The analytical transfer matrix method for quantum reflection*

Xu Tian(许 田)[a)†], Cao Zhuang-Qi(曹庄琪)[b)], and Fang Jing-Huai(方靖淮)[a)]

[a)] *Physics Department, Nantong University, Nantong* 226001, *China*
[b)] *Institute of Optics and Photonics, Shanghai Jiao Tong University, Shanghai* 200240, *China*

(Received 12 June 2008; revised manuscript received 4 July 2009)

In this paper, the analytical transfer matrix method (ATMM) is applied to study the properties of quantum reflection in three systems: a sech^2 barrier, a ramp potential and an inverse harmonic oscillator. Our results agree with those obtained by Landau and Lifshitz [Landau L D and Lifshitz E M 1977 *Quantum Mechanics (Non-relativistic Theory)* (New York: Pergamon)], which proves that ATMM is a simple and effective method for quantum reflection.

Keywords: analytical transfer matrix method, quantum reflection, reflection coefficient, transmission coefficient, reflection time

PACC: 0365S, 0365G

1. Introduction

With the development of experiments, we can obtain accurate velocities of atoms by advanced cooling[1−3] and launching[4] techniques. The atoms can be described by the adjustable potential that drives us to consider the quantum nature of the dynamics. Quantum reflection is an important effect which happens to an atom moving through a classically allowed region without reaching a classical turning point.[5] This effect is sometimes caused by the long range part of an atom-surface interaction. So it avoids the incident atom interacting with shorter-range forces and being scattered or adsorbed.[6]

The analytical transfer matrix method (ATMM) has taken into account the phase contribution of the sub-waves, and is used to prove that the phase shift at the classical turning point is exactly equal to π in Ref. [7]. Here we apply the ATMM to two situations: 1) $E \leq V_{\max}$, 2) $E > V_{\max}$. Corresponding to the classical reflection, the former is always considered as a good approximation. The latter belongs to the category of quantum reflection. The WKB approximation is helpless in such a situation, but the ATMM makes us solve the problems of quantum reflection easily. In Section 2, we introduce the theory of the ATMM. In Section 3, the ATMM is applied to a sech^2 barrier, a ramp potential and the inverse harmonic oscillator respectively. Then, we define a quantum reflection time t_{R} which is calculated in the above two instances. Finally, the conclusion and discussion are presented.

2. Analytical transfer matrix method

Now we introduce ATMM,[7−12] which will be applied in the next section.

In the one-dimensional potential $V(x)$, the wave function $\psi(x)$ satisfies the Schrödinger equation

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

where μ is the mass of a particle. In Fig. 1, $\psi(x)$ is in the region of $[x_0, x_m]$. Now we divide this region $[x_0, x_m]$ into m layers with the width d. The transfer matrix in each layer can be written as[7]

$$\boldsymbol{M}_j = \begin{bmatrix} \cos(k_j d) & -\dfrac{1}{k_j}\sin(k_j d) \\ k_j \sin(k_j d) & \cos(k_j d) \end{bmatrix}, \quad j = 1, 2, \ldots, m, \tag{2}$$

the matrix equation is

$$\begin{bmatrix} \psi(x_0) \\ \psi'(x_0) \end{bmatrix} = \prod_{j=1}^{m} M_j \begin{bmatrix} \psi(x_m) \\ \psi'(x_m) \end{bmatrix}. \tag{3}$$

The wave number $k_j = \sqrt{2\mu(E - V_j)}/\hbar$. We assume that $x_0 = 0$ and the particle is incident on the potential from the left, then the wave function for $x < x_0$

