

APPLICATION OF THE SPPS METHOD TO THE ONE-DIMENSIONAL QUANTUM SCATTERING

V. RABINOVICH*

National Polytechnic Institute
ESIME Zacatenco
D. F. México, CP 07738, México

F. URBANO-ALTAMIRANO†

National Polytechnic Institute
UPIITA
D. F. México, CP 07340, México

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Abstract

The transmission and reflection coefficients for the scattering of a particle on one-dimensional potential are calculated by means of Spectral Parameter Power Series (SPPS). The results were compared with known results.

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Keywords: potential barrier, scattering, Schrödinger equation, Spectral Parameter Power Series (SPPS)

1 Introduction

We consider the scattering of a one-dimensional particle of complete energy E on the potential barrier. The scattering process is described by a Schrödinger equation

$$\mathcal{H}\psi(x) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E\psi(x), x \in \mathbb{R} \quad (1.1)$$

where \hbar is the Planck constant, $m > 0$ is an effective mass of the particle, V is an electric potential of an external field, ψ is a wave function.

*E-mail address: vladimir.rabinovich@gmail.com

†E-mail address: edurbano06@gmail.com

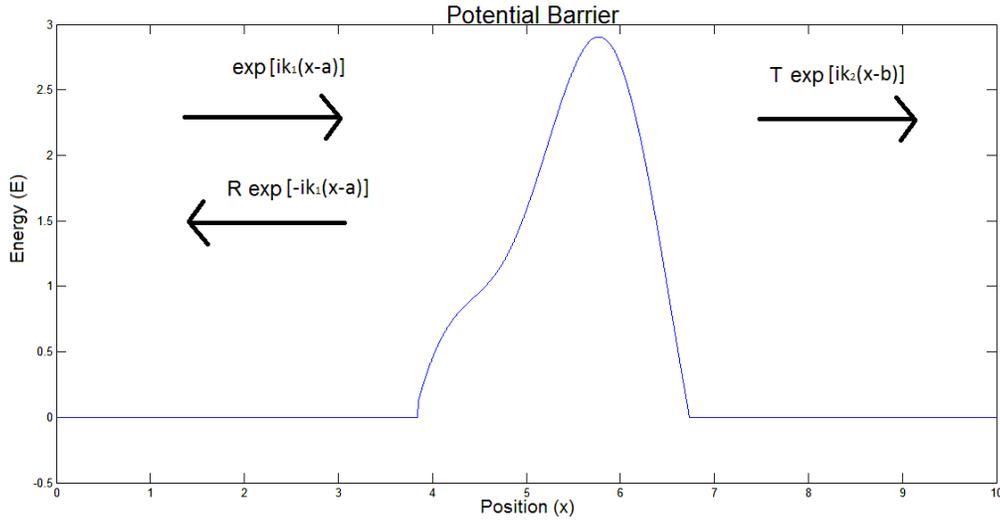


Figure 1. (Potential barrier and input-output wave functions. $a=3.85$, $b=6.73$)

We suppose that V is a real piecewise continuous function on \mathbb{R} , such that

$$V(x) = \begin{cases} V_1, & x \in (-\infty, a) \\ V_0(x), & x \in [a, b] \\ V_2, & x \in (b, +\infty) \end{cases}$$

We suppose for the definiteness, that $V_1 \leq V_2$. It yields that \mathcal{H} is a self-adjoint operator in $L^2(\mathbb{R})$ with a domain $H^2(\mathbb{R})$ with a continuous spectrum $[V_1, \infty)$.

We rewrite equation (1.1) as

$$\mathcal{H}_1 \psi(x) = \left(-\frac{d^2}{dx^2} + q(x) \right) \psi(x) = \lambda \psi(x), \lambda \in \mathbb{R}, x \in \mathbb{R}, \quad (1.2)$$

where

$$q(x) = \begin{cases} q_1, & x \in (-\infty, a) \\ q_0(x), & x \in [a, b] \\ q_2, & x \in (b, +\infty) \end{cases}$$

$$q_0(x) = \frac{2mV_0(x)}{\hbar^2}, q_j = \frac{2mV_j}{\hbar^2}, j = 1, 2, \lambda = \frac{2mE}{\hbar^2}.$$

