Reflection and transmission resonances and accuracy of the WKB method

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Abstract

In this paper, we calculate the transmission and reflection amplitudes of wave functions for different potentials such as the delta function, the rectangular barrier, the Eckart potential, and the Hulthen potential. We describe the relationship between these amplitudes and compute the reflection resonances between each potential. We describe the transmission and reflection probabilities using the WKB formula and compare the results with ones obtained from matching the boundary conditions. Furthermore, we use a two by two transfer matrix to calculate a rigorous bound on the transmission and reflection probabilities.

Keywords: Resonance, The WKB method

1 Introduction

One-dimensional quantum problems widely appear in any textbook on quantum mechanics \cite{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16}. Although they are simple in mathematics and clear in physics, they lead to important and new results \cite{17, 18, 19, 20, 21, 22, 23}. In physics, there are a number of applications of one-dimensional quantum problems. For example, in acoustics, one might be interested in the propagation of sound waves down a long pipe, while in electromagnetism, one might be interested in the physics of wave-guides \cite{23}.

In this paper, we study one-dimensional quantum problems for four selected potentials, the delta function, the rectangular barrier, the Eckart potential, and the Hulthen potential \cite{24}. We will calculate exact and approximate transmission and reflection probabilities by matching boundary conditions and by using the WKB method respectively, and compare
them to each other. We will also use a $2 \times 2$ transfer matrix to obtain a rigorous bound on these probabilities. Moreover, we will derive resonances of transmission and reflection probabilities.

## 2 Conventions

We are interested in solving the time-independent Schrödinger equation \([1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16]\),

\[
-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \psi(x) = E \psi(x). \tag{1}
\]

We concentrate on a potential which is asymptotically constant, that is $V(x) \to V_{\pm \infty}$ as $x \to \pm \infty$. For $E > V(x)$ for all $x$, the asymptotic wave functions are given by

\[
\psi(x) \to \begin{cases} 
  t \exp(-ik_{+\infty}x) \sqrt{k_{+\infty}}, & \text{if } x \to +\infty \\
  \sqrt{k_{-\infty}} \left( \exp(-ik_{-\infty}x) + r \exp(ik_{-\infty}x) \right) \sqrt{k_{-\infty}}, & \text{if } x \to -\infty
\end{cases}, \tag{2}
\]

where wave numbers are defined by

\[
k_{\pm \infty}^2 = \frac{2m (E - V_{\pm \infty})}{\hbar^2}. \tag{3}
\]

We identify $t$ and $r$ as transmission and reflection amplitudes respectively. Therefore, the conservation of flux leads to the condition

\[
T + R = 1, \tag{4}
\]

where $T \equiv |t|^2$ and $R \equiv |r|^2$ are transmission and reflection probabilities respectively. A position at which a transmission or reflection probability is in unity, it is thus referred to as the occurrence of resonance.

Moreover, we can obtain a rigorous bound on the transmission probabilities by using a $2 \times 2$ transfer matrix. It gives

\[
T_{\text{transmission}} \geq \text{sech}^2 \left( \frac{1}{2} \int_{x_1}^{x_2} \left| k_0 - \frac{k^2(x)}{k_0} \right| dx \right), \tag{5}
\]

where

\[
k^2(x) = \frac{2m [E - V(x)]}{\hbar^2}. \tag{6}
\]

and $k(x) \to k_0$ if $x$ is outside the interval $(x_1, x_2)$.

On the other hand, for $E < V(x)$ in the range $x_1 < x < x_2$ we can obtain the transmission probability for any potential by using a useful technique called the WKB method. The result is given by \[25\]

\[
T_w = \exp \left[ -2 \sqrt{\frac{2m}{\hbar^2}} \int_{x_1}^{x_2} \sqrt{V(x) - E} \, dx \right]. \tag{7}
\]
3 One-dimensional problems

In this section, we review main results in some one-dimensional problems. Four types of potentials are selected to discuss in this paper.