*Project supported by Science Foundation of Nantong University (Grant Nos. 03080122 and 09ZY001).
†Corresponding author. E-mail: tianxu@gmail.com
© 2010 Chinese Physical Society and IOP Publishing Ltd

and $x > x_m$ can be written as

$$\psi(x) = \begin{cases} A_0\,\mathrm{e}^{\mathrm{i}k_0 x} + B_0\,\mathrm{e}^{-\mathrm{i}k_0 x}, & x < 0, \\ A_{m+1}\,\mathrm{e}^{\mathrm{i}k_{m+1}x}, & x > x_m. \end{cases} \tag{4}$$

where i is in imaginary units. Depending on the boundary condition at x_0 and x_m, we can change Eq. (3) into

$$\left[-\frac{\psi'(x_0)}{\psi(x_0)}, 1\right] \prod_{j=1}^{m} M_j \begin{bmatrix} 1 \\ \dfrac{\psi'(x_m)}{\psi(x_m)} \end{bmatrix} = 0. \tag{5}$$

Defining

$$-P_j = \frac{\psi'(x_j)}{\psi(x_j)}, \tag{6}$$

and applying Eq. (4) into Eq. (5), then we obtain

$$\left[-\mathrm{i}k_0 \frac{A_0 - B_0}{A_0 + B_0}, 1\right] \prod_{j=1}^{m} M_j \begin{bmatrix} 1 \\ -P_{m+1} \end{bmatrix} = 0, \tag{7}$$

$$P_1 = -\mathrm{i}k_0 \frac{A_0 - B_0}{A_0 + B_0}, \tag{8}$$

$$-P_{m+1} = \mathrm{i}k_{m+1}, \tag{9}$$

$$P_j = k_j \tan\left[\tan^{-1}\left(\frac{P_{j+1}}{k_j}\right) - k_j d\right], \quad j = 1, 2, \ldots, m. \tag{10}$$

Let $\phi_j = \tan^{-1}(P_j/k_j)$ and P_j is replaced by Eq. (10),

$$\phi_j = l_j\pi + \tan^{-1}\left(\frac{P_{j+1}}{k_j}\right) - k_j d, \quad j = 1, 2, \ldots, m-1, l_j = 0, \pm 1, \pm 2, \ldots. \tag{11}$$

Sorting Eq. (11), we get

$$k_j d + \left[\phi_{j+1} - \tan^{-1}\left(\frac{k_{j+1}\tan\phi_{j+1}}{k_j}\right)\right] = l_j\pi + (\phi_{j+1} - \phi_j). \tag{12}$$

If $j = m$ in Eq. (12), we can obtain

$$k_m d = l_m\pi + \tan^{-1}\left(\frac{P_{m+1}}{k_m}\right) - \phi_m. \tag{13}$$

Integrating Eq. (12) with Eq. (13) and summing j, we obtain

$$\sum_{j=1}^{m} k_j d + \sum_{j=1}^{m-1}\left[\phi_{j+1} - \tan^{-1}\left(\frac{k_{j+1}\tan\phi_{j+1}}{k_j}\right)\right] = l\pi + \tan^{-1}\left(\frac{P_{m+1}}{k_m}\right) - \phi_1. \tag{14}$$

Equation (14) can be written as

$$\begin{aligned} &\exp(-\mathrm{i}2\phi_1) \\ &= \exp\left(\mathrm{i}2\left\{\sum_{j=1}^{m} k_j d + \sum_{j=1}^{m-1}\left[\phi_{j+1} - \tan^{-1}\left(\frac{k_{j+1}\tan\phi_{j+1}}{k_j}\right)\right] - \tan^{-1}\left(\frac{P_{m+1}}{k_m}\right)\right\}\right). \end{aligned} \tag{15}$$

For an arbitrary potential[12]

$$\sum_{j=1}^{m} k_j d = \int_0^{x_m} k(x)\,\mathrm{d}x, \tag{16}$$

$$\sum_{j=1}^{m-1}\left[\phi_{j+1} - \tan^{-1}\left(\frac{k_{j+1}\tan\phi_{j+1}}{k_j}\right)\right] = \int_0^{x_m} \frac{P}{P^2 + k^2}\frac{\mathrm{d}k}{\mathrm{d}x}\,\mathrm{d}x, \tag{17}$$

