

Scattering of Woods-Saxon Potential in Schrödinger Equation

Altuğ Arda,^{1,*} Oktay Aydoğdu,^{2,†} and Ramazan Sever^{3,‡}

¹*Department of Physics Education, Hacettepe University, 06800, Ankara, Turkey*

²*Department of Physics, Mersin University, 33343, Mersin, Turkey*

³*Department of Physics, Middle East Technical University, 06531, Ankara, Turkey*

Abstract

The scattering solutions of the one-dimensional Schrödinger equation for the Woods-Saxon potential are obtained within the position-dependent mass formalism. The wave functions, transmission and reflection coefficients are calculated in terms of Heun's function. These results are also studied for the constant mass case in detail.

Keywords: Schrödinger equation, Woods-Saxon potential, Heun Function, Scattering, Position-dependent mass

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*E-mail: arda@hacettepe.edu.tr

†E-mail: oktaydogdu@gmail.com

‡E-mail: sever@metu.edu.tr

I. INTRODUCTION

The quantum mechanical systems could be investigated in the view of two basic points. One of them is the studying of bound states to handle the necessary information about the system under consideration. The other point is solving of scattering problem for a given quantum mechanical system under the effect of a potential. So, one has to study both of bound states and scattering states of a quantum mechanical system under consideration to achieve a complete information about it. Some efforts have been made about the scattering problem for a relativistic and/or non-relativistic system under the influence of different types of potentials, such as Manning-Rosen potential [1, 2], Eckart potential [3, 4], Pöschl-Teller potential [5], Hulthén potential [6], Woods-Saxon potential [7-9], cusp potential [10], and Coulomb potential [11]. The scattering problem in the case where the mass depends on spatially coordinate has become a particular part of that problem, and has been received great attention to study of scattering states for a given quantum system [12-15]. The position-dependent mass formalism is a useful ground to explain the electronic properties of quantum wells and quantum dots [16], semiconductor heterostructures [17], and impurities in crystals [18-20].

In this paper, we solve the following one-dimensional Schrödinger equation ($\hbar = 1$)

$$\left\{ \frac{d^2}{dx^2} - \frac{dm(x)/dx}{m(x)} \frac{d}{dx} + 2m(x)[E - V(x)] \right\} \psi(x) = 0, \quad (1)$$

obtained from the Hamiltonian [14]

$$H = \frac{1}{2} \left(\hat{p} \frac{1}{m} \hat{p} \right) + V. \quad (2)$$

for the Woods-Saxon potential to study the scattering states within the framework of position-dependent mass formalism. The effective-mass Schrödinger equation could be transformed into Heun's equation [21] which is a Fuchsian-type equation with four singularities [14] by using a coordinate transformation. We obtain the wave function in terms of Heun's function and then we find transmission and reflection coefficients by studying the asymptotic behavior of the wave function at infinity. We write also the transmission and reflection coefficients for the case of constant mass by using the properties of Heun's function and also the continuity conditions of the wave function at $x = 0$. We find the wave function for the case of constant mass in terms of hypergeometric functions and plot the wave functions for

completeness. In nuclear physics, the Woods-Saxon potential is used to construct a shell model to describe the single-particle motion in a fusing system [22] and the potential plays an important role within the microscopic physics because of describing the interaction of a nucleon with a heavy nucleus [23].

The work is organized as follows. In Section II we obtain exactly scattering state solutions of the Woods-Saxon potential and transmission and reflection coefficients in the case of position-dependent mass. We study also the same quantities in the case of constant mass. The conclusions are given in Section III. In Appendix A we list some equalities related with Heun's function required for this work.

II. SCATTERING STATE SOLUTIONS

The Woods-Saxon potential has the form

$$V(x) = -\frac{V_0}{1 + e^{\delta x}}, \quad (3)$$

and we parameterize the mass function as

$$m(x) = (m_0 - m_1)\left(M - \frac{1}{1 + e^{\delta x}}\right), \quad (4)$$

where $M = (m_0 + m_1)/(m_0 - m_1)$ and V_0, δ, m_0 and m_1 are positive parameters. The form of the mass function is strongly similar to that of the potential. We could exactly solve the problem because of this form and also study the results for the case of constant mass. By using the transformation $y = (1 + e^{\delta x})^{-1}$ and inserting Eq.(4) and Eq.(3) into Eq.(1), we obtain the differential equation ($0 < y < 1$)

$$\begin{aligned} & \psi''(y) + \left(\frac{1}{y} + \frac{1}{y-1} - \frac{1}{y-M}\right)\psi'(y) \\ & + \frac{1}{y(y-1)(y-M)}\left\{-a_1^2 y - \frac{a_2^2}{y}M + \frac{a_3^2}{y-1}(M-1) + Ma_1^2 + a_2^2 - a_3^2\right\}\psi(y) = 0, \end{aligned} \quad (5)$$

where

$$a_1^2 = (2/\delta^2)(m_0 - m_1)V_0 ; \quad -a_2^2 = (2/\delta^2)(m_0 + m_1)E ; \quad -a_3^2 = (4/\delta^2)m_1(E + V_0). \quad (6)$$