3.1 A delta function potential

A delta function potential takes the form

\[ V(x) = \alpha \delta(x), \]  

(8)

where \( \alpha \) is a positive constant and the delta function is defined by

\[ \delta(x) = \begin{cases} 0, & \text{if } x \neq 0 \\ \infty, & \text{if } x = 0 \end{cases}. \]  

(9)

We are interested in a scattering state \( E > 0 \). We define

\[ k^2 = \frac{2mE}{\hbar^2} \quad \text{and} \quad k_0 = \frac{m\alpha}{\hbar^2}. \]  

(10)

The transmission and reflection amplitudes for this potential are given by (see \cite{3,4})

\[ t = \frac{k}{k - ik_0} \quad \text{and} \quad r = \frac{ik_0}{k - ik_0}. \]  

(11)

Therefore, the transmission and reflection probabilities are

\[ T = \frac{k^2}{k^2 + k_0^2} \quad \text{and} \quad R = \frac{k_0^2}{k^2 + k_0^2}. \]  

(12)

Note that

\[ T + R = 1. \]  

(13)

The transmission and reflection probabilities varying with \( k \) are shown in Fig. \ref{fig:delta_function}. We have seen that the transmission probability tends to unify as \( k \) goes to infinity. We say, however, that this potential has no transmission resonances. On the other hand, the reflection resonances occur at \( k = 0 \). Moreover, from the plotting if the potential is strongest, the total reflection happens. That is when the potential is stronger, penetration of a particle or wave through the potential is more difficult.

3.2 Rectangular barrier potential

The rectangular barrier potential has the form (see \cite{2,7})

\[ V(x) = \begin{cases} V_0, & \text{if } |x| \leq a \\ 0, & \text{if otherwise} \end{cases}. \]  

(14)

The shape of the rectangular barrier is shown in Fig. \ref{fig:rectangular_barrier}. We are interested in two cases \( E > V_0 > 0 \) and \( V_0 > E > 0 \).
Figure 1: Plotting of transmission and reflection probabilities varying as $k$ for the delta function potential with (a) $k_0 = 1$, (b) $k_0 = 2$, (c) $k_0 = 10$, (d) $k_0 = 100$ and (e) $k_0 = 1000$. 
3.2.1 Case I: $E > V_0 > 0$

We define

$$k^2 = \frac{2mE}{\hbar^2}, \quad q^2 = \frac{2m(E-V_0)}{\hbar^2}, \quad \text{and} \quad k_0^2 = \frac{2mV_0}{\hbar^2} = k^2 - q^2.$$  \hspace{1cm} (15)

The transmission and reflection amplitudes for this potential are given by (see [13, 26])

$$t = \frac{4kq \exp(2ika)}{(k+q)^2 \exp(2iqa) - (k-q)^2 \exp(-2iqa)}$$ \hspace{1cm} (16)

and

$$r = \frac{2i(k^2 - q^2) \sin(2qa) \exp(2ika)}{(k+q)^2 \exp(2iqa) - (k-q)^2 \exp(-2iqa)}.$$ \hspace{1cm} (17)

Therefore, the transmission and reflection probabilities are

$$T = \frac{4k^2q^2}{4k^2q^2 + k_0^4 \sin^2(2qa)} \quad \text{and} \quad R = \frac{k_0^4 \sin^2(2qa)}{4k^2q^2 + k_0^4 \sin^2(2qa)}.$$ \hspace{1cm} (18)

Note that

$$T + R = 1.$$ \hspace{1cm} (19)

The transmission and reflection probabilities varying with $q$ are shown in Fig. 3 and Fig. 4. Fig. 3 compares the effects of barrier heights $V_0$ of the potential on the probabilities when the width $a$ of the potential is fixed. It has been found that the higher the barrier of the potential is, the more the number of reflection resonances. This is similar to the case of the delta function potential: penetration of a particle or wave through the potential is hard to occur when the barrier height of the potential is large. Fig. 4 compares the effects of the widths of the potential on the probabilities when the barrier height of the potential is fixed. The results are that the reflection resonance can occur when the width increases. Analytically, the transmission resonances occur at

$$q = \frac{n\pi}{2a},$$ \hspace{1cm} (20)

where $n = 1, 2, 3, \ldots$, while the reflection resonance is at $k = 0$ for this potential.

