1}$ and $\pm x_{t2}$. According to the analysis of Ref. [10], if the two potential minima are infinitely separated, the half-phase losses at both the inner and outer turning points will approach $\pi/2$ with the increase of the layer number. When the two potential wells approach, the half-phase losses at the inner turning points $\pm x_{t1}$ strongly depend on the quantum tunnelling. With the increase of λ, which means the tunnelling is more and more appreciable, the deviation from $\pi/2$ of the half-phase losses at $\pm x_{t1}$ also increases, while the half-phase losses at $\pm x_{t2}$ almost keep constant. This is illustrated in Fig. 2.

IV. SUMMARY

We have derived the quantization conditions for energy splitting of symmetric double-well potentials by the analytic transfer matrix method. The half-phase losses at the outer turning points are $\pi/2$, while those at the inner points are smaller than $\pi/2$ and strongly depend on the quantum tunnelling, which is totally different from the WKB method and other modified WKB methods. With the aid of the correct phase losses and the phase contribution of subwaves, theoretically, as the number of segment layer approaches infinitely, the exact results can be obtained.

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