Reflection and transmission coefficients from the superposition of various potentials

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Abstract. The reflection and transmission coefficients describe the behavior of the matter wave incident on a potential barrier. They can be expressed in terms of the probability with which the matter wave can be reflected or transmitted. The central equation accounting for the behavior of the matter wave is the Schrödinger equation. The Schrödinger equation is the second order partial differential equation. However, in a stationary state, the Schrödinger equation is reduced to the time independent Schrödinger equation. This time independent Schrödinger equation is the second order linear ordinary differential equation. Since the time independent Schrödinger equation is linear, superposition of any of the two solutions to the time independent Schrödinger equation is also a solution. In this paper, we focus on the superposition of various potentials. The reflection and transmission coefficients from the superposition of various potentials are obtained. A comparison between the exact coefficients and those obtained by the $2 \times 2$ transfer matrix is made. The relationship between the transmission coefficient of the superposed potential and that of each individual potential is found. The results show that the transmission coefficient obtained from the $2 \times 2$ transfer matrix is of a lower bound on the exact transmission coefficient.

1. Introduction

Quantum mechanics describes the behaviors of small particles not seen by our eyes such as those in atoms and molecules. The central equation in quantum mechanics is the Schrödinger equation by which the behaviors of these small particles are governed [1, 2, 3, 4, 5, 6, 7, 8]. Using the Schrödinger equation, the behavior of a particle is described by its wave function. Many physical phenomena in quantum mechanics have motion in one dimension such as the scattering of particles from a potential. In this scattering problem, what fraction of particles is transmitted and what fraction is reflected are calculated. They are called reflection coefficient and transmission coefficient, respectively. One of the potentials in scattering problems is a rectangular barrier potential [9, 10]. One might ask what happen if there is more than one barrier. A. Dutt and S. Kar analyzed quantum mechanical tunnelling across smooth double barrier potentials [11]. G. Rastelli derived a useful and succinct expression for the tunnelling amplitude $\nu$ in asymmetric double-well potentials [12]. He found that there are no systematic effects of asymmetry on quantum tunneling. V. Jelic and F. Marsiglio obtained eigenenergies and eigenstate for a square double well potential and a parabolic double well potential [13].
They found that the particle can be viewed as being in a superposition of two states; in the first the particle is in the left well, while in the second the particle is in the right well. Ahmed Z. et.al. studied a general double Dirac delta potential [14]. Their results showed that the general double Dirac delta potential is the simplest solvable potential to introduce double wells, avoided crossings, resonances and perfect transmission. Cai C. and Zhu R. studied transport properties of the nonadiabatically pumped double-quantum-well (DQW) structure [15]. They found that two Fano resonances are excited while one of the Floquet sidebands coincides with the bonding and antibonding quasibound states, respectively. J. Boos, V. P. Frolov, and A. Zelnikov discussed scattering and resonant states of the ghost-free scalar massless particle in the presence of a \( \delta \)-like potential [16]. They demonstrated that the quantum mechanical scattering of a particle on a \( \delta \)-like potential is exactly solvable. In this paper, the reflection and transmission coefficients for superposition of various potentials will be investigated.

This paper is organized as follows. In section 2, the Schrödinger equation is solved, and the reflection and transmission coefficients are obtained for the superposition of various potentials. In section 3, the rigorous bounds on the reflection and transmission coefficients are calculated. Finally, conclusions are given in section 4.

2. Scattering problem in one dimension

Many physical phenomena in quantum mechanics have motion in one dimension. These phenomena are governed by the Schrödinger equation in one dimension

\[
\frac{i\hbar}{\partial t} \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t),
\]

where \( \Psi(x,t) \) is a wave function of a particle, \( m \) is the particle’s mass, \( \hbar \) is the reduced Plank constant, and \( V(x,t) \) is the particle’s potential energy.

Mathematically, the Schrödinger equation is the second order partial differential equation. However, in a stationary state, the Schrödinger equation is reduced to the time-independent Schrödinger equation

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

where \( \psi(x) \) is a time-independent wave function of a particle, \( E \) is the particle’s total energy and \( V(x) \) is the particle’s time-independent potential energy. The time-independent Schrödinger equation can be solved if the potential energy \( V(x) \) is specified.

