Explicit expression for the reflection and transmission probabilities through an arbitrary potential barrier

2008 J. Phys. A: Math. Theor. 41 465301

(http://iopscience.iop.org/1751-8121/41/46/465301)

J. Phys. A: Math. Theor. **41** (2008) 465301 (7pp) doi:10.1088/1751-8113/41/46/465301

Explicit expression for the reflection and transmission probabilities through an arbitrary potential barrier

Pengyi Su[1,2,3], **Zhuangqi Cao**[1,2], **Kaisheng Chen**[1,2], **Cheng Yin**[1,2] **and Qishun Shen**[1,2]

[1] Department of Physics, State Key Laboratory on Fiber-Optic Local Area Network and Advanced Optical Communication Systems, Shanghai Jiao Tong University, Shanghai 200240, People's Republic of China
[2] R&D Center, SemiMask Corporation, Shanghai 200233, People's Republic of China

E-mail: patton.su@semimask.com

Received 21 April 2008, in final form 23 September 2008
Published 16 October 2008
Online at stacks.iop.org/JPhysA/41/465301

Abstract
Without solving the Schrödinger equation, exact and general expressions of the reflection and transmission probabilities for a quantum particle through an arbitrary potential barrier are presented by using the analytical transfer matrix method. It is seen that in addition to the parameters of the ambience and both the start and the final point of the barrier, the unique dependence on the formulae is the total phase shift accumulated by the mainwaves and the subwaves.

PACS numbers: 04.20.Jb, 73.40.Gk

1. Introduction

Quantum tunneling which is associated with a quantum particle through a potential barrier is a subject of profound importance in many areas of physics [1–5]. One of the reasons for an increased interest in the problem is that recent advances in molecular-beam-epitaxy (MBE) technology have opened up new possibilities of building next-generation nanometer-scale electronic devices [6]. On the other hand, a better fundamental understanding of quantum transport theory becomes an urgent challenge. The most straightforward method to study the quantum tunneling is to solve the Schrödinger equation, such as solving numerically the time-dependent Schrödinger equation by the use of the numerical techniques [7, 8] and the analytical approximations [9–12]. However, since exact solutions of the Schrödinger equation are not possible except for a few of the simplest potentials, theoretical description of the tunneling problems, even in its basic one-dimensional form, turns out to be rather difficult. There has been a large amount of literature on the subject, in which, either an approximate or a numerical approach is used. No doubt that using numerical methods one gets the solution to the

[3] Author to whom any correspondence should be addressed.

desired accuracy, but a considerable deal of physical insight is lost in the process. Among the approximate methods, the most famous method is certainly the semiclassical WKB approach [13]. In addition to the quantum mechanics, it has been widely used in various branches of physics, such as, nuclear physics, solid-state physics and, in particular, atomic physics. However, the WKB approximation is essentially restricted to slowly varying potential, many physically interesting situations do not fulfill the conditions of the semiclassical limit. For example, the semiclassical approach yields an oversimplified expression for the transmission amplitude through a potential barrier [14]. For these reasons, many features of quantum tunneling are found lie beyond the reach of the WKB approximations. Therefore, it is apparent that the conventional WKB method needs important modifications. Since two decade ago, various sophisticated techniques have been developed to improve the WKB method, such as the path-integral method [15], Airy function method [3], instanton method [16] and postclassical approximation [17]. Although these methods can give more accurate results than that of the WKB method, but different approaches often results in different final expressions with different valid conditions for the tunneling transmission amplitude, there is still no a generally accepted method available for calculating the quantum tunneling. In this paper, we present a general analysis of a quantum particle through an arbitrary potential barrier based on the analytical transfer matrix (ATM) method [18–20]. Although transfer matrix technique has been used to describe the transport processes and the scattering of quantum wires [21–25], however it in general acts as a numerical method but does not act as an analytical method. In our analysis, without solving the Schrödinger equation, exact and general expressions for the transmission and reflection probabilities are presented in a very explicit way. Different from the WKB method and its refined versions, subwaves, which inherently exist in an inhomogeneous system and is always neglected in the semiclassical approaches, are taken into account, results in a total phase shift of a quantum particle across an arbitrary potential barrier.

