Scattering of the Woods–Saxon potential in the Schrödinger equation

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

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1. Introduction
Quantum mechanical systems can be investigated in view of two basic points. One is the studying of bound states to handle the necessary information about the system under consideration. The other is solving the scattering problem for a given quantum mechanical system under the effect of a potential. So, one has to study both bound and scattering states of the quantum mechanical system under consideration to achieve a complete understanding about it. Efforts have been made regarding the scattering problem for a relativistic and/or non-relativistic system under the influence of different types of potential, such as Manning–Rosen [1, 2], Eckart [3, 4], Pöschl–Teller [5], Hulthén [6], Woods–Saxon [7–9], cusp [10] and Coulomb [11]. The scattering problem in the case where the mass depends on the spatial coordinate has become a particular part of that problem, and has received great attention when studying scattering states for a given quantum system [12–15]. The position-dependent mass formalism is a useful basis for explaining 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 (\(\hbar = 1\)):

\[
\left\{ \frac{d^2}{dx^2} - \frac{dm(x)/dx}{m(x)} \frac{d}{dx} + 2m(x)[E - V(x)] \right\} \psi(x) = 0, \tag{1}
\]
obtained from the Hamiltonian \[14\]

\[ H = \frac{1}{2} \left( \hat{p} \cdot \frac{1}{m} \hat{p} \right) + V \] (2)

for the Woods–Saxon potential to study the scattering states within the framework of the 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 wavefunction in terms of Heun’s function and then we find transmission and reflection coefficients by studying the asymptotic behavior of the wavefunction at infinity. We also write 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 wavefunction at \( x = 0 \). We find the wavefunction for the case of constant mass in terms of hypergeometric functions and plot the wavefunctions for completeness. In nuclear physics, the Woods–Saxon potential is used to construct a shell model which describes single-particle motion in a fusing system [22]. The potential plays an important role within microscopic physics because it describes the interaction of a nucleon with a heavy nucleus [23].

The paper is organized as follows. In section 2 we obtain exact scattering state solutions of the Woods–Saxon potential, plus transmission and reflection coefficients in the case of position-dependent mass. We also study the same quantities in the case of constant mass. The conclusions are given in section 3. In the appendix we list some equalities related with Heun’s function required for this work.

2. Scattering state solutions

The Woods–Saxon potential has the form

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

and we parameterize the mass function as

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

where \( M = (m_0 + m_1)/(m_0 - m_1) \) and \( V_0, \delta, m_0 \) 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 equations (4) and (3) into equation (1), we obtain the differential equation \((0 < y < 1)\)

\[ \psi''(y) + \left( \frac{1}{y} + \frac{1}{y - 1} - \frac{1}{y - M} \right) \psi'(y) + \frac{1}{y(y - 1)(y - M)} \times \left\{ -a_1^2 y - \frac{a_2^2}{y} M + \frac{a_3^2}{y - 1} (M - 1) + Ma_1^2 + a_2^2 - a_3^2 \right\} \psi(y) = 0, \] (5)

where

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

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

\[ \psi(y) = y^{a_1}(y - 1)^{a_2} f(y), \] (7)
which gives a Heun’s-type equation shown in equation (A.1) in the appendix:
\[
\begin{align*}
  f''(y) + \left( \frac{1 + 2a_2}{y} + \frac{1 + 2a_1}{y - 1} - \frac{1}{y - M} \right) f'(y) + \frac{1}{y(y - 1)(y - M)} f(y) &= 0.
\end{align*}
\]

The general solution of equation (8), which is regular in the neighborhood of \( y = 0 \), is written in terms of Heun’s function as [14]
\[
f(y) = AH \left( M, \left[ -a_1^2 + (a_2 + a_3)(1 + a_2 + a_3) \right] M + a_2; a_2 + a_3 - a_1, 1 + 2a_2, -1; y \right),
\]
where the constant \( A \) will be determined below.

Let us first investigate the limit \( x \to \infty(y \simeq e^{-kx} \to 0) \), which gives \( f(0) = A \) in equation (9) and the solution \( \psi(y) \to Ay^{a_2} = Ae^{-kx} \) becomes
\[
\psi(x) = Ae^{-ikx},
\]
where \( k_1 = \sqrt{2(\alpha_0 + \alpha_1)E} \) and we have used the property of \( H(\alpha, \beta; \gamma, \delta; 0) = 1 \).