This time-independent Schrödinger equation is the second order linear ordinary differential equation. Since the time-independent Schrödinger equation is linear, superposition of any of the two solutions to the time-independent Schrödinger equation is also a solution.

In this paper, the superposition of various potentials is chosen to solve the time-independent Schrödinger equation given above. Moreover, an unbound state, where the total energy is greater than the potential energy \( E > V(x) \), is focused on.

2.1. Rectangular double barrier potential

A rectangular double barrier potential is the superposition of two rectangular barrier potentials. It is given by

\[
V(x) = \begin{cases} 
0, & x < a \\
V_1, & a \leq x \leq b \\
0, & b < x < c \\
V_2, & c \leq x \leq d \\
0, & x > d
\end{cases}
\]
Figure 1. The rectangular double barrier potential with \( a = 1, b = 2, c = 4, d = 7, V_1 = 2.5, \) and \( V_2 = 3.5. \)

The rectangular double barrier potential is plotted as shown in Figure 1. The solution to the time-independent Schrödinger equation with this rectangular double barrier potential is given by

\[
\psi(x) = \begin{cases} 
Ae^{ikx} + Be^{-ikx}, & x < a \\
Ce^{iK_1x} + De^{-iK_1x}, & a \leq x \leq b \\
Ee^{ikx} + Fe^{-ikx}, & b < x < c \\
Ge^{iK_2x} + He^{-iK_2x}, & c \leq x \leq d \\
Ie^{ikx}, & x > d 
\end{cases}
\]

where

\[
k = \sqrt{\frac{2mE}{\hbar^2}}, \quad K_1 = \sqrt{\frac{2m}{\hbar^2}(E - V_1)}, \quad \text{and} \quad K_2 = \sqrt{\frac{2m}{\hbar^2}(E - V_2)}. \tag{2}
\]

The boundary conditions are the continuity of the wave functions and their first derivatives. At point \( a, \) we have

\[
Ae^{ika} + Be^{-ika} = Ce^{iK_1a} + De^{-iK_1a} \\
ika Ae^{ika} - ikBe^{-ika} = iK_1Ce^{iK_1a} - iK_1De^{-iK_1a}. \tag{3}
\]

At point \( b, \) we have

\[
Ce^{iK_1b} + De^{-iK_1b} = Ee^{ikb} + Fe^{-ikb} \\
iK_1Ce^{iK_1b} - iK_1De^{-iK_1b} = ikEe^{ikb} - ikFe^{-ikb}.
\]

At point \( c, \) we have

\[
Ee^{ikc} + Fe^{-ikc} = Ge^{iK_2c} + He^{-iK_2c} \\
ika Ee^{ikc} - ikFe^{-ikc} = iK_2Ge^{iK_1c} - iK_2He^{-iK_2c}.
\]
At point \( d \), we have
\[
G e^{iK_2d} + He^{-iK_2d} = I e^{ikd},
\]
\[
iK_2Ge^{iK_2d} - iK_2He^{-iK_2d} = ikIe^{ikd}.
\]  
(4)

Let us now evaluate the reflection and transmission coefficients, \( R \) and \( T \), as defined by
\[
R = \left| \frac{J_{\text{ref}}}{J_{\text{inc}}} \right| \quad \text{and} \quad T = \left| \frac{J_{\text{tra}}}{J_{\text{inc}}} \right|,
\]  
(5)

where \( J_{\text{ref}} \) is a reflected current density, \( J_{\text{tra}} \) is a transmitted current density, and \( J_{\text{inc}} \) is an incident current density. The current density is given by
\[
J = \frac{i\hbar}{2m} \left[ \psi(x) \frac{d\psi^*(x)}{dx} - \psi^*(x) \frac{d\psi(x)}{dx} \right].
\]

Therefore, we obtain
\[
J_{\text{ref}} = \frac{i\hbar}{2m} \left[ \psi_{\text{ref}}(x) \frac{d\psi_{\text{ref}}^*(x)}{dx} - \psi_{\text{ref}}^*(x) \frac{d\psi_{\text{ref}}(x)}{dx} \right] = -\frac{\hbar k}{m} |B|^2,
\]
where
\[
\psi_{\text{ref}}(x) = Be^{-ikx}.
\]