To obtain a Fuchsian-type differential equation from Eq. (5), we use a new transformation

$$\psi(y) = y^{a_2}(y-1)^{a_3}f(y), \quad (7)$$

which gives a Heun's-type equation given as in Eq. (A1) in Appendix A

$$f''(y) + \left(\frac{1+2a_2}{y} + \frac{1+2a_3}{y-1} - \frac{1}{y-M} \right) f'(y) + \frac{1}{y(y-1)(y-M)} \left\{ [-a_1^2 + (a_2 + a_3)^2]y - [-a_1^2 + (a_2 + a_3)(1 + a_2 + a_3)]M + a_2 \right\} f(y) = 0. \quad (8)$$

The general solution of Eq. (8), which is regular in the neighborhood of $y = 0$, is written in terms of the Heun's function as [14]

$$f(y) = AH(M, -[-a_1^2 + (a_2 + a_3)(1 + a_2 + a_3)]M + a_2; a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; y), \quad (9)$$

where the constant A will be determined below.

Let us first investigate the limit $x \rightarrow \infty (y \simeq e^{-\delta x} \rightarrow 0)$, which gives $f(0) = A$ in Eq. (9) and the solution $\psi(y) \rightarrow Ay^{a_2} = Ae^{-\delta a_2 x}$ becomes

$$\psi(x) = Ae^{-ik_1 x}, \quad (10)$$

where $k_1 = \sqrt{2(m_0 + m_1)E}$ and we have used the property of $H(a, b; \alpha, \beta, \gamma, \delta; 0) = 1$.

To study the behavior of the solution Eq. (9) for $x \rightarrow -\infty (y \rightarrow 1), 1 - y \simeq e^{\delta x}$, we use Eq. (A5) of Appendix A, which changes the argument y to $1 - y$. Thus, we obtain the Heun's function in Eq. (9) as

$$\begin{aligned} & H(M, -[-a_1^2 + (a_2 + a_3)(1 + a_2 + a_3)]M + a_2; a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; y) = \\ & D_1 H(1 - M, [-a_1^2 + (a_2 + a_3)(1 + a_2 + a_3)]M + a_1^2 - (a_2 + a_3)^2 - a_2; \\ & a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_3, -1; 1 - y) + D_2 (1 - y)^{-2a_3} \\ & \times H(1 - M, [-a_1^2 + (a_2 - a_3)(1 + a_2 - a_3)]M + a_1^2 - (a_2 - a_3)^2 - a_2; \\ & a_2 - a_3 + a_1, a_2 - a_3 - a_1, 1 - 2a_3, -1; 1 - y), \end{aligned} \quad (11)$$

where the constants D_1 and D_2 are written by using Eq. (A6) in Appendix A

$$D_1 = H(M, -[-a_1^2 + (a_2 + a_3)(1 + a_2 + a_3)]M + a_2; a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; 1), \quad (12)$$

$$D_2 = H(M, -[-a_1^2 + (a_2 - a_3)(1 + a_2 - a_3)]M + a_2; a_2 - a_3 + a_1, a_2 - a_3 - a_1, 1 + 2a_2, -1; 1). \quad (13)$$

Using Eq. (11) we obtain the solution in Eq. (9) as

$$\psi(y) \rightarrow A(-1)^{a_3} \{D_1 e^{\delta a_3 x} + D_2 e^{-\delta a_3 x}\}, \quad (14)$$

which gives

$$\psi(x) = e^{ik_2 x} + \frac{D_2}{D_1} e^{-ik_2 x}, \quad (15)$$

where $k_2 = \sqrt{4m_1(E + V_0)}$ and we set $A = (-1)^{-a_3}/D_1$. Thus, we achieve the following form of the wave function for the limit $x \rightarrow \pm\infty$

$$\psi(x) = \begin{cases} e^{ik_2 x} + R e^{-ik_2 x}, & x \rightarrow -\infty, \\ T' e^{ik_1 x}, & x \rightarrow +\infty, \end{cases} \quad (16)$$

As a result, we recover the asymptotic behavior of a plane wave coming from the left-hand side.