$$\begin{aligned} &\exp\left[-\mathrm{i}2\tan^{-1}\left(\frac{P_{m+1}}{k_m}\right)\right] \\ &= \exp\left[-\mathrm{i}2\tan^{-1}\left(\frac{-\mathrm{i}k_{m+1}}{k_m}\right)\right] \\ &= \frac{k_m - k_{m+1}}{k_m + k_{m+1}} \\ &= r_{m,m+1}, \end{aligned} \tag{18}$$

so

$$\begin{aligned} &\exp(-\mathrm{i}2\phi_1) \\ &= r_{m,m+1}\cdot\exp\left[\mathrm{i}2\int_0^{x_m}\left(k + \frac{P}{P^2 + k^2}\frac{\mathrm{d}k}{\mathrm{d}x}\right)\mathrm{d}x\right]. \end{aligned} \tag{19}$$

Multiplying $1/k_1$ at both sides of Eq. (8), we get

$$\frac{\mathrm{i}P_1}{k_1} = \frac{k_0}{k_1}\frac{A_0 - B_0}{A_0 + B_0}, \tag{20}$$

then acquire the reflection coefficient easily

$$\begin{aligned} &R_{\mathrm{ATMM}} \\ &= \frac{B_0}{A_0} \\ &= \frac{r_{01} + \exp(-\mathrm{i}2\phi_1)}{1 + r_{01}\exp(-\mathrm{i}2\phi_1)} \\ &= \frac{r_{01} + r_{m,m+1}\exp\left[\mathrm{i}2\displaystyle\int_0^{x_m} H(x)\,\mathrm{d}x\right]}{1 + r_{01}r_{m,m+1}\exp\left[\mathrm{i}2\displaystyle\int_0^{x_m} H(x)\,\mathrm{d}x\right]}, \end{aligned} \tag{21}$$

where

$$r_{01} = (k_0 - k_1)/(k_0 + k_1), \tag{22}$$

and the total wave vector

$$H(x) = k + \frac{P}{P^2 + k^2}\frac{\mathrm{d}k}{\mathrm{d}x}, \tag{23}$$

where the first term in the above equation is the wave vector of the dominant scattering wave and the second one is the contribution of the scattering sub-wave between the neighbouring layers in Fig. 1.

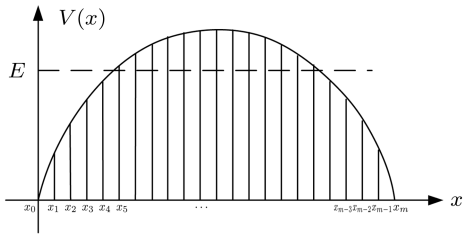


Fig. 1. Arbitrary potential $V(x)$, $x_{0,m}$ are truncation points.

The reflection coefficient $R_{\mathrm{ATMM}} = |R_{\mathrm{ATMM}}|\,\mathrm{e}^{\mathrm{i}\delta(E)}$, in which $\delta(E)$ is the phase of R_{ATMM}. $|R_{\mathrm{ATMM}}|^2$ is the reflection probability.

3. Application

In this part, we apply Eq. (5) to two simple examples at first.

A sech^2 barrier: $V(x) = V_0\mathrm{sech}^2(ax)$.

A ramp potential: $V(x) = V_0/(1 + \mathrm{e}^{-ax})$.

We obtain the corresponding potentials for the above two systems in Figs. 2 and 3 respectively. Figures 2 and 3 show that $V_0 = V_{\max}$, where $V_{\max}$ is the height of the potentials. For simplicity, we let $\hbar = m = 1$. Reflection coefficients can be obtained easily by Eqs. (21)–(23). Given some values of V_0, we get the results in Figs. 4 and 5. In general, reflection coefficients become smaller when E gets larger and $E \leq V_{\max}$. When V_0 gets larger and E is near or above $V_{\max}$, the shape of reflection probability $|R_{\mathrm{ATMM}}|^2$ does not change. Thus quantum reflection occurs.