Similarly,
\[
J_{\text{tra}} = \frac{\hbar k}{m} |I|^2 \quad \text{and} \quad J_{\text{inc}} = \frac{\hbar k}{m} |A|^2.
\]

From equation (5), the reflection and transmission coefficients are given by
\[
R = \frac{|B|^2}{|A|^2} \quad \text{and} \quad T = \frac{|I|^2}{|A|^2}.
\]

Solving equations (3) - (4), we obtain
\[
T = \frac{64k^2K_2^2}{|\alpha|^2},
\]
where
\[
\alpha = \left\{ 2kK_2 \cos[K_2(d - c)] - i \left( k^2 + K_2^2 \right) \sin[K_2(d - c)] \right\} \times
\]
\[
\left\{ 2kK_1 \cos[K_1(b - a)] - i \left( k^2 + K_1^2 \right) \sin[K_1(b - a)] \right\}
\]
\[
\times e^{-ik(d+c)+ik(b-a)} kK_1
\]
\[
+ \left( k^2 - K_1^2 \right) \left( k^2 - K_2^2 \right) \sin[K_1(b - a)] \sin[K_2(d - c)]
\]
\[
e^{-ik(d-c)-ik(b+a)} kK_1.
\]

2.2. Parabolic double barrier potential

A parabolic double barrier potential is the superposition of two parabolic barrier potentials. It is given by
\[
V(x) = \begin{cases} 
0, & x < a \\
(1/2)m\omega^2(x - b)^2, & a \leq x \leq c \\
0, & c < x < d \\
(1/2)m\omega^2(x - c)^2, & d \leq x \leq f \\
0, & x > f 
\end{cases}
\]  
(6)
Figure 2. The parabolic double barrier potential with $a = 1$, $b = 1.5$, $c = 2$, $d = 4$, $e = 5.5$, $f = 7$, $m = 3$, and $\omega = 1.1$.

The parabolic double barrier potential is plotted as shown in Figure 2. The solution to the time-independent Schrödinger equation with this parabolic double barrier potential is given by

$$
\psi(x) = \begin{cases} 
Ae^{ikx} + Be^{-ikx} & , x < a \\
Cf(x)e^{m\omega(x-b)^2/2h} + Df(x)e^{-m\omega(x-b)^2/2h} & , a \leq x \leq c \\
Ee^{ikx} + F e^{-ikx} & , c < x < d \\
Gf(x)e^{m\omega(x-e)^2/2h} + Hf(x)e^{-m\omega(x-e)^2/2h} & , d \leq x \leq f \\
Ie^{ikx} & , x > f
\end{cases}
$$

where $k$ is given by equation (2) and $f(x)$ is given by power series.

3. The rigorous bound on the transmission probability

In some complicated cases where the exact reflection and transmission coefficients cannot be obtained, their rigorous bounds can be found. These bounds can provide some qualitative understanding despite the potential energy of a complicated form.

The general formula of the rigorous bounds on the reflection and transmission coefficients derived from the method of $2 \times 2$ transfer matrix are given by [17, 18, 19, 20, 21, 22]

$$
R \leq \tanh^2 \left( \int_{-\infty}^{\infty} \frac{\sqrt{[h'(x)]^2 + \left( \frac{2m}{\hbar^2} \{ E - V(x) \} - h^2(x) \}^2 } 2h(x) \, dx \right)
$$

and

$$
T \geq \text{sech}^2 \left( \int_{-\infty}^{\infty} \frac{\sqrt{[h'(x)]^2 + \left( \frac{2m}{\hbar^2} \{ E - V(x) \} - h^2(x) \}^2 } 2h(x) \, dx \right),
$$

where $h(x)$ is a positive function which satisfies

$$
h(\pm \infty) = \sqrt{\frac{2m}{\hbar^2} [E - V(\pm \infty)]}.
$$
If a potential energy asymptotically vanishes $V(\pm \infty) = 0$, the simple choice we can adopt is $h(x) = k$, where $k$ is given in equation (2). Therefore,

$$R \leq \tanh^2 \left( \frac{m}{\hbar^2} \int_{-\infty}^{\infty} |V(x)| \, dx \right) \quad \text{and} \quad T \geq \text{sech}^2 \left( \frac{m}{\hbar^2} \int_{-\infty}^{\infty} |V(x)| \, dx \right).$$