We can write the wave function explicitly

$$\begin{aligned} \psi(x) &= (-1)^{2a_3} (1 + e^{\delta x})^{-(a_2+a_3)} e^{\delta a_3 x} \\ &\times \frac{H(M, b + a_2; a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; \frac{1}{1+e^{\delta x}})}{H(M, b + a_2; a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; 1)}, \end{aligned} \quad (17)$$

where $b = -[-a_1^2 + (a_2 + a_3)(1 + a_2 + a_3)]M$. Finally, we give the reflection and transmission coefficients for the case of position-dependent mass, respectively

$$|R|^2 = \left| \frac{H(M, b' + a_2; a_2 - a_3 + a_1, a_2 - a_3 - a_1, 1 + 2a_2, -1; 1)}{H(M, b + a_2; a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; 1)} \right|^2, \quad (18)$$

where $b' = -[-a_1^2 + (a_2 - a_3)(1 + a_2 - a_3)]M$, and

$$|T|^2 = \frac{k_1}{k_2} \frac{1}{|H(M, b + a_2; a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; 1)|^2}. \quad (19)$$

In order to investigate the dependence of the reflection coefficient to the energy E , we rewrite Eq. (18) in the following form by interchanging $\alpha \leftrightarrow \beta$ in Heun's function

$$\begin{aligned} |R|^2 &= \left| \frac{H(M, b' + a_2; a_2 - a_3 + a_1, a_2 - a_3 - a_1, 1 + 2a_2, -1; 1)}{H(M, b + a_2; a_2 + a_3 + a_1, a_2 + a_3 - a_1, 1 + 2a_2, -1; 1)} \right| \\ &\times \left| \frac{H(M, b' + a_2; a_2 - a_3 - a_1, a_2 - a_3 + a_1, 1 + 2a_2, -1; 1)}{H(M, b + a_2; a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; 1)} \right|, \end{aligned} \quad (20)$$

By using Eq. (A7) in Appendix A and keeping in mind that $a_1^2 = a_2^2/M - a_3^2/(M - 1)$, Eq. (20) gives

$$|R|^2 = \frac{[(M - 1)a_2 + Ma_3]^2}{[(M - 1)a_2 - Ma_3]^2} \times \left| \frac{H(M, b' + a_3 - a_1; a_2 - a_3 + a_1, a_2 - a_3 - a_1 + 1, 2 + 2a_2, 0; 1)}{H(M, b - a_3 - a_1; a_2 + a_3 + a_1, a_2 + a_3 - a_1 + 1, 2 + 2a_2, 0; 1)} \right| \times \left| \frac{H(M, b' + a_3 + a_1; a_2 - a_3 - a_1, a_2 - a_3 + a_1 + 1, 2 + 2a_2, 0; 1)}{H(M, b - a_3 + a_1; a_2 + a_3 - a_1, a_2 + a_3 + a_1 + 1, 2 + 2a_2, 0; 1)} \right|, \quad (21)$$

This equation enables us to analyze the dependence of reflection coefficient to the energy E when the energy goes to infinity. In this case, Eq. (21) gives

$$|R|^2 =_{E \rightarrow \infty} \left(\frac{\sqrt{2m_1} - \sqrt{m_0 + m_1}}{\sqrt{2m_1} + \sqrt{m_0 + m_1}} \right)^2 \left| \frac{H(M, -M(a_2 - a_3)^2; a_2 - a_3, a_2 - a_3, 2a_2, 0; 1)}{H(M, -M(a_2 + a_3)^2; a_2 + a_3, a_2 + a_3, 2a_2, 0; 1)} \right|^2, \quad (22)$$

Using the equality $H(a, b; \alpha, \beta, \gamma, 0; y) = {}_2F_1(\alpha, \beta; \gamma; y)$ (for $b = -a\alpha\beta$) [14] and also ${}_2F_1(\alpha, \alpha; \gamma; 1) \rightarrow_{\alpha, \gamma \rightarrow \infty} e^{\alpha^2/\gamma}$, we obtain

$$|R|^2 =_{E \rightarrow \infty} \left(\frac{\sqrt{2m_1} - \sqrt{m_0 + m_1}}{\sqrt{2m_1} + \sqrt{m_0 + m_1}} \right)^2. \quad (23)$$

Eq. (23) shows that the reflection coefficient increases up to the value obtained in Eq. (23) while changing with energy. Fig. (1) shows the variation of the reflection and transmission coefficients as a function of the energy E in the position dependent mass case. In Fig. (2), the effect of the mass parameters m_0 and m_1 on the reflection and transmission coefficients are given. It is seen that the reflection coefficient decreases linearly with mass parameters while the transmission coefficient increases with the growing values of the parameters. In the Figs. (1) and (2), It could be seen that the unitarity condition $|R|^2 + |T|^2 = 1$ is satisfied in the constant and position dependent mass cases. In Fig. (2), we see that the reflection coefficient can not take zero value for the case of $E < V_0$ which is agreed with quantum mechanical results.