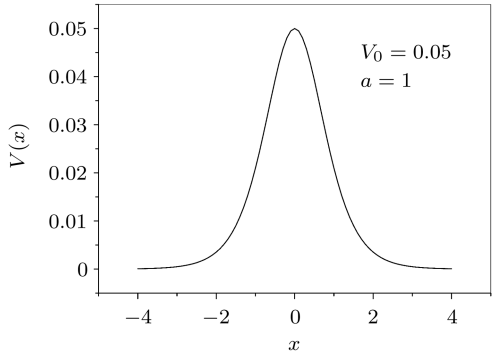


Fig. 2. Potential for the sech^2 barrier as a function of the coordinate x when $V_0 = 0.05$ and $a = 1$.

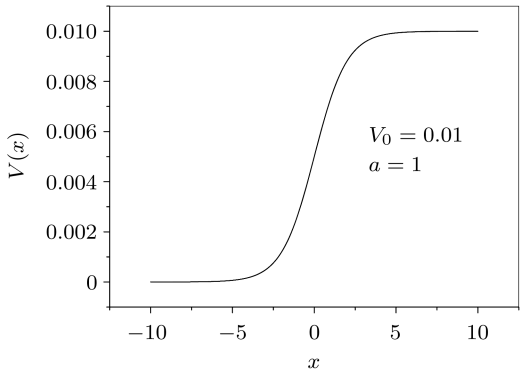


Fig. 3. Plot of the ramp potential as a function of the coordinate x when $V_0 = 0.01$ and $a = 1$.

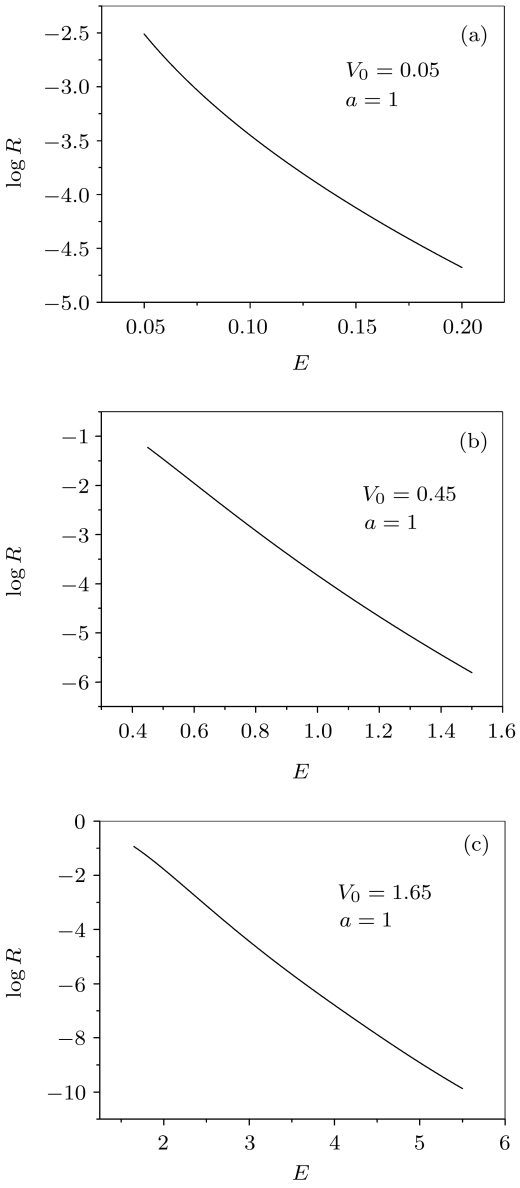


Fig. 4. Reflection coefficients for the sech^2 barrier: (a) $V_0 = 0.05$ and $a = 1$; (b) $V_0 = 0.45$ and $a = 1$; (c) $V_0 = 1.65$ and $a = 1$.