Moreover, we can obtain a lower bound of the transmission probability by using a $2 \times 2$ transfer matrix

$$T \geq \text{sech}^2\left(\frac{k_0^2a}{\sqrt{k_0^4 + q^2}}\right).$$ \hspace{1cm} (21)

This rigorous bound is compared with the exact solution in Fig. 5. It is found that the lower bound approaches the exact solution when a particle is at high energy.
3.2.2 Case II: $V_0 > E > 0$

We define

$$Q^2 = \frac{2m(V_0 - E)}{\hbar^2}.$$ \hfill (22)

The transmission and reflection amplitudes for this potential are given by

$$t = \frac{2iQke^{-2ika}}{(k^2 - Q^2)\sinh(2Qa) + 2ikQ\cosh(2Qa)}$$ \hfill (23)

and

$$r = \frac{(k^2 + Q^2)\sinh(2Qa)e^{-2ika}}{(k^2 - Q^2)\sinh(2Qa) + 2ikQ\cosh(2Qa)}. \hfill (24)$$

Therefore, the transmission and reflection probabilities are

$$T = \frac{4k^2Q^2}{(k^2 - Q^2)^2\sinh^2(2Qa) + 4k^2Q^2\cosh^2(2Qa)} \hfill (25)$$

and

$$R = \frac{k_0^4\sinh^2(2Qa)}{(k^2 - Q^2)^2\sinh^2(2Qa) + 4k^2Q^2\cosh^2(2Qa)} \hfill (26)$$

We have seen that in this case $T \neq 0$. It follows that a particle can penetrate the barrier from one side to the other although the potential energy of the particle exceeds its total energy, which does not appear in classical physics. This is called tunneling. Note that in this case

$$T + R \neq 1. \hfill (27)$$

By the WKB method, we obtain

$$T_w = \exp(-4Qa). \hfill (28)$$

In Fig. 6, the result from the WKB method is compared with the exact result. It is found that the larger the height of the potential, the more accurate the WKB approximation becomes.

3.3 An Eckart potential

The Eckart potential takes the form

$$V(x) = \frac{V_\infty + V_-\infty}{2} + \frac{V_\infty - V_-\infty}{2}\tanh\left(\frac{x}{a}\right) + \frac{V_0}{\cosh^2(x/a)}.\hfill (29)$$

The shape of the Eckart potential is shown in Fig. 7.

We define

$$k_{\pm\infty}^2 = \frac{2m(E - V_{\pm\infty})}{\hbar^2} \quad \text{and} \quad \bar{k} = \frac{k_\infty + k_-\infty}{2}. \hfill (30)$$
The transmission amplitude for this potential is given by (see [27, 28])

\[
\begin{align*}
t &= -\frac{i}{\sqrt{k_{\infty}k_{-\infty}a}} \frac{\Gamma[i\bar{ka} + (1/2) + \sqrt{(1/4) - 2mV_0a^2/\hbar^2}]}{\Gamma(i\bar{ka})} \\
&\times \frac{\Gamma[i\bar{ka} + (1/2) - \sqrt{(1/4) - 2mV_0a^2/\hbar^2}]}{\Gamma(i\bar{ka})}.
\end{align*}
\] (31)

Therefore, the transmission and reflection probabilities are

\[
\begin{align*}
T &= \frac{\sinh(\pi k_{-\infty}a) \sinh(\pi k_{\infty}a)}{\sinh^2(\pi ka) + \cos^2 \left( \pi \sqrt{(1/4) - 2mV_0a^2/\hbar^2} \right)} \quad (32) \\
\end{align*}
\]

and

\[
\begin{align*}
R &= \frac{\cosh \left[ \pi a \left( k - \sqrt{k_{\infty}^2 + k_{-\infty}^2 - k^2} \right) \right] - \cos \pi b}{\cosh \left[ \pi a \left( k + \sqrt{k_{\infty}^2 + k_{-\infty}^2 - k^2} \right) \right] - \cos \pi b},
\end{align*}
\] (33)

where \( k = \sqrt{2mE/\hbar^2} \) and \( b = \sqrt{1 - 8mV_0a^2/\hbar^2} \). Fig. 8 shows the transmission and reflection probabilities vary as \( V_0 \). Fig. 8 (a) and (b) compare the effects of \( a \) on the probabilities for \( a = 1 \) and \( a = 2 \) respectively. When \( a \) increases, the transmission probability approaches unity. Analytically, the transmission resonances occur at

\[
V_0 = -\frac{\hbar^2}{2ma^2}n(n + 1). \quad (34)
\]

In contrast, there are no reflection resonances for this potential.