Now, we begin to give the results for the case of constant mass, which means that $m_0 = m_1$, starting from the wave function. With the help of Eq. (A8) in Appendix A, we write the wave function

$$\psi(x)_{m_0=m_1} = (-1)^{2a_3} (1 + e^{\delta x})^{-(a_2+a_3)} e^{\delta a_3 x} \times \frac{{}_2F_1(1 + a_2 + a_3, a_2 + a_3; 1 + 2a_2; \frac{1}{1+e^{\delta x}})}{{}_2F_1(1 + a_2 + a_3, a_2 + a_3; 1 + 2a_2; 1)}, \quad (24)$$

which can be written in terms of Gamma functions

$$\begin{aligned} \psi(x)_{m_0=m_1} &= (-1)^{2a_3} (1 + e^{\delta x})^{-(a_2+a_3)} e^{\delta a_3 x} \frac{\Gamma(a_2 - a_3)\Gamma(1 + a_2 - a_3)}{\Gamma(1 + 2a_2)\Gamma(-2a_3)} \\ &\times {}_2F_1(1 + a_2 + a_3, a_2 + a_3; 1 + 2a_2; \frac{1}{1 + e^{\delta x}}). \end{aligned} \quad (25)$$

where used the relation of hypergeometric function ${}_2F_1(\alpha, \beta; \gamma; 1) = \frac{\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)}$. The parameters given in Eq. (6) in the case of constant mass become ($m_0 = m_1 = m$)

$$-a_2^2 = (4/\delta^2)mE ; \quad -a_3^2 = (4/\delta^2)m(E + V_0). \quad (26)$$

We depict the wave function for two different values of parameter sets in Fig. (3). It is seen that the wave function exhibit an oscillatory behaviour for $x < 0$ and exponentially decreasing in the region $x > 0$. The oscillating behaviour of the wave function given in Eq. (16) for $x < 0$ is a purely quantum mechanical interference effect between the incident and reflected waves [23]. The wave function in the region $x > 0$ goes to zero due to the potential given in Eq. (3).

We give the reflection and transmission coefficients for the case of constant mass. Using Eq. (A8) in Appendix A and the relation ${}_2F_1(\alpha, \beta; \gamma; 1) = \frac{\Gamma(\gamma)\Gamma(\gamma-\alpha-\beta)}{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)}$ in Eq. (18), we obtain

$$|R|_{m_0=m_1}^2 = \left| \frac{{}_2F_1(a_2 - a_3 + 1, a_2 - a_3; 1 + 2a_2; 1)}{{}_2F_1(a_2 + a_3 + 1, a_2 + a_3; 1 + 2a_2; 1)} \right|^2 = \left| \frac{\Gamma(2a_3)\Gamma(a_2 - a_3)\Gamma(a_2 - a_3 + 1)}{\Gamma(-2a_3)\Gamma(a_2 + a_3)\Gamma(a_2 + a_3 + 1)} \right|^2, \quad (27)$$

and similarly from Eq. (19)

$$|T|_{m_0=m_1}^2 = \frac{k_1}{k_2} \frac{1}{|{}_2F_1(a_2 + a_3 + 1, a_2 + a_3; 1 + 2a_2; 1)|^2} = \frac{k_1}{k_2} \left| \frac{\Gamma(a_2 - a_3)\Gamma(a_2 - a_3 + 1)}{\Gamma(1 + 2a_2)\Gamma(-2a_3)} \right|^2. \quad (28)$$

It should be noted that we must apply the continuity condition to obtain a relation between the coefficients written in Eq. (16). The condition that the wave function and its derivative must be continuous at $x = 0$ gives $k_2(1 - |R|^2) = k_1|T|^2$ [24, 25]. In Fig. (4), we plot the variation of the reflection and transmission coefficients according to the energy E in the case of constant mass. The reflection coefficient goes to zero when the energy increases while the transmission coefficient goes to unity. It could be interesting to study the limiting case of $\delta \rightarrow \infty$. In that case the potential function becomes $V(x) \rightarrow 0$ and the mass function

goes to $2m$. It means that the reflection and transmission can not appear (Eqs. (27) and (28)) as expected. In addition, in the limiting case $\delta \rightarrow -\infty$ we obtain a step potential from Eq. (3) and Eq. (4) gives us $m(x) \rightarrow 2m$. Thus, we get the reflection coefficient as

$$|R|_{m_0=m_1}^2 =_{\delta \rightarrow -\infty} \left| \frac{a_2 - a_3}{a_2 + a_3} \right|^2 =_{\delta \rightarrow -\infty} \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2. \quad (29)$$

where $k_1 = \sqrt{4mE}$ and $k_2 = \sqrt{4m(E + V_0)}$.