Let the complete energy of the particle $E \in (V_2, \infty)$. It implies that $\lambda > q_2 \geq q_1$. We set

$$k_j = \sqrt{\lambda - q_j} > 0, j = 1, 2$$

We define the solutions of the equation (1.2) of the form

$$\psi(x) = \begin{cases} e^{ik_1(x-a)} + R e^{-ik_1(x-a)}, & x < a \\ c_1 \psi_1(x) + c_2 \psi_2(x), & x \in (a, b) \\ T e^{ik_2(x-b)}, & x > b \end{cases}, \quad (1.3)$$

where $\psi_1(x), \psi_2(x)$ are linearly independent solutions of equation (1.2) on (a, b) . The wave function $\psi(x)$ describes the process of the scattering of a particle with energy $E > V_2$ moving from the left to right. The complex number $R = R(\lambda)$ is called the reflection coefficient, and $T = T(\lambda)$ is called the transmission coefficient. We will find the coefficients R and T using the continuity of ψ and ψ' on \mathbb{R} . It is well known that the coefficients R and T satisfied the relation

$$|R|^2 + \frac{k_1}{k_2} |T|^2 = 1. \quad (1.4)$$

Let ψ_1, ψ_2 be linear independent solutions of (1.1) on $[a, b]$ satisfying the conditions of the Cauchy problem

$$\psi_1(a) = 1, \psi_1'(a) = 0, \quad (1.5)$$

$$\psi_2(a) = 0, \psi_2'(a) = 1. \quad (1.6)$$

Applying (1.3), (1.5), (1.6) we obtain the equations

$$1 + R = c_1, \quad (1.7)$$

$$ik_1(1 - R) = c_2,$$

$$T = c_1\psi_1(b) + c_2\psi_2(b),$$

$$ik_2T = c_1\psi_1'(b) + c_2\psi_2'(b).$$

Equations (1.7) imply that

$$(1 + R)\psi_1(b) + ik_1(1 - R)\psi_2(b) = T, \quad (1.8)$$

$$(1 + R)\psi_1'(b) + ik_1(1 - R)\psi_2'(b) = ik_2T,$$

and

$$R = \frac{\psi_1'(b) + k_2k_1\psi_2(b) + i[k_1\psi_2'(b) - k_2\psi_1(b)]}{k_2k_1\psi_2(b) - \psi_1'(b) + i[k_2\psi_1(b) + k_1\psi_2'(b)]}, \quad (1.9)$$

$$T = [(1 + R)\psi_1(b) + ik_1(1 - R)\psi_2(b)]. \quad (1.10)$$

It is clear that $k_j = k_j(\lambda) = \sqrt{\lambda - q_j} > 0, j = 1, 2, \psi_j(b) = \psi_j(b, \lambda), j = 1, 2$ and hence $R = R(\lambda), T = T(\lambda)$ depend on the spectral parameter $\lambda = \frac{2mE}{\hbar^2}$, and therefore from the energy E of the particle.

Remark 1.1. As usual the reflection and transmission coefficients are defined for wave functions ψ of the form

$$\psi(x) = \begin{cases} e^{-ik_1x} + R_1e^{ik_1x}, & x < a, \\ T_1e^{ik_2x}, & x > b. \end{cases}$$

Hence

$$R_1 = Re^{-2ik_1a}, T_1 = e^{-ik_2b}T,$$

and $|R| = |R_1|, |T| = |T_1|$.

There is an extensive literature devoted to finding the reflection and transmission coefficients by analytical and numerical methods (see for instance [1],[6], [7], [8], [15], [14], [16], [17], [18], etc.).

A numerical implementation of R and T are based on solutions of the Cauchy problem for the equation (1.2) on the interval (a, b) . Of course one can use the canonical Runge-Kutta method or its improving for the numerical calculation of solutions ψ_1, ψ_2 . But if we are interesting in the behavior of $R(\lambda), T(\lambda)$ on a large interval of the energy the Runge-Kutta method demands big machinery resources. In this paper solutions of Cauchy problem (1.5), (1.6) are sought of the form of a power series

$$\psi(z, \lambda) = \sum_{k=0}^{\infty} a_k(z) \lambda^k \quad (1.11)$$

with respect to a spectral parameter $\lambda \in \mathbb{C}$ with coefficients a_k defined by some recursive formulas (Spectral parameter power series method, abbreviated SPPS method). The SPPS method has been discovered by V.V. Kravchenko [11], [12] and has been successfully applied to different problems of Mathematical Physics which are reduced to spectral Sturm-Liouville problems [4], [5], [10], [13]. In [3] the SPPS method was applied to the analysis of electromagnetic waveguides.