2. Theory

We start with the effective-mass approximation, time-independent Schrödinger equation,

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

where $m(x)$ represents position-dependent effective mass, and $\hbar = h/2\pi$, h is Planck's constant, $V(x)$ and $\psi(x)$ are the potential energy and the wavefunction, respectively, E represents particle energy. As shown in figure 1, consider an arbitrary potential barrier $V(x)$ is situated between $x = 0$ and $x = s$. V_0 and m_0 are the potential energy and the effective mass at $x \leqslant 0$, respectively; V_s and m_s represent the potential energy and the effective mass at $x \geqslant s$, respectively. We then divide the region $(0, s)$ into l segments with homogeneous potential energy $V_j = V(x_{j-1} + d_j/2)$ and effective mass $m_j = m(x_{j-1} + d_j/2)$ and the thickness d_j $(j = 1, 2, \ldots, l)$. According to the analytical transfer matrix (ATM) method, the transfer matrix corresponding to the jth segment can be written as

$$M(d_j)=\begin{bmatrix}\cos(\kappa_j d_j) & -\frac{m_j}{\kappa_j}\sin(\kappa_j d_j)\\ \frac{\kappa_j}{m_j}\sin(\kappa_j d_j) & \cos(\kappa_j d_j)\end{bmatrix}\qquad (j=1,2,\ldots,l), \tag{2}$$

where $\kappa_j = \sqrt{2m_j(E - V_j)}/\hbar$.

We assume that the wavefunctions at $x \leqslant 0$ and $x \geqslant s$ can be described as

$$\psi(x)=\begin{cases}A_0\exp(\mathrm{i}\kappa_0 x)+B_0\exp(-\mathrm{i}\kappa_0 x) & (x\leqslant 0)\\ A_s\exp(\mathrm{i}\kappa_s x) & (x\geqslant s),\end{cases} \tag{3}$$

where $\kappa_0 = \sqrt{2m_0(E - V_0)}/\hbar$ and $\kappa_s = \sqrt{2m_s(E - V_s)}/\hbar$.

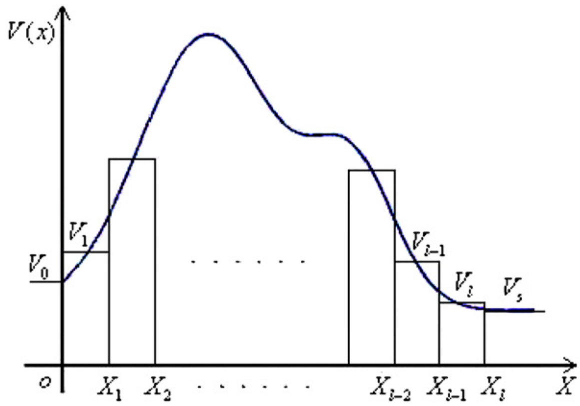

Figure 1. Arbitrary potential barrier.

On applying the boundary conditions at $x = 0$ and $x = s$, we have

$$\begin{bmatrix} \psi(0) \\ \frac{1}{m_0}\psi'(0) \end{bmatrix} = \prod_{j=1}^{l} M_j(d_j) \begin{bmatrix} \psi(s) \\ \frac{1}{m_s}\psi'(s) \end{bmatrix}, \tag{4}$$

Equation (4) can be changed into the following form:

$$\begin{bmatrix} -\frac{1}{m_0}\frac{\psi'(0)}{\psi(0)} & 1 \end{bmatrix} \prod_{j=1}^{l} M_j(d_j) \begin{bmatrix} 1 \\ \frac{1}{m_s}\frac{\psi'(s)}{\psi(s)} \end{bmatrix} = 0. \tag{5}$$

We set

$$\psi'(s)/\psi(s) = -q_s, \tag{6}$$

since $s = x_l$ $(d_j \to 0)$, the use of equation (3) yields

$$q_s = -\mathrm{i}\kappa_s. \tag{7}$$

Thus, equation (5) becomes

$$\begin{bmatrix} -\frac{\mathrm{i}\kappa_0}{m_0}\frac{A_0 - B_0}{A_0 + B_0} & 1 \end{bmatrix} \prod_{j=1}^{l} M_j(d_j) \begin{bmatrix} 1 \\ -\frac{q_s}{m_s} \end{bmatrix} = 0. \tag{8}$$