III. CONCLUSION

We have exactly solved the one-dimensional effective mass Schrödinger equation for the Woods-Saxon potential. We have found the wave functions in terms of Heun's function. The reflection and transmission coefficients are calculated by using the asymptotic behaviour of the wave function at infinity. To analyze these coefficients in the case of position-dependent mass, we calculate the reflection coefficient in the limit $E \rightarrow \infty$. They are plotted as a function of mass parameters in Fig. (2). One can see that the unitarity condition in the scattering problem given as $|R|^2 + |T|^2 = 1$ is satisfied in the position dependent mass case also. We have also obtained the wave function, reflection and transmission coefficients in the constant mass case. They are presented in the Figs. (3) and (4).

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Appendix A: Useful Equalities of Heun's Function

Heun's equation with the following form

$$\left\{ \frac{d^2}{dy^2} + \left(\frac{\gamma}{y} + \frac{1 + \alpha + \beta - \gamma - \delta}{y - 1} - \frac{\delta}{y - a} \right) \frac{d}{dy} + \frac{\alpha\beta y + b}{y(y - 1)(y - a)} \right\} f(y) = 0, \quad (A1)$$

has a solution in the neighborhood of $y = 0$

$$f(y) = H(a, b; \alpha, \beta, \gamma, \delta; y), \quad (A2)$$

and two linearly independent solutions in the neighborhood of $y = 1$ [14]

$$f(y) = H(1 - a, -b - \alpha\beta; \alpha, \beta, 1 + \alpha + \beta - \gamma - \delta, \delta; 1 - y), \quad (\text{A3})$$

and

$$f(y) = (1 - y)^{\gamma + \delta - \alpha - \beta} H(1 - a, -b - \alpha\beta - (\gamma + \delta - \alpha - \beta)(\gamma + \delta - a\gamma); \gamma + \delta - \alpha, \gamma + \delta - \beta, 1 - \alpha - \beta + \gamma + \delta, \delta; 1 - y), \quad (\text{A4})$$

The solution in the neighborhood of $y = 0$ can be written as a linear combination of last two Heun's functions [14]

$$\begin{aligned} H(a, b; \alpha, \beta, \gamma, \delta; y) &= D_1 H(1 - a, -b - \alpha\beta; \alpha, \beta, 1 + \alpha + \beta - \gamma - \delta, \delta; 1 - y) \\ &+ D_2 (1 - y)^{\gamma + \delta - \alpha - \beta} \\ &\times H(1 - a, -b - \alpha\beta - (\gamma + \delta - \alpha - \beta)(\gamma + \delta - a\gamma); \\ &\gamma + \delta - \alpha, \gamma + \delta - \beta, 1 - \alpha - \beta + \gamma + \delta, \delta; 1 - y), \end{aligned} \quad (\text{A5})$$

where the constants are given

$$\begin{aligned} D_1 &= H(a, b; \alpha, \beta, \gamma, \delta; 1), \\ D_2 &= H(a, b - a\gamma(\gamma + \delta - \alpha - \beta); \gamma + \delta - \alpha, \gamma + \delta - \beta, \gamma, \delta; 1). \end{aligned} \quad (\text{A6})$$

The following identity links the arguments (β, γ, δ) to $(\beta + 1, \gamma + 1, \delta + 1)$, respectively,

$$\begin{aligned} &(\gamma a\beta + b)H(a, b - \alpha; \alpha, \beta + 1, \gamma + 1, \delta + 1; y) \\ &= a\gamma H(a, b; \alpha, \beta, \gamma, \delta; y) + a\gamma(y - 1) \frac{d}{dy} H(a, b; \alpha, \beta, \gamma, \delta; y). \end{aligned} \quad (\text{A7})$$

Finally, in the limit of $a \rightarrow \infty$, Heun's function turns into a hypergeometric function [14]

$$\begin{aligned} H(a, a\Delta; \alpha, \beta, \gamma, \delta; y) &=_{a \rightarrow \infty} {}_2F_1 \left(\frac{1}{2}(\alpha + \beta - \delta) + \sqrt{\left[\frac{1}{2}(\alpha + \beta - \delta)\right]^2 + \Delta}, \right. \\ &\left. \frac{1}{2}(\alpha + \beta - \delta) - \sqrt{\left[\frac{1}{2}(\alpha + \beta - \delta)\right]^2 + \Delta}; \gamma; y \right). \end{aligned} \quad (\text{A8})$$

with $\gamma \neq -n (n = 0, 1, 2, \dots)$.