### 3.1. Rectangular double barrier potential

Since the rectangular double barrier potential energy $V(x)$, given by equation (1), is always non-negative, the absolute sign can be removed

$$R \leq \tanh^2 \left( \frac{m}{\hbar^2} \int_a^d V(x) \, dx \right) \quad \text{and} \quad T \geq \text{sech}^2 \left( \frac{m}{\hbar^2} \int_a^d V(x) \, dx \right).$$

By substituting $V(x)$ from equation (1) and performing an integration, we obtain

$$R \leq \tanh^2 \left[ \frac{m}{\hbar^2} \{V_1(b - a) + V_2(d - c)\} \right] \quad \text{and} \quad T \geq \text{sech}^2 \left[ \frac{m}{\hbar^2} \{V_1(b - a) + V_2(d - c)\} \right]. \quad (7)$$

From the hyperbolic function identities,

$$\tanh(x + y) = \frac{\tanh(x) + \tanh(y)}{1 + \tanh(x) \tanh(y)} \quad (8)$$

and

$$\text{sech}(x + y) = \left[ \frac{1}{\text{sech}(x) \text{sech}(y)} + \left\{ \frac{1}{\text{sech}^2(x)} - 1 \right\} \left\{ \frac{1}{\text{sech}^2(y)} - 1 \right\} \right]^{-1}, \quad (9)$$

we can obtain the relationship between the reflection and transmission coefficients of the superposed potential and those of individual potentials. From equation (7), this relationship is given by [23]

$$R \leq \frac{R_1 + 2\sqrt{R_1 R_2} + R_2}{1 + 2\sqrt{R_1 R_2} + R_1 R_2} \quad \text{and} \quad T \geq \left[ \frac{1}{\sqrt{T_1 T_2} + \sqrt{\left( \frac{1}{T_1} - 1 \right) \left( \frac{1}{T_2} - 1 \right)}} \right]^{-2},$$

where $R_1$ and $R_2$ are the rigorous bounds on the reflection coefficients for potential $V_1$ and potential $V_2$, respectively, given by

$$R_1 \leq \tanh^2 \left[ \frac{mV_1}{\hbar^2}(b - a) \right] \quad \text{and} \quad R_2 \leq \tanh^2 \left[ \frac{mV_2}{\hbar^2}(d - c) \right]$$

and $T_1$ and $T_2$ are the rigorous bounds on the transmission coefficients for potential $V_1$ and potential $V_2$, respectively, given by

$$T_1 \geq \text{sech}^2 \left[ \frac{mV_1}{\hbar^2}(b - a) \right] \quad \text{and} \quad T_2 \geq \text{sech}^2 \left[ \frac{mV_2}{\hbar^2}(d - c) \right].$$

Figure 3 shows the variation in the rigorous bounds on the transmission coefficients for the rectangular double barrier potential, with potential $V_1$ in the left panel and potential $V_2$ in the right panel. The rigorous bounds decrease with increasing potential $V_1$ or potential $V_2$.

Figure 4 shows the variation in the rigorous bounds on the transmission coefficients for the rectangular double barrier potential, with the width of potential $V_1$ in the left panel and the width of potential $V_2$ in the right panel. The rigorous bounds decrease with the increase in the width of potential $V_1$ or the width of potential $V_2$.

From equation (7), the rigorous bounds on the transmission coefficients for the rectangular double barrier potential vary with the height and the width of individual potentials, but not with the separation between them.
Figure 3. The rigorous bounds on the transmission coefficients for the rectangular double barrier potential with $a = 1$, $b = 2$, $c = 4$, $d = 7$, and $m = 3$. In the left panel, potential $V_1$ is fixed at 2.5, while potential $V_2$ varies. In the right panel, potential $V_2$ is fixed at 3.5, while potential $V_1$ varies.

Figure 4. The rigorous bounds on the transmission coefficients for the rectangular double barrier potential with $b = 2$, $c = 4$, $V_1 = 2.5$, $V_2 = 3.5$, and $m = 3$. In the left panel, the width of potential $V_2$ is fixed, while the width of potential $V_1$ varies. In the right panel, the width of potential $V_1$ is fixed, while the width of potential $V_2$ varies.