By using the similar procedures in [11], we have

$$-\frac{\mathrm{i}\kappa_0}{m_0}\frac{A_0 - B_0}{A_0 + B_0} = \frac{q_1}{m_1}, \tag{9}$$

where q_1 can be obtained from the recursion formula

$$q_j = \kappa_j \tan\left[\tan^{-1}\left(\frac{m_j}{m_{j+1}}\frac{q_{j+1}}{q_j}\right) - \kappa_j d_j\right] \qquad (j = 1, 2, \ldots, l), \tag{10}$$

and $q_{l+1} = q_s$. In order to obtain an expression with clear physical insight, we set

$$\phi_j = \tan^{-1}\left(\frac{m_j}{m_j}\frac{q_j}{\kappa_j}\right), \tag{11}$$

which, by use of equation (10), becomes

$$\begin{aligned}\phi_j &= n\pi + \tan^{-1}\left(\frac{m_j}{m_{j+1}}\frac{q_{j+1}}{\kappa_j}\right) - \kappa_j d_j \\ &= n\pi + \tan^{-1}\left(\frac{m_j}{m_{j+1}}\frac{\kappa_{j+1}}{\kappa_j}\tan\phi_{j+1}\right) - \kappa_j d_j, \\ &\quad (n = 0, 1, 2, \ldots;\ j = 1, 2, \ldots, l-1).\end{aligned} \tag{12}$$

Rearranging equation (12) yields

$$\kappa_j d_j + \left[\phi_{j+1} - \tan^{-1}\left(\frac{m_j}{m_{j+1}}\frac{\kappa_{j+1}}{\kappa_j}\tan\phi_{j+1}\right)\right] = n\pi + (\phi_{j+1} - \phi_j). \tag{13}$$

The solution for $j = l$ is

$$\kappa_l d_l = l\pi + \tan^{-1}\left(\frac{m_l}{m_s}\frac{q_s}{\kappa_l}\right) - \phi_{l.} \tag{14}$$

Using equations (13) and (14), and summing all the indices j, we have

$$\sum_{j=1}^{l}\kappa_j d_j + \sum_{j=1}^{l-1}\left[\phi_{j+1} - \tan^{-1}\left(\frac{m_j}{m_{j+1}}\frac{\kappa_{j+1}}{\kappa_j}\tan\phi_{j+1}\right)\right] = n\pi + \tan^{-1}\left(\frac{m_l}{m_s}\frac{q_s}{\kappa_l}\right) - \phi_{1,} \tag{15}$$

which gives

$$\begin{aligned}\exp(-\mathrm{i}2\phi_1) = \exp\Bigg\{\mathrm{i}2\Bigg[\sum_{j=1}^{l}\kappa_j d_j + \sum_{j=1}^{l-1}\left(\phi_{j+1} - \tan^{-1}\left(\frac{m_j}{m_{j+1}}\frac{\kappa_{j+1}}{\kappa_j}\tan\phi_{j+1}\right)\right) \\ - \tan^{-1}\left(\frac{m_l}{m_s}\frac{q_s}{\kappa_l}\right)\Bigg]\Bigg\}.\end{aligned} \tag{16}$$

By using a well-known relation between the inverse hyperbolic tangent function and the natural logarithm [26],

$$\tanh^{-1} u = \frac{1}{2}\ln\left(\frac{1+u}{1-u}\right). \tag{17}$$

According to equations (7) and (17), we have

$$\exp\left[-\mathrm{i}2\tan^{-1}\left(\frac{m_l}{m_s}\frac{q_s}{\kappa_l}\right)\right] = \frac{m_s\kappa_l - m_l\kappa_s}{m_s\kappa_l + m_l\kappa_s} = r_{ls.} \tag{18}$$

Evidently, r_{ls} denotes the reflection coefficient at the final point of potential barrier. For a continuously varying potential energy $V(x)$ and the effective mass $m(x)$, letting $l \to \infty$ $(d_j \to 0)$, we obtain

$$\sum_{j=1}^{l}\kappa_j d_j = \int_0^s \kappa(x)\,\mathrm{d}x, \tag{19}$$

$$\sum_{j=1}^{l-1}\left[\phi_{j+1} - \tan^{-1}\left(\frac{m_j}{m_{j+1}}\frac{\kappa_{j+1}}{\kappa_j}\tan\phi_{j+1}\right)\right] = \int_0^s \frac{q(\kappa m' - m\kappa')}{m(q^2+\kappa^2)}\,\mathrm{d}x, \tag{20}$$

where $q' = \mathrm{d}q/\mathrm{d}x$ and $m' = \mathrm{d}m/\mathrm{d}x$.