The paper is organized as follows. In Section 2 we give some known analytical expressions for reflection and transmission coefficients R, T which will be used later for the comparison with R, T obtained by the SPPS method. Section 3 is devoted to the numerical calculations of R, T . We show that the results of calculations obtained by this method give a good coincidence with results obtained from analytical formulas.

2 Analytical form of the transmission and reflection coefficient

1⁰. *Rectangular barrier.* Let

$$V(x) = \begin{cases} U_0 > 0, x \in [0, b] \\ 0, x \notin [0, b] \end{cases},$$

and $E > U_0$. We set

$$k_1 = \frac{\sqrt{2mE}}{\hbar}, k_2 = \frac{\sqrt{2m(E - U_0)}}{\hbar}.$$

Then simple calculations taking into account the continuity of solutions and their derivatives of equation (1.1) implies the formulas for T and R (see for instance [18])

$$T = \left[1 + \frac{1}{4} \left(\frac{k_1^2 + k_2^2}{k_1 k_2} \right)^2 \sinh^2(k_2 b) \right]^{-1}, \quad (2.1)$$

$$R = \frac{1}{4} T \left(\frac{k_1^2 + k_2^2}{k_1 k_2} \right)^2 \sinh^2(k_2 b). \quad (2.2)$$

2⁰. *Potential* $V(x) = \frac{U_0}{\cosh^2(\alpha x)}$, where $U_0 > 0, \alpha > 0$ are constants. A graph of this potential is shown in Figure 2.

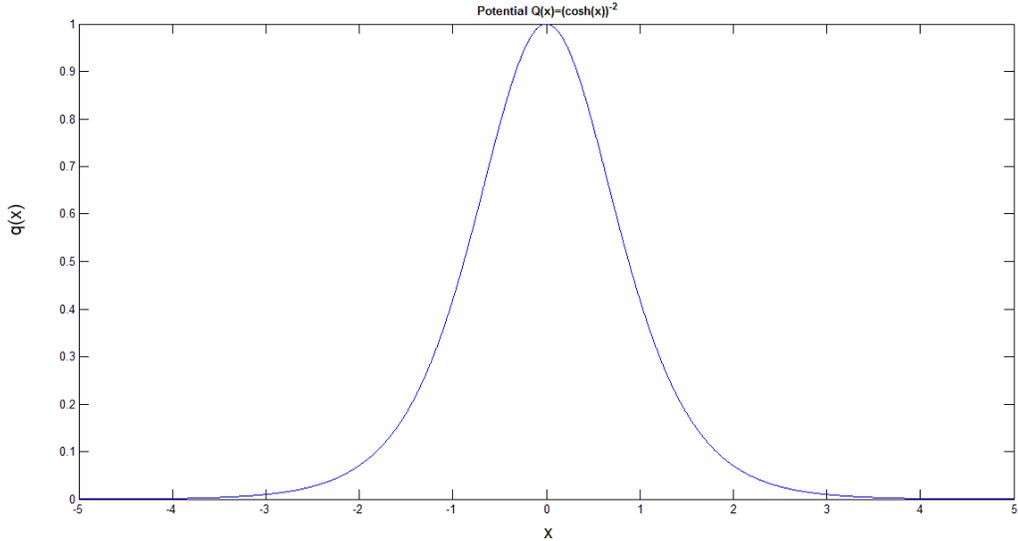


Figure 2. Graph of the potential $q(x) = \frac{U_0}{\cosh^2(\alpha x)}$ with $U_0 = 1 \text{ eV}$ and $\alpha = 1 \times 10^9 \text{ nm}^{-1}$ in the interval $x \in [-5, 5]$

This potential is not finite, but $V(x)$ is exponentially decreasing at infinity, that is

$$V(x) \leq C e^{-2\alpha|x|}, C > 0.$$

Then we can consider the solution ψ of the equation (1.1) with the asymptotics

$$\psi(x) \sim \begin{cases} e^{ikx} + R e^{-ikx}, & x \rightarrow -\infty \\ T e^{ikx}, & x \rightarrow +\infty \end{cases}, \quad k = \frac{\sqrt{2mE}}{\hbar},$$

where R and T are transmission and reflection coefficients. In the classical book [14] the solution $\psi(x)$ of equation (1.1) with potential $\frac{U_0}{\cosh^2(\alpha x)}$ has been obtained as