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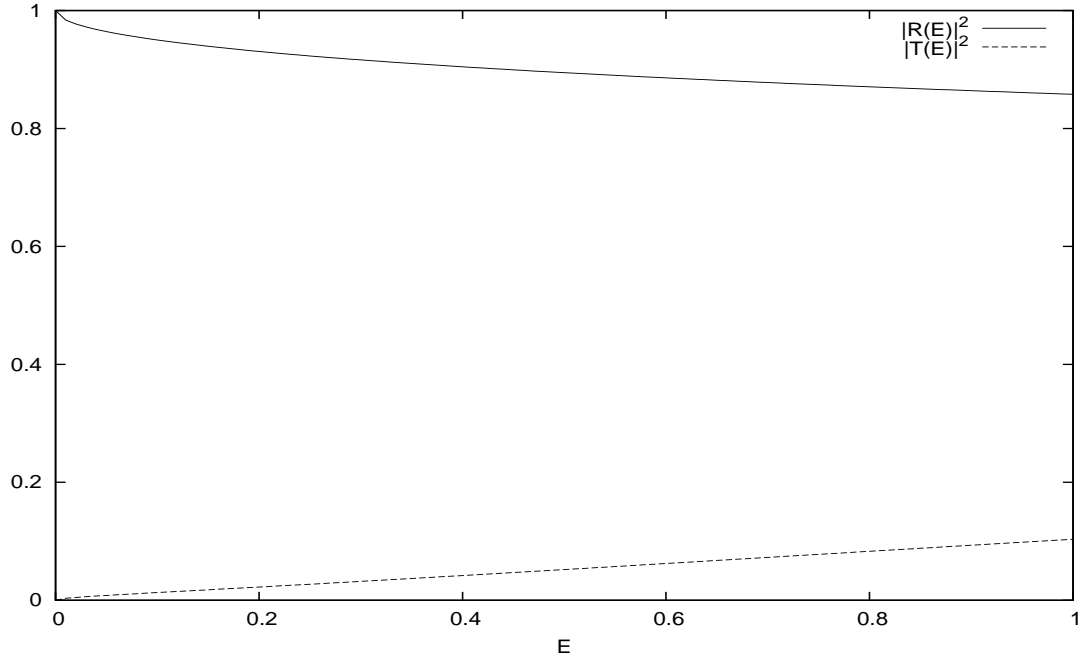
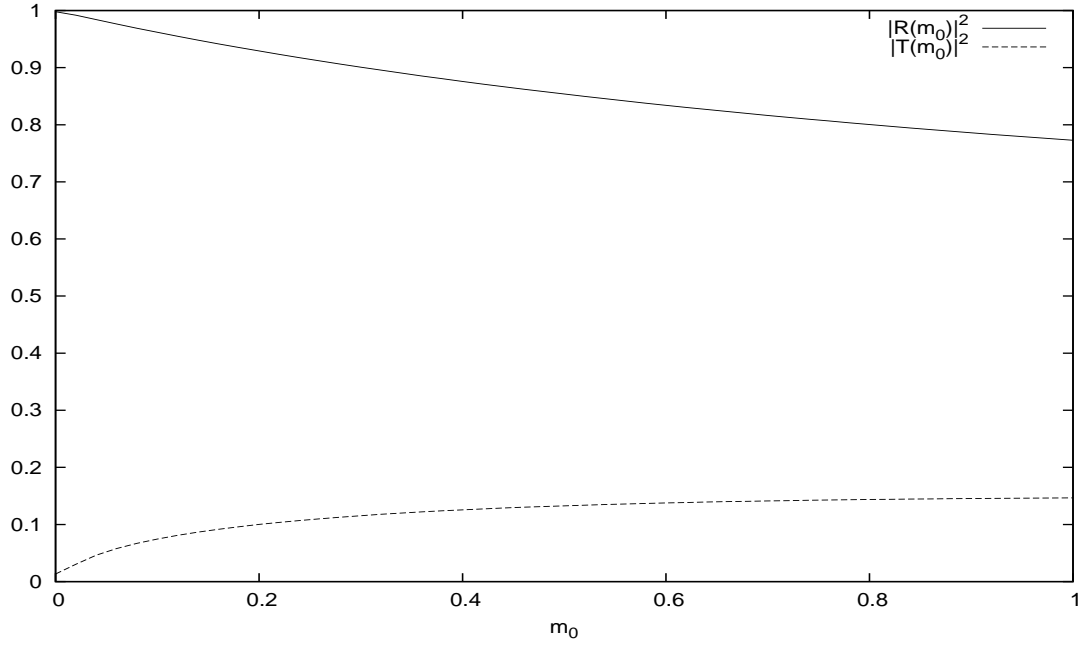
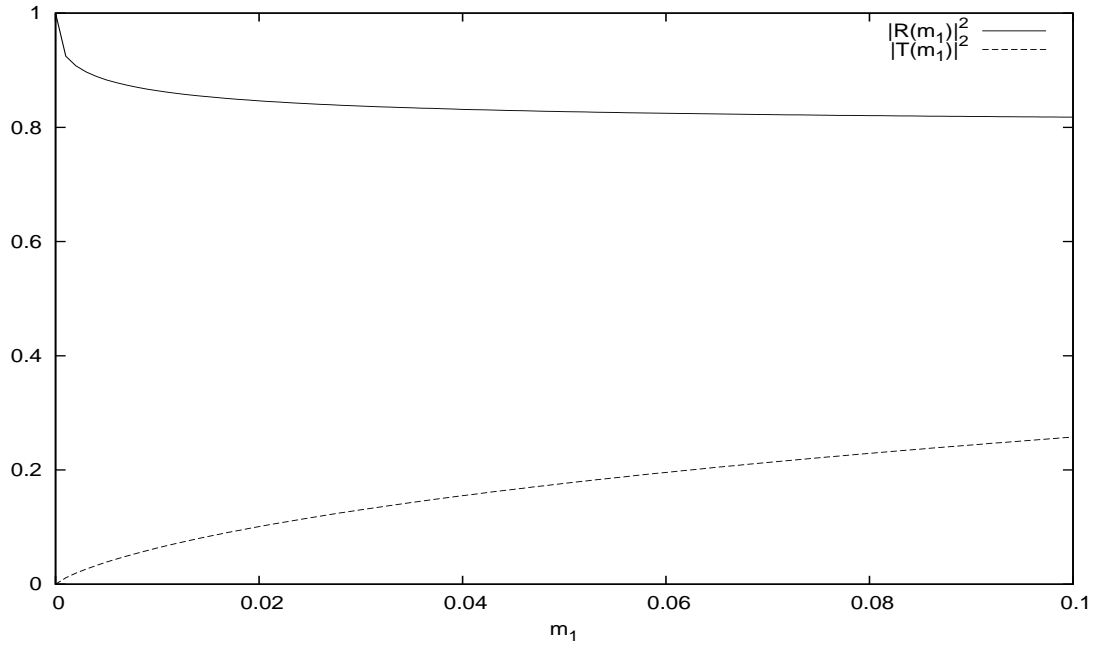