We have pointed out in our previous works [11] that equations (19) and (20) represent phase shifts accumulated by the main waves and the subwaves through the potential barrier, respectively.

If we define general wavenumber $K(x)$,

$$K(x) = \kappa(x) + \frac{q(\kappa m' + m\kappa')}{m(q^2 + \kappa^2)}, \tag{21}$$

which leads to

$$\exp(-\mathrm{i}2\phi_1) = r_{ls} \exp\left[\mathrm{i}2 \int_0^s K(x)\,\mathrm{d}x\right]. \tag{22}$$

Since equation (9) can be recast in the form

$$\frac{m_1\kappa_0}{m_0\kappa_1}\frac{A_0 - B_0}{A_0 + B_0} = \frac{\mathrm{i}q_1}{\kappa_1}, \tag{23}$$

we then obtain

$$r = \frac{B_0}{A_0} = \frac{r_{01} + \exp(-\mathrm{i}2\phi_1)}{1 + r_{01}\exp(-\mathrm{i}2\phi_1)}. \tag{24}$$

where

$$r_{01} = \frac{m_1\kappa_0 - m_0\kappa_1}{m_1\kappa_0 + m_0\kappa_1}. \tag{25}$$

Which represents the reflection coefficient at the start point of the potential barrier. Combining equations (22) and (24), we finally obtain the reflection coefficient of a quantum particle through an arbitrary potential barrier,

$$r = \frac{r_{01} + r_{ls}\exp\left[\mathrm{i}2\int_0^s K(x)\,\mathrm{d}x\right]}{1 + r_{01}r_{ls}\exp\left[\mathrm{i}2\int_0^s K(x)\,\mathrm{d}x\right]}. \tag{26}$$

The reflection and the transmission probabilities can easily be expressed as $R = rr^*$ and $T = 1 - R$, respectively.

We would like to emphasize that (i) the general wavenumber $K(x)$ in equation (26) contains another function $q(x) = -\psi'(x)/\psi(x)$, which looks like to relate the solution of the Schrödinger equation. In fact, $q(x)$can be completely specified by equations (7) and (10) without solving the Schrödinger equation, therefore, equation (26) is a closed expression. (ii) The algorithm proposed in this paper is general, it does not involve any approximations. The expression of the reflection coefficient, which is presented in a simple and explicit form, is exact. (iii) In addition to the parameters of the ambience, the start point and the final point of the potential barrier, the unique dependence on the reflection coefficient is the total phase shift accumulated by the mainwaves and the subwaves. (iv) Different from the semiclassical approaches, this method is free from the 'stumbling blocks' of turning points; moreover, it is not subject to the requirement of the de Broglie wavelength and the range of the energy E. As a consequence, this expression may extensively be applied to many basic quantum phenomena, such as quantum tunneling, quantum reflection, the time related to a tunneling particle and the resonant tunneling.

3. Special case

In order to illustrate the reliability of our results, test calculations have been performed with a potential profile

$$V(x) = \frac{V_0}{\cosh^2(\alpha x)} \qquad (V_0 > 0), \tag{27}$$

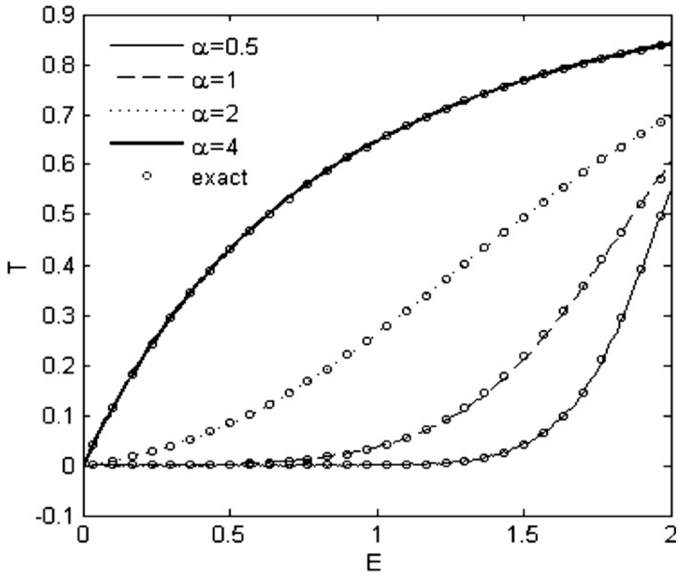

Figure 2. Transmission probability as a function of the incident particle energy for the potential (27) with $V_0 = 2$.