$$\psi(x) = (1 - \xi^2)^{-ik/2\alpha} F \left[(-ik/\alpha) - s, (-ik/\alpha) + s + 1, (-ik/\alpha) + 1, \frac{1}{2}(1 - \xi) \right] \quad (2.3)$$

where F is a hypergeometric function, $\xi = \tanh(\alpha x)$, $k = \frac{\sqrt{2mE}}{\hbar}$, and $s = \frac{1}{2} \left(-1 + \sqrt{1 - \frac{8mU_0}{\hbar^2 \alpha^2}} \right)$. The asymptotics of the solution $\psi(x)$ for $x \rightarrow -\infty$ is

$$\psi(x) \sim e^{-ikx} \frac{\Gamma(ik/\alpha) \Gamma(1 - (ik/\alpha))}{\Gamma(-s) \Gamma(1 + s)} + e^{ikx} \frac{\Gamma(-ik/\alpha) \Gamma(1 - (ik/\alpha))}{\Gamma((-ik/\alpha) - s) \Gamma((-ik/\alpha) + s + 1)}. \quad (2.4)$$

Taking into account that $\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin x\pi}$ one can obtain

$$|R|^2 = \frac{\cos^2 \left(\frac{1}{2} \pi \sqrt{1 - \frac{8mV_0}{\hbar^2 \alpha^2}} \right)}{\left[\sinh^2(\pi k/\alpha) + \cos^2 \left(\frac{1}{2} \pi \sqrt{1 - \frac{8mV_0}{\hbar^2 \alpha^2}} \right) \right]}, \quad (2.5)$$

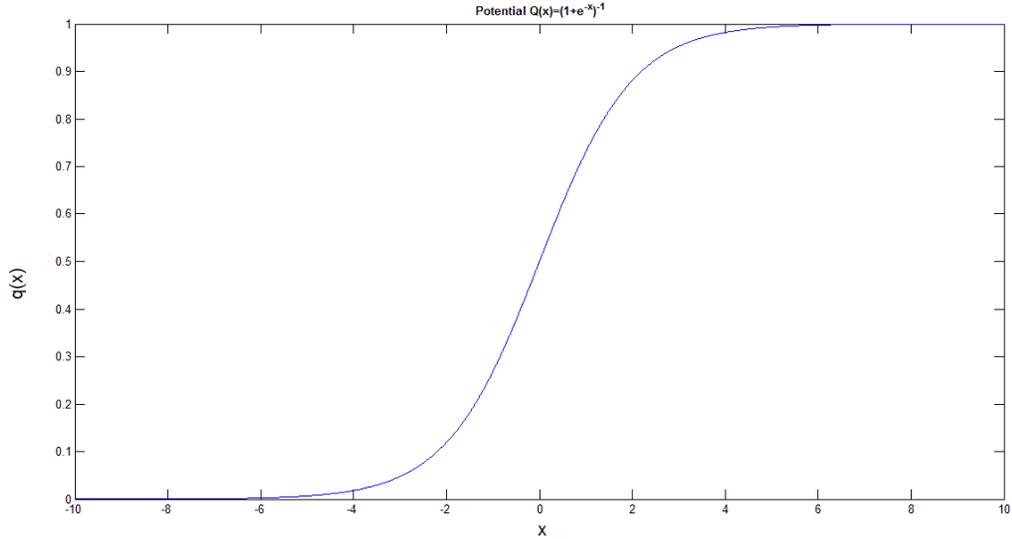


Figure 3. Graph of the potential $q(x) = \frac{U_0}{1+e^{-\alpha x}}$ with $U_0 = 1 \text{ eV}$ and $\alpha = 1 \times 10^9 \text{ nm}^{-1}$ in the interval $x \in [-10, 10]$

if $\frac{8mV_0}{\hbar^2\alpha^2} < 1$ and otherwise

$$|R|^2 = \frac{\cos^2\left(\frac{1}{2}\pi\sqrt{1 - \frac{8mV_0}{\hbar^2\alpha^2}}\right)}{\left[\sinh^2(\pi k/\alpha) + \cos^2\left(\frac{1}{2}\pi\sqrt{\frac{8mV_0}{\hbar^2\alpha^2} - 1}\right)\right]}. \quad (2.6)$$