### 3.4 A Hulthen potential

A Hulthen potential takes the form [29]

\[
V(x) = \theta(-x) \frac{V_0}{e^{-ax} - q} + \theta(x) \frac{V_0}{e^{ax} - q},
\] (35)

where \( V_0, a, \) and \( q \) all are real and positive with \( q < 1 \). \( \theta(x) \) is the Heaviside step function defined by

\[
\theta(x) = \begin{cases} 
1, & \text{if } x > 0 \\
0, & \text{if } x < 0
\end{cases}.
\] (36)

The shape of the Hulthen potential is shown in Fig. 9. We are interested in two cases \( E > V(x) > 0 \) and \( V(x) > E > 0 \).
3.4.1 Case I: \( E > V(x) > 0 \)

The transmission and reflection amplitudes for this potential are given, in terms of a hypergeometric function, by (see [29])

\[
    t = \frac{(1 - q)2^{\lambda}q^{2\mu}}{1 + 2\mu} \left\{ (q(1 + 2\mu)(\lambda^2 - 2\lambda\mu + \mu^2 - \nu^2)F(1 + \lambda - \mu - \nu, 1 + \lambda - \mu + \nu, 2 - 2\mu; q) 
    \right.
\]

\[
    F(\lambda + \mu - \nu, \lambda + \mu + \nu, 1 + 2\mu; q) \right\} - \{q(1 - 2\mu)(\lambda^2 + 2\lambda\mu + \mu^2 - \nu^2) 
    \]

\[
    F(1 + \lambda + \mu - \nu, 1 + \lambda + \mu + \nu, 2 + 2\mu; q)F(\lambda - \mu - \nu, \lambda - \mu + \nu, 1 - 2\mu; q) \right\} 
    \]

\[
    - \{((1 - 2\mu)(2\mu)(1 + 2\mu)F(\lambda + \mu - \nu, \lambda + \mu + \nu, 1 + 2\mu; q) 
    \right]
\]

\[
    F(\lambda - \mu - \nu, \lambda - \mu + \nu, 1 - 2\mu; q) \right\} 
    \]

\[
    /[\{q(\lambda^2 + 2\lambda\mu + \mu^2 - \nu^2)F(1 - \lambda - \mu - \nu, 1 - \lambda - \mu + \nu, 2 - 2\mu; q) 
    \right.
    \]

\[
    F(\lambda + \mu - \nu, \lambda + \mu + \nu, 1 - 2\mu; q) \right\} + \{q(\lambda^2 - 2\lambda\mu + \mu^2 - \nu^2) 
    \]

\[
    F(1 + \lambda - \mu - \nu, 1 + \lambda - \mu + \nu, 2 - 2\mu; q)F(-\lambda - \mu - \nu, -\lambda - \mu + \nu, 1 - 2\mu; q) \right\} 
    \]

\[
    - \{(2\mu)(1 - 2\mu)F(\lambda - \mu - \nu, \lambda - \mu + \nu, 1 - 2\mu; q) 
    \right]
\]

\[
    F(-\lambda - \mu - \nu, -\lambda - \mu + \nu, 1 - 2\mu; q) \right\} \] \quad (37)

and

\[
    r = -\frac{q^{1+2\mu}(\lambda^2 + 2\lambda\mu + \mu^2 - \nu^2) \sqrt{E + k}}{1 + 2\mu} \left\{ (1 + 2\mu)F(\lambda + \mu - \nu, \lambda + \mu + \nu, 1 + 2\mu; q) 
    \right.
\]

\[
    F(1 - \lambda - \mu - \nu, 1 - \lambda - \mu + \nu, 2 - 2\mu; q) \right\} + \{(1 - 2\mu) 
    \]

\[
    F(1 + \lambda + \mu - \nu, 1 + \lambda + \mu + \nu, 2 + 2\mu; q)F(-\lambda - \mu - \nu, -\lambda - \mu + \nu, 1 - 2\mu; q) \right\} 
    \]

\[
    /[\{q(\lambda^2 + 2\lambda\mu + \mu^2 - \nu^2)F(1 - \lambda - \mu - \nu, 1 - \lambda - \mu + \nu, 2 - 2\mu; q) 
    \right.
    \]

\[
    F(\lambda - \mu - \nu, \lambda - \mu + \nu, 1 - 2\mu; q) \right\} + \{q(\lambda^2 - 2\lambda\mu + \mu^2 - \nu^2) 
    \]