for which the exact expression for transmission probability is known by Landau and Lifshitz [7] and can be written as

$$T = \frac{\sinh^2\left(\frac{\pi\kappa}{\alpha}\right)}{\sinh^2\left(\frac{\pi\kappa}{\alpha}\right) + \cosh^2\left(\frac{\pi}{2}\sqrt{1-\frac{8mV_0}{\hbar^2\alpha^2}}\right)}. \qquad (28)$$

The calculation results of equation (28) and the proposed expression are plotted in figure 2. It is demonstrated that the numerical results for the ATM method and equation (28) are exactly same for arbitrary settled accuracy, as long as the segments of the potential are divided finer enough in the proposed scheme. The validity of the formula is also well examined in quantum tunneling and resonant tunneling for several typical potential barriers.

4. Conclusion

In conclusion, the analytical transfer matrix (ATM) method is used to treat one-dimensional quantum problems. Owing to the consideration of the phase shift contributed by the subwaves, which inherently exist in the inhomogeneous potential and is always neglected in the semiclassical approaches, exact and general expressions of the reflection and transmission probabilities for a quantum particle through an arbitrary potential barrier are presented in a closed and clear form.

Acknowledgment

This work was supported by the National Nature Science Foundation of China under grants 60677029.

References

[1] Ferry D K and Goodnick S M 1997 *Transport in Nanostructures* (Cambridge: Cambridge University Press)
[2] Leo J and Toombs G A 1991 *Phys. Rev.* B **43** 9944
[3] Roy S, Ghatak A K, Goyal I C and Gallawa R L 1993 *IEEE J. Quantum Electron.* **29** 340
[4] Steinberg A M 1995 *Phys. Rev. Lett.* **27** 2405
[5] Hagino K and Balantekin A B 2004 *Phys. Rev.* A **70** 032106
[6] Chebotarev L V 1998 *Phys. Stat. Sol.* B **208** 69
[7] Stovneng J A and Hauge E H 1991 *Phys. Rev.* B **44** 13582
[8] Konsek S L and Pearsall T P 2003 *Phys. Rev.* B **67** 045306
[9] Garcla-CalderOn G and Rubio A 1997 *Phys. Rev.* A **55** 3361
[10] Yamada N, Garcla-CalderOn G and Villavicencio J 2005 *Phys. Rev.* A **72** 012106
[11] Wulf U and Skalozub V V 2005 *Phys. Rev.* B **72** 165331
[12] Villavicencio J, Romo R and Cruz E 2007 *Phys. Rev.* A **75** 012111
[13] Berry M V and Mount K E 1972 *Rep. Prog. Phys.* **35** 315
[14] Landau L D and Lifshitz E M 1965 *Quantum Mechanics (Non-Relativistic Theory)* (Oxford: Pergamon)
[15] Sokolovski D, Brouard S and Connor J N L 1994 *Phys. Rev.* A **50** 1240
[16] Holstein B R 1996 *Am. J. Phys.* **64** 1061
[17] Chebotarev L V 1997 *Eur. J. Phys* **18** 188
[18] Cao Z, Liu Q, Shen Q, Dou X and Chen Y 2001 *Phys. Rev.* A **63** 054103
[19] Zhou F, Cao Z and Shen Q 2003 *Phys. Rev.* A **67** 062112
[20] Ou Y C, Cao Z and Shen Q 2004 *J. Chem. Phys.* **121** 1
[21] James H M 1949 *Phys. Rev.* B **76** 1602
[22] Mello P A, Pereyra P and Kumar N 1988 *Ann. Phys., NY* **181** 290
[23] Pereyra P and Castillo E 2002 *Phys. Rev.* B **65** 205120
[24] Garcla-CalderOn G, Romo R and Rubio A 1993 *Phys. Rev.* B **47** 9572
[25] Garcla-CalderOn G, Romo R and Rubio A 1997 *Phys. Rev.* B **56** 4845
[26] Azzam R M A and Bashara N M 1977 *Ellipsometry and Polarized Light* (Amsterdam: North-Holland)