3.2. Parabolic double barrier potential

Since the parabolic double barrier potential energy $V(x)$, given by equation (6), is always non-negative, the absolute sign can be removed

$$R \leq \tanh^2 \left( \frac{m}{\hbar^2} \int_a^f V(x)dx \right) \quad \text{and} \quad T \geq \text{sech}^2 \left( \frac{m}{\hbar^2} \int_a^f V(x)dx \right).$$
By substituting $V(x)$ from equation (6) and performing an integration, we obtain

$$R \leq \tanh^2 \left[ \frac{m^2 \omega^2}{6kh^2} \left\{ (c - b)^3 - (a - b)^3 + (f - e)^3 - (d - e)^3 \right\} \right]$$

and

$$T \geq \text{sech}^2 \left[ \frac{m^2 \omega^2}{6kh^2} \left\{ (c - b)^3 - (a - b)^3 + (f - e)^3 - (d - e)^3 \right\} \right].$$

From the hyperbolic function identities, equations (8) and (9), we can obtain the relationship between the reflection and transmission coefficients of the superposed potential and those of individual potentials. From equations (10) and (11), this relationship is given by

$$R \leq R_1 + 2\sqrt{R_1R_2 + R_1R_2}$$

and

$$T \geq \left[ \frac{1}{T_1T_2} + \sqrt{\frac{1}{T_1^2} - 1} \left( \frac{1}{T_2^2} - 1 \right) \right]^{-2},$$

where $R_1$ and $R_2$ are the rigorous bounds on the reflection coefficients for potential $V_1(x) = (1/2)m\omega^2(x - b)^2$ and potential $V_2(x) = (1/2)m\omega^2(x - e)^2$, respectively, given by

$$R_1 \leq \tanh^2 \left[ \frac{m^2 \omega^2}{6kh^2} \left\{ (c - b)^3 - (a - b)^3 \right\} \right] \quad \text{and} \quad R_2 \leq \tanh^2 \left[ \frac{m^2 \omega^2}{6kh^2} \left\{ (f - e)^3 - (d - e)^3 \right\} \right]$$

and $T_1$ and $T_2$ are the rigorous bounds on the transmission coefficients for potential $V_1(x) = (1/2)m\omega^2(x - b)^2$ and potential $V_2(x) = (1/2)m\omega^2(x - e)^2$, respectively, given by

$$T_1 \geq \text{sech}^2 \left[ \frac{m^2 \omega^2}{6kh^2} \left\{ (c - b)^3 - (a - b)^3 \right\} \right] \quad \text{and} \quad T_2 \geq \text{sech}^2 \left[ \frac{m^2 \omega^2}{6kh^2} \left\{ (f - e)^3 - (d - e)^3 \right\} \right].$$

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{The left panel shows the rigorous bounds on the transmission coefficients for the parabolic double barrier potential with $a = 1$, $c = 2$, $d = 4$, $e = 5.5$, $f = 7$, $\omega = 1.1$, and $m = 3$. The right panel shows the maximum values of potential $V_1(x)$.}
\end{figure}

Figure 5 shows the variation in the rigorous bounds on the transmission coefficients for the parabolic double barrier potential, with the maximum value of potential $V_1(x)$. The rigorous bounds decrease with the increase in the maximum value of potential $V_1(x)$. Similarly, the rigorous bounds decrease with the increase in the maximum value of potential $V_2(x)$ as shown in Figure 6.
Figure 6. The left panel shows the rigorous bounds on the transmission coefficients for the parabolic double barrier potential with $a = 1$, $b = 1.5$, $c = 2$, $d = 4$, $f = 7$, $\omega = 1.1$, and $m = 3$. The right panel shows the maximum of potential $V_2(x)$.

4. Conclusions

In this paper, the reflection and transmission coefficients from the superposition of the rectangular potentials and the superposition of the parabolic potentials are obtained. The results show that for a rectangular double barrier potential, the rigorous bounds on these coefficients decrease with the increase in the height and the width of the individual potentials, but remain unchanged when the separation distance between the individual potential changes. For a parabolic double barrier potential, the rigorous bounds on these coefficients decrease with the increase in the maximum value of the individual potentials.

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