Applying formula $|R|^2 + |T|^2 = 1$ we obtain that

$$|T|^2 = \frac{\sinh^2(\pi k/\alpha)}{\sinh^2(\pi k/\alpha) + \cos^2\left(\frac{1}{2}\pi\sqrt{1 - \frac{8mV_0}{\hbar^2\alpha^2}}\right)} \quad (2.7)$$

if $\frac{8mV_0}{\hbar^2\alpha^2} < 1$. Otherwise

$$|T|^2 = \frac{\sinh^2(\pi k/\alpha)}{\sinh^2(\pi k/\alpha) + \cos^2\left(\frac{1}{2}\pi\sqrt{\frac{8mV_0}{\hbar^2\alpha^2} - 1}\right)}. \quad (2.8)$$

3⁰. Potential $V(x) = \frac{U_0}{1+e^{-\alpha x}}$ where $U_0 > 0$, $\alpha > 0$ are constants. A graph of an example of this kind of potential is shown in Figure 3.

One can see that $\lim_{x \rightarrow -\infty} V(x) = 0$ and $\lim_{x \rightarrow +\infty} V(x) = U_0$. As above we consider so-

lutions of the equation (1.1) with the asymptotics

$$\psi(x) \sim \begin{cases} e^{ik_1x} + Re^{-ik_1x}, & x \rightarrow -\infty \\ Te^{ik_2x}, & x \rightarrow +\infty \end{cases},$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar}, k_2 = \frac{\sqrt{2m(E-U_0)}}{\hbar}, E > U_0.$$

Following to [14] the solution to the Schrödinger equation (1.1) with potential $V(x) = \frac{U_0}{1+e^{-\alpha x}}$ is equal to

$$\psi(x) = F \left[i[k_1 - k_2]/\alpha, -i[k_1 + k_2]/\alpha, \frac{-2ik_2}{\alpha} + 1, \xi \right]$$

where $\xi = -e^{-\alpha x}$, $k_1 = \frac{\sqrt{2mE}}{\hbar}$ and $k_2 = \frac{\sqrt{2m(E-U_0)}}{\hbar}$. The asymptotic form of the solution ($x \rightarrow -\infty$) is

$$u(x) \approx (-1)^{-ik_2/\alpha} [C_1 e^{ik_1x} + C_2 e^{-ik_1x}]$$

where

$$C_1 = \frac{\Gamma(-2ik_1/\alpha)\Gamma(-2ik_2/\alpha + 1)}{\Gamma(-i(k_1 + k_2)/\alpha)\Gamma(-i(k_1 + k_2)/\alpha + 1)}$$

$$C_2 = \frac{\Gamma(2ik_1/\alpha)\Gamma(-2ik_2/\alpha + 1)}{\Gamma(i(k_1 - k_2)/\alpha)\Gamma(i(k_1 - k_2)/\alpha + 1)}$$

and applying the formula $\Gamma(x)\Gamma(1-x) = \pi/\sin(\pi x)$ one can find the module of the reflection coefficient

$$|R|^2 = \left| \frac{C_2}{C_1} \right|^2 = \frac{\sinh^2(\pi(k_1 - k_2)/\alpha)}{\sinh^2(\pi(k_1 + k_2)/\alpha)}, k_1 > k_2. \quad (2.9)$$

Applying the formula (1.4) we obtain the module of the transmission coefficient

$$|T|^2 = \frac{k_2}{k_1}(1 - |R|^2). \quad (2.10)$$

3 Spectral parameter power series method (SPPS method)

We shortly describe here the SPPS method. Let

$$-\psi'' + q(x)\psi = \lambda\psi, x \in (a, b) \quad (3.1)$$

be a Schrödinger equation on the interval (a, b) with a piecewise continuous potential $q(x)$ on $[a, b]$. Since $q \in L^1([a, b])$ every generalized solution ψ of the equation (3.1) belongs to $C^{(1)}([a, b])$. Following to the SPPS method the general solution ψ of (3.1) is equal to

$$\psi = c_1\psi_1 + c_2\psi_2,$$

where C_1, C_2 are arbitrary complex constant, and

$$\begin{aligned}\psi_1 &= u_0 \sum_{n=0}^{\infty} \lambda^n \widetilde{X}^{(2n)}, \\ \psi_2 &= u_0 \sum_{n=0}^{\infty} \lambda^n X^{(2n+1)},\end{aligned}\tag{3.2}$$

where u_0 is a particular solution of equation (3.1) such that u_0 is a solution of the homogeneous equation

$$-u''(x) + q(x)u(x) = 0, \quad x \in (a, b),\tag{3.3}$$

such that $u_0^{-1} \in C([a, b])$. $\widetilde{X}^{(2n)}, X^{(2n+1)}$ are found by the recursive formulas

$$\begin{aligned}\widetilde{X}^{(0)} &\equiv 1, X^{(0)} \equiv 1, \\ \widetilde{X}^{(n)}(x) &= (-1)^{n-1} \int_a^x \widetilde{X}^{(n-1)}(s) (u_0^2(s))^{(-1)^{n-1}} ds, \\ X^{(n)}(x) &= (-1)^n \int_a^x X^{(n-1)}(s) (u_0^2(s))^{(-1)^n} ds.\end{aligned}\tag{3.4}$$