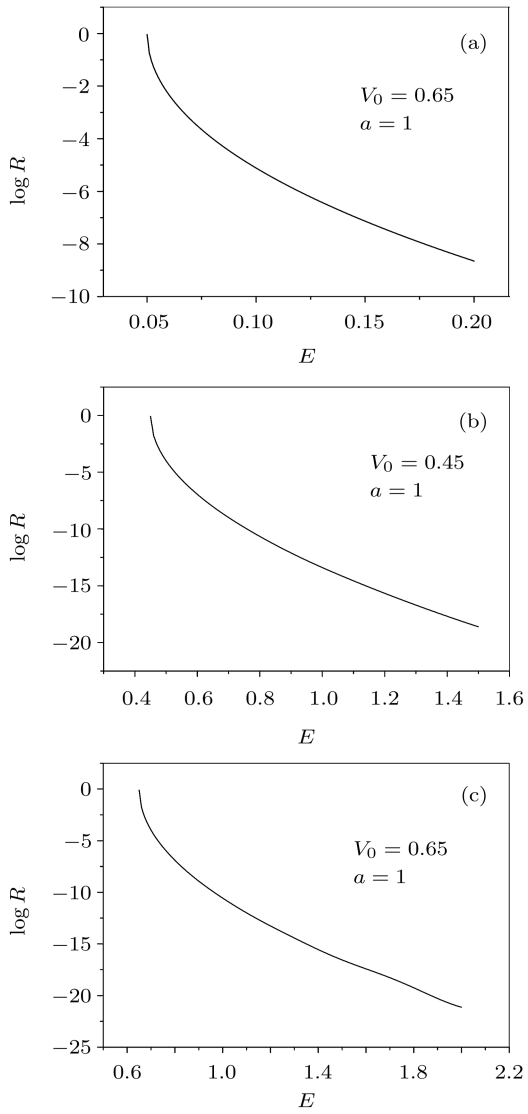


Fig. 5. Reflection coefficients for the ramp potentials: (a) $V_0 = 0.05$ and $a = 1$; (b) $V_0 = 0.45$ and $a = 1$; (c) $V_0 = 0.65$ and $a = 1$.

In order to use the ATMM in more general problems, we compute the nonclassical transmission in the inverse harmonic oscillator, when E is near or above $V_{\max}$. Here the tunneling coefficient is similar to the reflection coefficient, where $T_{\rm ATMM} = |T_{\rm ATMM}|\,{\rm e}^{{\rm i}\eta}$ and η is the phase of $T_{\rm ATMM}$. The reflection and the transmission probability, i.e., $|R_{\rm ATMM}|^2$ and $|T_{\rm ATMM}|^2$ satisfy $\mid T_{\rm ATMM} \mid^2 = 1 - \mid R_{\rm ATMM} \mid^2$. So

$$\begin{aligned} &\mid T_{\rm ATMM} \mid^2 \\ &= 1 - \mid R_{\rm ATMM} \mid^2 \\ &= 1 - \left| \frac{r_{01} + r_{m,m+1} \exp\left[{\rm i}2 \int_0^{x_m} H(x)\,{\rm d}x \right]}{1 + r_{01} r_{m,m+1} \exp\left[{\rm i}2 \int_0^{x_m} H(x)\,{\rm d}x \right]} \right|^2 . \end{aligned} \tag{24}$$

Figure 6 shows the potential of the inverse harmonic oscillator $V(x) = V_0 - 0.5x^2$. Figure 7 is the transmission probability through the inverse harmonic oscillator for different V_0. The transmission probability gets larger when the incident energy increases. If E is larger to an extent, the transmission probability converges to 1 gradually. In contrast, the reflection probability is convergent to 0 by degrees. These results show that quantum reflection occurs in the 'turning point' at which the particle reverses its direction of motion. The 'turning point' is in the complex coordinate, that is, the complex root of the equation $V(x) = E$.