FIG. 1: The reflection and transmission coefficients in the case of position-dependent mass for $m_0 = 0.1, m_1 = 10, \delta = 5, V_0 = 5$.



(a) reflection and transmission coefficients for $m_1 = 0.01, \delta = 3, V_0 = 1$ and $E = 0.05$.



(b) reflection and transmission coefficients for $m_0 = 1, \delta = 5, V_0 = 1$ and $E = 0.1$.

FIG. 2: Reflection and transmission coefficients in the case of position-dependent mass.

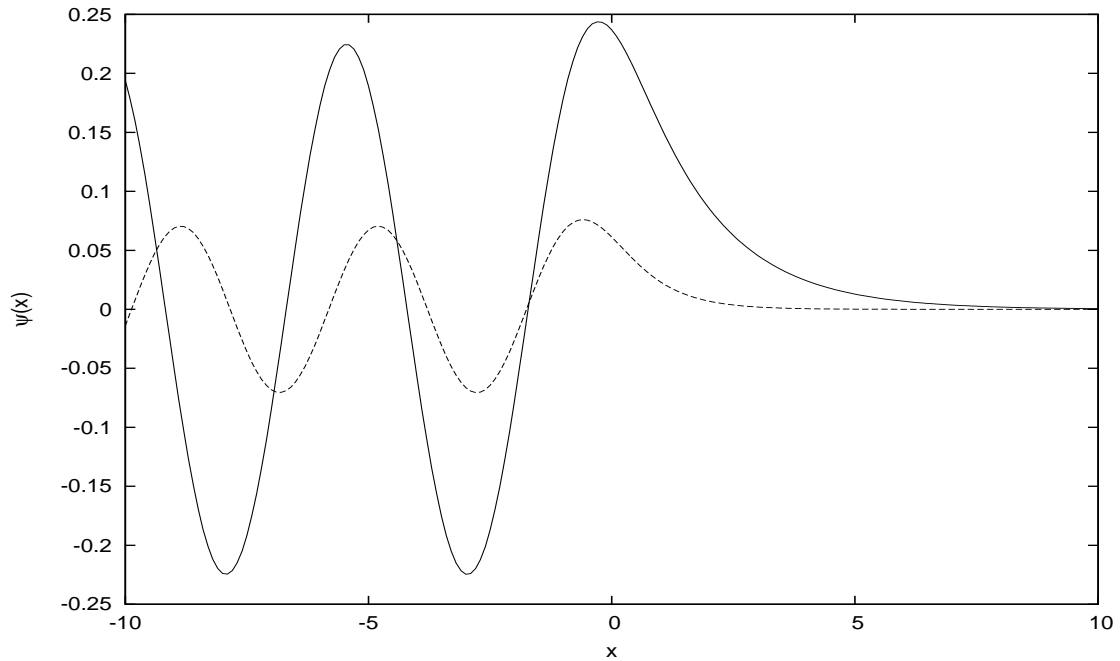