\[
    F(1 + \lambda - \mu - \nu, 1 + \lambda - \mu + \nu, 2 - 2\mu; q)F(-\lambda - \mu - \nu, -\lambda - \mu + \nu, 1 - 2\mu; q) \right\} 
    \]

\[
    - \{(2\mu)(1 - 2\mu)F(\lambda - \mu - \nu, \lambda - \mu + \nu, 1 - 2\mu; q) 
    \right]
\]

\[
    F(-\lambda - \mu - \nu, -\lambda - \mu + \nu, 1 - 2\mu; q) \right\} \] \quad (38)

where \( \mu = ik/a, \nu = ip/a, \lambda = iV_0/\alpha q, p^2 = (E + V_0/q)^2 - m^2, \) and \( k^2 = E^2 - m^2. \) The transmission and reflection probabilities are derived from

\[
    T = |t|^2 \quad \text{and} \quad R = |r|^2. \quad (39)
\]

We can check that

\[
    T + R = 1. \quad (40)
\]

The transmission and reflection probabilities for varying \( E \) are shown in Fig. [10] There are both transmission and reflection resonances. Fig. [10] (a) and [10] (b) describe how the diffuseness \( a \) has an effect on the probabilities with the other parameters \( m, V_0, \) and \( q \) fixed.
3.4.2 Case II: $V(x) > E > 0$

By the WKB method, we obtain

$$T_w = \exp \left[ -2\sqrt\frac{2m}{\hbar^2} \int_{-1}^{1} \sqrt{\theta(-x) \frac{V_0}{e^{-ax} - q} + \theta(x) \frac{V_0}{e^{ax} - q} - E \, dx} \right]. \quad (41)$$

Fig. 11 shows the transmission probability for different heights of the Hulthen potential. The probability decreases if the height of the Hulthen potential increases.

4 Conclusions

In this paper, we introduced a $2 \times 2$ transfer matrix for a scattering process ($E > V(x)$) and the WKB method for a tunneling phenomenon ($E < V(x)$). It is found that the WKB method is high accurate when compared to exact solutions. We could use this WKB method to find reflection and transmission probabilities for difficult potentials which may give no exact solutions.

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Figure 2: The rectangular barrier with $a = 1$ and $V_0 = 1$. 
Figure 3: The effects of barrier heights $V_0$ of the potential on the probabilities for varying $q$ in the rectangular barrier with (a) $k_0 = 1$, (b) $k_0 = 2$, (c) $k_0 = 10$, (d) $k_0 = 100$ and (e) $k_0 = 1000$ for $a = 1$. 
Figure 4: The effects of the widths $a$ of the potential on the probabilities varying as $q$ in the rectangular barrier with (a) $a = 1$, (b) $a = 2$, (c) $a = 10$, and (d) $a = 100$ for $k_0 = 1$. 
Figure 5: Plot of the transmission probability and its lower bound. $T \times 2$ denotes the lower bound derived from a $2 \times 2$ transfer matrix.
Figure 6: The exact solution of the transmission probability compared to the WKB approximation with (a) $V_0 = 1$, (b) $V_0 = 10$, (c) $V_0 = 50$, and (d) $V_0 = 100$ for $m = h = a = 1$. 
Figure 7: The Eckart potential with $V_{-\infty} = 2$, $V_{\infty} = 1$, $a = 3$, and $V_0 = -1/9$. 
Figure 8: The effects of $a$ on the probabilities varying as $V_0$ in the Eckart potential with (a) $a = 1$ and (b) $a = 2$ for $k_{-\infty} = 1$, $k_{\infty} = 2$, and $m = \hbar = 1$. 
Figure 9: The Hulthen potential with $q = 0.9$, $a = 0.5$, and $V_0 = 1$.

Figure 10: Plotting of transmission and reflection probabilities for varying $E$ for a Hulthen potential with (a) $a = 0.5$ and (b) $a = 1$ when $m = 1$, $V_0 = 1$, and $q = 0.9$. 
Figure 11: The transmission probability obtained from the WKB approximation with (a) $V_0 = 1$, (b) $V_0 = 2$, (c) $V_0 = 10$, and (d) $V_0 = 50$ for $q = 0.9$, $a = 0.5$, and $m = \hbar = 1$. 