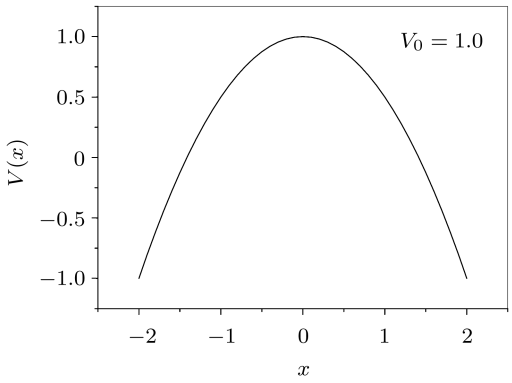
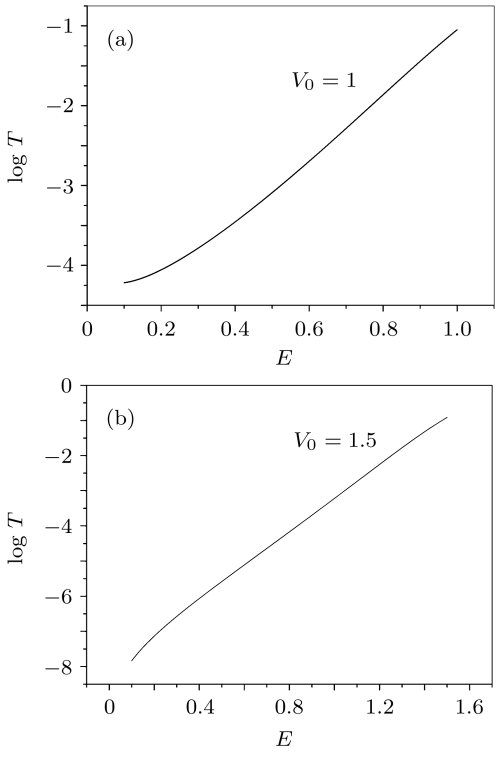


Fig. 6. Plot of the inverse harmonic oscillator as a function of the coordinate x when $V_0 = 1.0$.



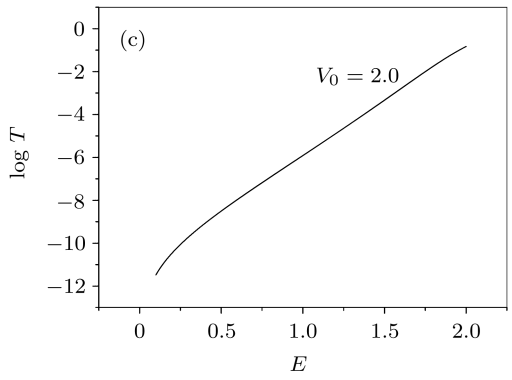


Fig. 7. Transmission coefficients for the inverse harmonic oscillator: (a) $V_0 = 1.0$; (b) $V_0 = 1.5$; (c) $V_0 = 2.0$.

We define another parameter $t_{\rm R}$ as quantum reflection time, where $t_{\rm R}$ is the time for the occurrence of quantum reflection when $E > V_{\max}$. Here,

$$t_{\rm R} = \hbar\,|R|^2 \left(\frac{{\rm d}\delta}{{\rm d}E}\right). \tag{25}$$

Equation (25) is applied to the sech^2 barrier and the ramp potential. The corresponding results are shown in Figs. 8 and 9. The quantum reflection time $t_{\rm R}$ decreases with the increase of the incident energy E. For the sech^2 barrier, $t_{\rm R}$ gets larger when a decreases in Fig. 8, whereas it is very interesting that $t_{\rm R}$ increases with the enhancement of a for the ramp potential. In Fig. 9, the separations between $t_{\rm R}$ for different a are small when $E \leqslant 0.05$ or $E \geqslant 0.15$. However, the separation is large when E is small for the sech^2 barrier in Fig. 8. If E increases to an extent, we can obtain $t_{\rm R} \longrightarrow 0$ easily from Figs. 8 and 9.

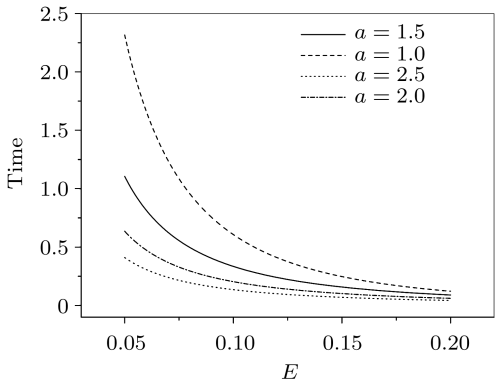


Fig. 8. Plot of quantum reflection time as a function of the coordinate E for the sech^2 barrier with different a: $a = 1$; $a = 1.5$; $a = 2$; $a = 2.5$.