To study the behavior of the solution (equation (9)) for \( x \to -\infty(y \to 1) \), \( 1 - y \simeq e^{ikx} \), we use equation (A.5) of the appendix, which changes the argument \( y \) to \( 1 - y \). Thus, we obtain Heun’s function in equation (9) as
\[
H(M, -\left[ -a_1^2 + (a_2 + a_3)(1 + a_2 + a_3) \right] M + a_2; a_2 + a_3 - a_1, 1 + 2a_2, -1; y) = D_1H(1 - M, -\left[ -a_1^2 + (a_2 + a_3)(1 + a_2 + a_3) \right] M + a_1^2 - (a_2 + a_3)^2 - a_2;
\]
\[
\begin{align*}
  &a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; 1 - y) + D_2(1 - y)^{-2a_1} \times H(1 - M, -\left[ -a_1^2 + (a_2 - a_3)(1 + a_2 - a_3) \right] M + a_1^2 - (a_2 - a_3)^2 - a_2;
\end{align*}
\]
\[
\begin{align*}
  &a_2 - a_3 + a_1, a_2 - a_3 - a_1, 1 - 2a_2, -1; 1 - y),
\end{align*}
\]
where the constants \( D_1 \) and \( D_2 \) are written by using equation (A.6) in the appendix:
\[
D_1 = H(M, -\left[ -a_1^2 + (a_2 + a_3)(1 + a_2 + a_3) \right] M + a_2;
\]
\[
\begin{align*}
  &a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; 1), \quad (12)
\end{align*}
\]
\[
D_2 = H(M, -\left[ -a_1^2 + (a_2 - a_3)(1 + a_2 - a_3) \right] M + a_2;
\]
\[
\begin{align*}
  &a_2 - a_3 + a_1, a_2 - a_3 - a_1, 1 + 2a_2, -1; 1). \quad (13)
\end{align*}
\]

Using equation (11) we obtain the solution in equation (9) as
\[
\psi(y) \to A(-1)^{a_2} \left[ D_1e^{ikx} + D_2e^{-ikx} \right],
\]
which gives
\[
\psi(x) = e^{ikx} + \frac{D_2}{D_1} e^{-ikx},
\]
where \( k_2 = \sqrt{4m_1(E + V_0)} \) and we set \( A = (-1)^{-a_2}/D_1 \). Thus, we achieve the following form of the wavefunction for the limit \( x \to \pm \infty \):
\[
\psi(x) = \begin{cases} 
  e^{ikx} + Re^{-ikx}, & x \to -\infty \\
  T'e^{ikx}, & x \to +\infty. 
\end{cases}
\]

As a result, we recover the asymptotic behavior of a plane wave coming from the left-hand side.
\( \psi(x) = \left( -1 \right)^\alpha e^{ix} \alpha(x) e^{i\beta x} \)

\[
\frac{H(M, b + a^2; a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; \frac{1}{4})}{H(M, b + a^2; a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; 1)}, \tag{17}
\]

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

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

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

\[
|T|^2 = \left| \frac{k_1}{k_2} \frac{1}{H(M, b + a^2; a_2 + a_3 - a_1, a_2 + a_3 + a_1, 1 + 2a_2, -1; 1)} \right|^2. \tag{19}
\]

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

\[
|R|^2 = \left| \frac{H(M, b'; a_2; a_2 + a_3 + a_1, a_2 + a_3 - a_1, 1 + 2a_2, -1; 1)}{H(M, b; a_2; a_2 + a_3 + a_1, a_2 + a_3 - a_1, 1 + 2a_2, -1; 1)} \right|^2 \times \left| \frac{H(M, b'; a_2; a_2 - a_3 - a_1, a_2 - a_3 + a_1, 1 + 2a_2, -1; 1)}{H(M, b; a_2; a_2 - a_3 - a_1, a_2 - a_3 + a_1, 1 + 2a_2, -1; 1)} \right|. \tag{20}
\]

By using equation (A.7) in the appendix and keeping in mind that \( a_1^2 = a_2^2/(M - a_2^2)/(M - 1) \), equation (20) gives

\[
|R|^2 = \left| \frac{(M - 1)a_2 + Ma_1}{(M - 1)a_2 - Ma_1} \right|^2 \times \left| \frac{H(M, b'; a_3 - a_1; a_2 - a_3 + a_1, a_2 - a_3 - a_1, 1 + 2a_2, 0; 1)}{H(M, b; a_3 - a_1; a_2 - a_3 + a_1, a_2 - a_3 - a_1, 1 + 2a_2, 0; 1)} \right|^2 \times \left| \frac{H(M, b'; a_3 + a_1; a_2 - a_3 - a_1, a_2 - a_3 + a_1, 1 + 2a_2, 0; 1)}{H(M, b; a_3 + a_1; a_2 - a_3 - a_1, a_2 - a_3 + a_1, 1 + 2a_2, 0; 1)} \right|. \tag{21}
\]
This equation enables us to analyze the dependence of the reflection coefficient on energy $E$ when energy goes to infinity. In this case, equation (21) gives

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

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

$$|R|^2 =_{E \to \infty} \left( \frac{\sqrt{2m_1} - \sqrt{m_0 + m_1}}{\sqrt{2m_1} + \sqrt{m_0 + m_1}} \right)^2. \quad \text{(23)}$$
Figure 3. The unnormalized wavefunctions in the case of constant mass for $m = 1, \delta = 2$, $V_0 = 0.5, E = -m/10$ (solid line) and for $m = 2, \delta = 2$, $V_0 = 0.5, E = -m/10$.