The solution u_0 can be find of the form

$$u_0 = y_1 + iy_2$$

where y_1 and y_2 are given by

$$y_1 = \sum_{n=0}^{\infty} \widetilde{Y}^{(2n)}, y_2 = \sum_{n=0}^{\infty} Y^{(2n+1)},$$

where

$$\begin{aligned}\widetilde{Y}^{(0)} &= 1, Y^{(0)} = 1, \\ \widetilde{Y}^{(n)}(x) &= \int_a^x \widetilde{Y}^{(n-1)}(s) (q(s))^{\frac{1+(-1)^{n-1}}{2}} ds, \\ Y^{(n)}(x) &= \int_a^x Y^{(n-1)}(s) (q(s))^{\frac{1+(-1)^n}{2}} ds.\end{aligned}$$

Applying particular solutions (3.2) of equation (3.1) we obtain the analytical expression for the reflection and transmission coefficients given by formulas (1.9), (1.10) where ψ_1, ψ_2 are defined by (3.2).

4 Numerical Implementation

We show here the results obtained using the SPPS method. For the numerical calculation of R and T we truncated the series in (3.2), that is

$$\begin{aligned}\psi_1 &= \psi_0 \sum_{n=0}^N \lambda^n \widetilde{X}^{(2n)}, \\ \psi_2 &= \psi_0 \sum_{n=0}^N \lambda^n X^{(2n+1)}.\end{aligned}\quad (4.1)$$

The calculations were performed in MATLAB and *spapi* routines for the calculations of the integrals in formulas (3.4).

In Figure 4 we present results for the reflection R and transmission T coefficients for a rectangular potential barrier which are obtained numerically by SPPS ($N = 120$) and compare with those obtained analytically. We considered a potential barrier $V_0 = 5 \text{ eV}$ and $a = 2 \text{ nm}$. The effective electron mass m is the effective mass of *GaAs* ($m = 0.067m_0 = 6.1030 \times 10^{-32} \text{ kg}$). Note that this material is widely used in the optoelectronics [1], [2], [9]. Tunneling occurs in the part of the graph corresponding to $E \in [0, 5] \text{ eV}$.

In Figure 5 we show the graphic of absolute errors versus the analytical values for the transmission and reflection coefficients of Figure 4.

In Figure 6 the results of the transmission coefficient T for the potential $\frac{U_0}{\cosh^2(\alpha x)}$ with values $U_0 = 1 \text{ eV}$ and $\alpha = 1 \times 10^9 \text{ nm}^{-1}$ obtained analytically and with SPPS are compared. For applying the SPPS method we changed $\frac{U_0}{\cosh^2(\alpha x)}$ by its truncation on the segment $[-5, 5] \text{ nm}$, because $\frac{U_0}{\cosh^2(\alpha x)} = 0$ for $|x| > 5$ with the precision machinery. For the comparison of the SPPS method and analytical method we apply formulas (2.5),(2.6),(2.7),(2.8) on the energy interval $[0, 1] \text{ eV}$.

In Figure 7 we show the absolute error for transmission coefficient of Figure 6.

In Figure 8 the results for the reflection coefficient R of the potential $\frac{U_0}{1+e^{-\alpha x}}$ with values $U_0 = 1 \text{ eV}$ and $\alpha = 1 \times 10^9 \text{ nm}^{-1}$ obtained analytically and with SPPS are compared. For the application of the SPPS method we change the potential $\frac{U_0}{1+e^{-\alpha x}}$ by

$$V(x) = \begin{cases} 0, & x < -10 \\ \frac{U_0}{1+e^{-\alpha x}}, & |x| \leq 10 \\ U_0, & x > 10 \end{cases},$$

because $\frac{U_0}{1+e^{-\alpha x}}$ coincides with $V(x)$ with the precision machinery.