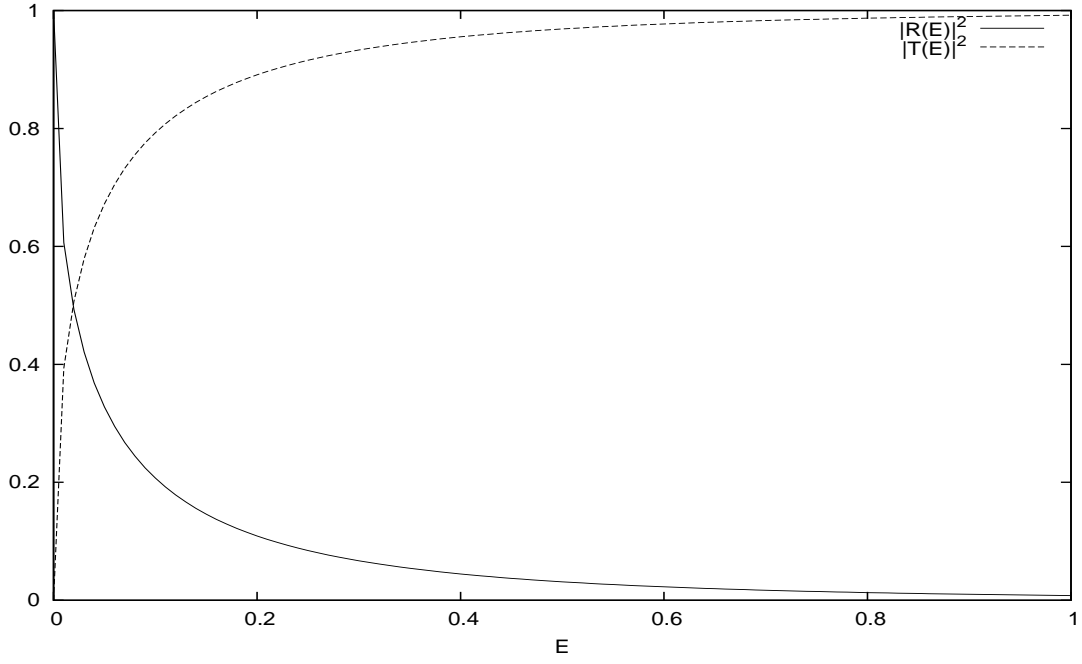
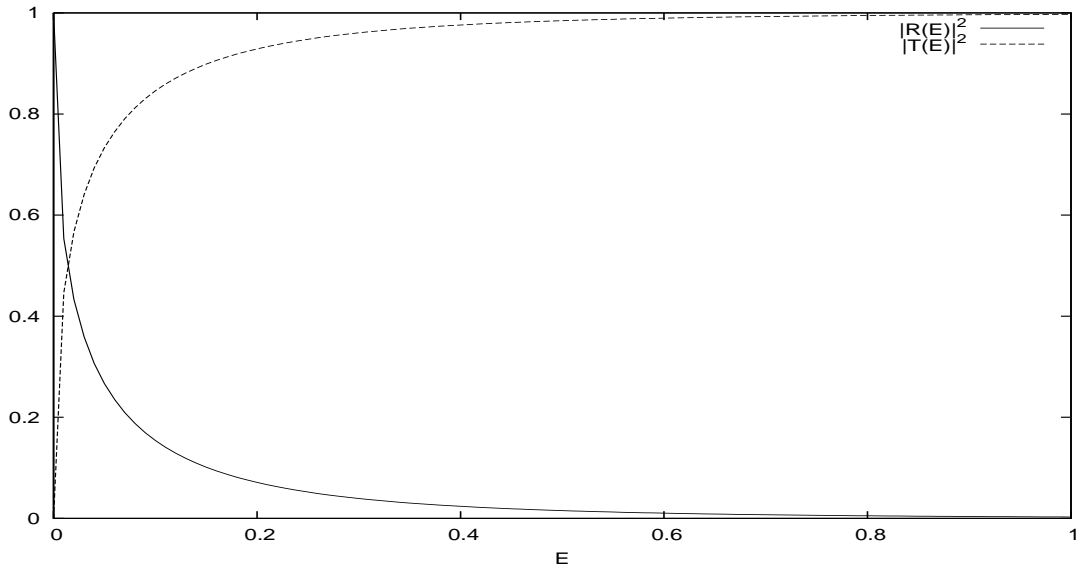


FIG. 3: The unnormalized wave functions in the case of constant mass for $m = 1, \delta = 2, V_0 = 0.5, E = -m/10$ (solid line) and for $m = 2, \delta = 2, V_0 = 0.5, E = -m/10$.



(a) reflection and transmission coefficients for $m = 0.5, \delta = 5, V_0 = 1$.



(b) reflection and transmission coefficients for $m = 1, \delta = 5, V_0 = 1$.

FIG. 4: Reflection and transmission coefficients in the case of constant mass.