Equation (23) shows that the reflection coefficient increases up to the value obtained in equation (23) while changing with energy. Figure 1 shows the variation of reflection and transmission coefficients as a function of energy $E$ in the position-dependent mass case. In figure 2, the effect of the mass parameters $m_0$ and $m_1$ on reflection and transmission coefficients is given. It is seen that the reflection coefficient decreases linearly with mass parameters while the transmission coefficient increases with increasing values of the parameters. In figures 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 figure 2, we see that the reflection coefficient cannot take zero value for the case of $E < V_0$ which is agreed with quantum mechanical results.

Now, we give the results for the case of constant mass, which means that $m_0 = m_1$, starting from the wavefunction. With the help of equation (A.8) in the appendix, we write the wavefunction

$$
\psi(x)_{m_0=m_1} = (-1)^{2a_0} (1 + e^{\delta x})^{-a_2} e^{a_3 x} \times \frac{\gamma(1 + a_2 + a_3, a_2 + a_3; 1 + 2a_2; 1 + e^{\delta x})}{\gamma(1 + a_2 + a_3, a_2 + a_3; 1 + 2a_2; 1)},
$$

(24)

which can be written in terms of Gamma functions

$$
\psi(x)_{m_0=m_1} = (-1)^{2a_0} (1 + e^{\delta x})^{-a_2} e^{a_3 x} \times \frac{\gamma(a_2 - a_3)\gamma(1 + a_2 - a_3)}{\gamma(1 + 2a_2)\gamma(-2a_3)} \times \gamma(1 + a_2 + a_3, a_2 + a_3; 1 + 2a_2; 1 + e^{\delta x}),
$$

(25)

where we used the relation of the hypergeometric function $\gamma(a_1, a_2; a; 0) = \gamma(a_1, a_2; a; 1)$.

The parameters given in equation (6) in the case of constant mass become $(m_0 = m_1 = m)$

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

(26)

We depict the wavefunction for two different values of parameter sets in figure 3. It is seen that the wavefunction exhibits an oscillatory behavior for $x < 0$ and exponentially decreases.
in the region $x > 0$. The oscillating behavior of the wavefunction given in equation (16) for $x < 0$ is a purely quantum mechanical interference effect between the incident and reflected waves [23]. The wavefunction in the region $x > 0$ goes to zero due to the potential given in equation (3).

We give the reflection and transmission coefficients for the case of constant mass. Using equation (A.8) in the appendix and the relation $\mathcal{F}_1(\alpha, \beta; \gamma; 1) = \frac{\Gamma(\gamma-\alpha)\Gamma(\gamma-\beta)}{\Gamma(\gamma-\alpha-\beta)}$ in equation (18), we obtain

$$|R|^2_{m=0.5} = \left| \frac{\mathcal{F}_1(a_2 - a_3 + 1, a_2 - a_3; 1 + 2a_2; |}{\mathcal{F}_1(a_2 + a_3 + 1, a_2 + a_3; 1 + 2a_2; 1)} \right|^2 = \left| \frac{\Gamma(2a_3)\Gamma(a_2 - a_3)\Gamma(a_2 - a_3 + 1)}{\Gamma(-2a_3)\Gamma(a_2 + a_3)\Gamma(a_2 + a_3 + 1)} \right|^2. \tag{27}$$

Figure 4. Reflection and transmission coefficients in the case of constant mass: (a) $m = 0.5$, $\delta = 5$, $V_0 = 1$; (b) for $m = 1$, $\delta = 5$, $V_0 = 1$. 