In Figure 9 we show the absolute error for reflection coefficient of Figure 8.

In Table 1 we present the maximum absolute errors for the transmission and reflection coefficients that previously we showed.

Finally, we work with a double rectangular barrier potential with $V_0 = 5 \text{ eV}$ and width of the barriers $b = 2 \text{ nm}$. The graphic of the potential is shown in Figure 10 and the transmission coefficient T obtained with SPPS is shown in Figure 11.

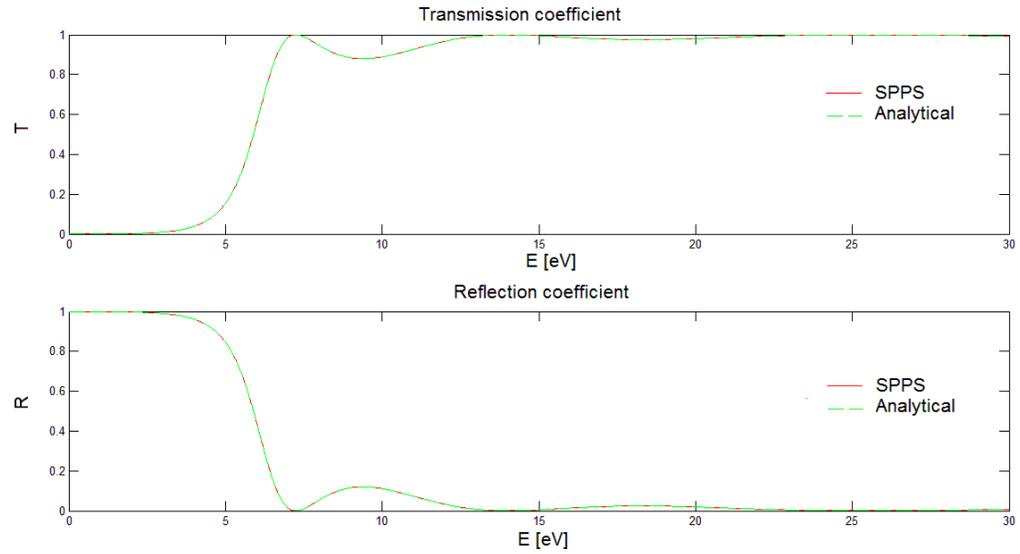


Figure 4. Comparison of the results for the reflection and transmission coefficients of a rectangular barrier potential ($V_0 = 5$ eV and $b = 2$ nm) obtained analytically and with SPPS.

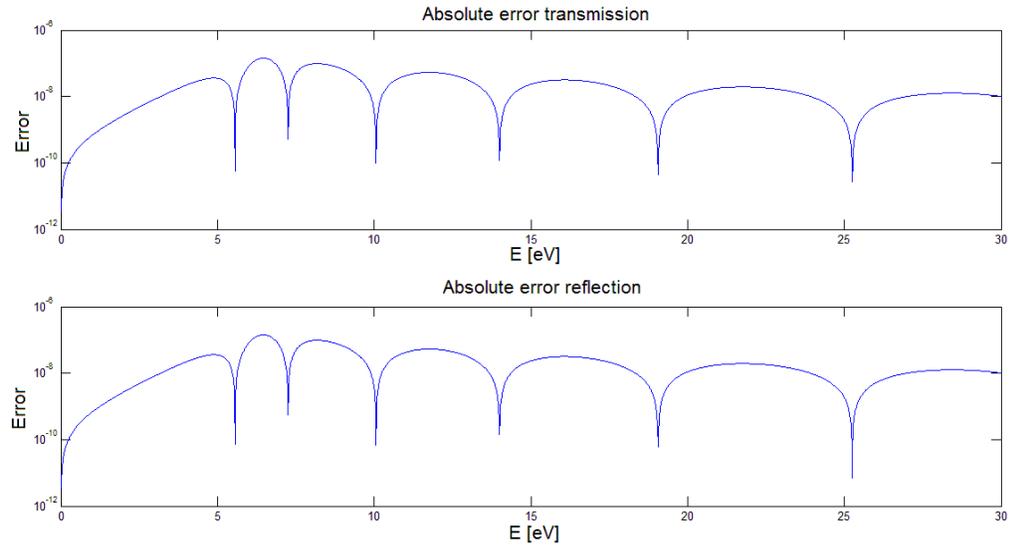


Figure 5. Absolute error for the SPPS results for coefficients of reflection R and transmission T of a rectangular barrier ($V_0 = 5$ eV and $b = 2$ nm).