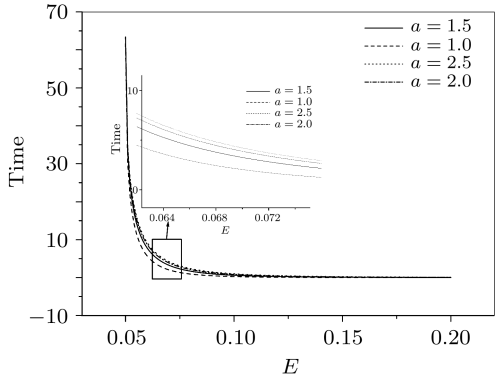


Fig. 9. Plot of quantum reflection time as a function of the coordinate E for the ramp potential with different a: $a = 1$; $a = 1.5$; $a = 2$; $a = 2.5$.

4. Conclusions

In this work, we have extended the ATMM to compute the quantum reflection coefficient and reflection time for the sech^2 barrier and the ramp potential. In addition, the ATMM is successfully applied to calculate the transmission probability in the inverse harmonic oscillator. As E increases and is larger than $V_{\max}$, the reflection coefficient decreases gradually until it converges to zero. In contrast, the tunneling coefficient increases to 1 by degrees. No matter how the parameter V_0 changes, the shapes of the reflection probability or transmission probability are similar when $E \leqslant V_{\max}$ or E is larger than $V_{\max}$. When E changes near or above $V_{\max}$, the change of reflection probability or transmission probability is continuous. During the changes, quantum reflection happens. In the sech^2 barrier, there is an inequality among quantum reflection times: $t_{{\rm R}_{a=1}} > t_{{\rm R}_{a=1.5}} > t_{{\rm R}_{a=2}} > t_{{\rm R}_{a=2.5}}$. However, in the ramp potential, there is a contrasting relation: that is, $t_{{\rm R}_{a=1}} < t_{{\rm R}_{a=1.5}} < t_{{\rm R}_{a=2}} < t_{{\rm R}_{a=2.5}}$. Since 2001, the ATMM has been used as a powerful tool for atomic physics to calculate the energies and the problem of scattering phase shift in the interaction between particles. This is the first attempt for us to apply the ATMM to investigate the properties of quantum reflection. However, the WKB approximation cannot be used in this situation. We look forward to finding more properties in the context of this field by this method.

References

[1] Kasevich M and Chu S 1992 *Phys. Rev. Lett.* **69** 1741

[2] Lawall J, Bardou F, Saubamea B, Shimizu K, Leduc M, Aspect A and Cohen-Tannoudji C 1994 *Phys. Rev. Lett.* **73** 1915

[3] Reichel J, Bardou F, Ben-Dahan M, Peik E, Rand S, Solomon C and Cohen-Tannoudji C 1995 *Phys. Rev. Lett.* **75** 4575

[4] Dahan M B, Peik E, Reichel J, Castin Y and Salomon C 1996 *Phys. Rev. Lett.* **76** 4508

[5] Jurisch A and Friedrich H 2004 *Phys. Rev.* A **70** 032711

[6] Friedrich H, Jacoby G and Meister C G 2002 *Phys. Rev.* A **65** 032902

[7] Cao Z Q, Liu Q, Shen Q S, Dou X M and Chen Y L 2001 *Phys. Rev.* A **63** 054103

[8] Xu T, Cao Z Q and Shen Q S 2005 *Chin. Phys. Lett.* **22** 2746

[9] Xu T, Cao Z Q, Shen Q S and Zhu G L 2006 *Chin. Phys.* **15** 1172

[10] Xu T, Cao Z Q and Fang J H 2008 *Chin. Phys.* B **17** 4379

[11] He Y, Cao Z Q and Shen Q S 2004 *Chin. Phys. Lett.* **21** 2089

[12] Ou Y C, Cao Z Q and Shen Q S 2004 *J. Chem. Phys.* **121** 8175