The oscillating behavior of the wavefunction given in equation (16) for $x < 0$ is a purely quantum mechanical interference effect between the incident and reflected waves [23].
and similarly from equation (19)

\[
|T|_{m_0=m_1} = \frac{k_1}{k_2} \frac{1}{2 F_1(a_2 + a_3 + 1, a_2 + a_3; 1 + 2a_2; 1)^2} = \frac{k_1}{k_2} \frac{\Gamma(a_2 - a_3)\Gamma(a_2 - a_3 + 1)}{\Gamma(1 + 2a_2)\Gamma(-2a_3)}.
\]

(28)

It should be noted that we must apply the continuity condition to obtain a relation between the coefficients written in equation (16). The condition that the wavefunction and its derivative must be continuous at \( x = 0 \) gives \( k_2(1 - |R|^2) = k_1 |T|^2 \) [24, 25]. In figure 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 \( \delta \to \infty \). In that case the potential function becomes \( V(x) \to 0 \) and the mass function goes to \( 2m \). It means that the reflection and transmission cannot appear (equations (27) and (28)) as expected. In addition, in the limiting case \( \delta \to -\infty \), we obtain a step potential from equation (3) and equation (4) gives us \( m(x) \to 2m \). Thus, we get the reflection coefficient as

\[
|R|^2_{m_0=m_1} \equiv \delta \to -\infty \left( \frac{a_2 - a_3}{a_2 + a_3} \right)^2 \equiv \delta \to -\infty \left( \frac{k_1 - k_2}{k_1 + k_2} \right)^2,
\]

(29)

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

3. Conclusion

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

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Appendix. Useful equalities of Heun’s function

Heun’s equation with the following form:

\[
\begin{aligned}
&\frac{d^2}{dy^2} \left( \frac{\gamma y + 1 + \alpha + \beta - y - \delta}{y - 1} \right) \frac{d}{dy} + \frac{\alpha \beta y + b}{y(y - 1)(y - a)} f(y) = 0.
\end{aligned}
\]

(A.1)
has a solution in the neighborhood of \( y = 0 \):

\[
f(y) = H(a, b; \alpha, \beta, \gamma, \delta; y),
\]

(A.2)

and two linearly independent solutions in the neighborhood of \( y = 1 \) [14]:

\[
f(y) = H(1 - a, -b - \alpha \beta; \alpha, \beta, 1 + \alpha + \beta - y - \delta, \delta; 1 - y),
\]

(A.3)

and

\[
f(y) = (1 - y)^{\gamma + \delta - \alpha - \beta} H(1 - a, -b - \alpha \beta - (\gamma + \delta - \alpha - \beta)(\gamma + \delta - a \gamma); \gamma + \delta - \alpha,
\]

\[
\gamma + \delta - \beta, 1 - \alpha - \beta + \gamma + \delta, \delta; 1 - y),
\]

(A.4)

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

\[
H(a, b; \alpha, \beta, \gamma, \delta; y) = D_1 H(1 - a, -b - \alpha \beta; \alpha, \beta, 1 + \alpha + \beta - y - \delta, \delta; 1 - y) + D_2 (1 - y)^{\gamma + \delta - \alpha - \beta} H(1 - a, -b - \alpha \beta - (\gamma + \delta - \alpha - \beta)(\gamma + \delta - a \gamma); \gamma + \delta - \alpha,
\]

\[
\gamma + \delta - \beta, 1 - \alpha - \beta + \gamma + \delta, \delta; 1 - y),
\]

(A.5)

where the constants are given as

\[
D_1 = H(a, b; \alpha, \beta, \gamma, \delta; 1),
\]

\[
D_2 = H(a, b - a \gamma (\gamma + \delta - \alpha - \beta); \gamma + \delta - \alpha, \gamma + \delta - \beta, \gamma, \delta; 1).
\]

(A.6)

The following identity links the arguments \((\beta, \gamma, \delta)\) to \((\beta + 1, \gamma + 1, \delta + 1)\), respectively:

\[
(\gamma a \beta + b) H(a, b - a \gamma (\gamma + \delta - \alpha - \beta); \gamma + \delta - \alpha, \gamma + \delta - \beta, \gamma, \delta; y) = a \gamma H(a, b; \alpha, \beta, \gamma, \delta; y) + a \gamma (y - 1) \frac{d}{dy} H(a, b; \alpha, \beta, \gamma, \delta; y).
\]

(A.7)

Finally, in the limit of \( a \to \infty \), Heun’s function turns into a hypergeometric function [14]

\[
H(a, a \Delta; \alpha, \beta, \gamma, \delta; y) \approx_{y \to \infty} 2 F_1 \left( \frac{1}{2}(\alpha + \beta - \delta) + \sqrt{\left[ \frac{1}{2}(\alpha + \beta - \delta) \right]^2 + \Delta} ; \gamma; y \right) \frac{1}{2}(\alpha + \beta - \delta) - \sqrt{\left[ \frac{1}{2}(\alpha + \beta - \delta) \right]^2 + \Delta ; \gamma; y},
\]

(A.8)

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

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