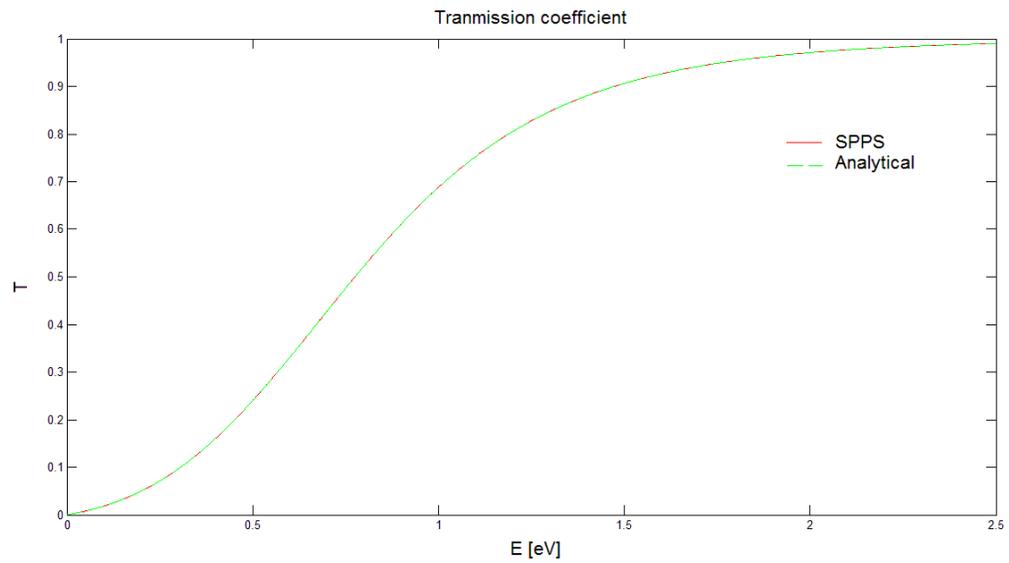


Figure 6. Comparison of the results for the transmission coefficient T for the potential $V_0(x) = \frac{U_0}{\cosh^2(\alpha x)}$ where $U_0 = 1 \text{ eV}$ and $\alpha = 1 \times 10^9 \text{ nm}^{-1}$ obtained analytically and with SPPS.

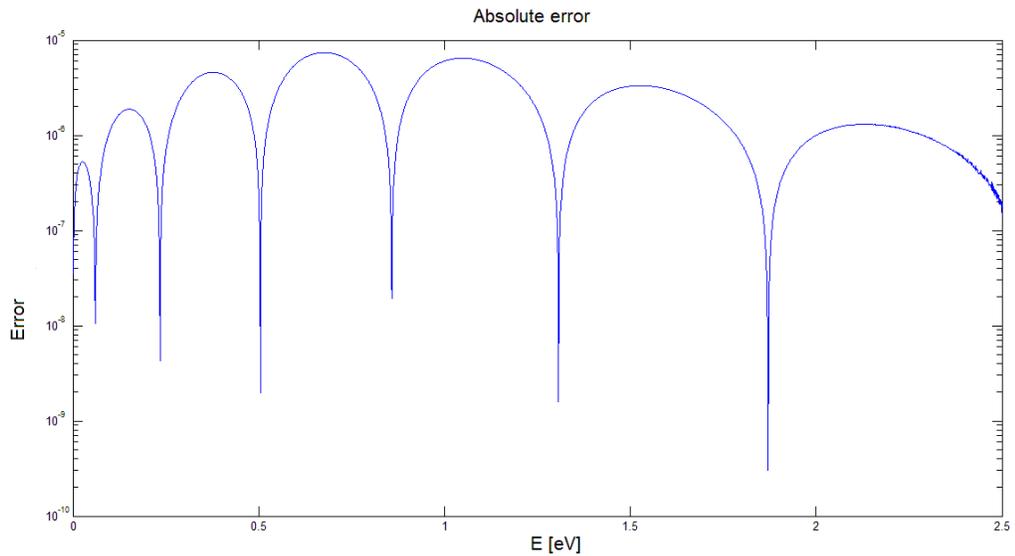


Figure 7. Absolute error for SPPS results for transmission coefficient T of the potential $V_0(x) = \frac{U_0}{\cosh^2(\alpha x)}$ where $U_0 = 1 \text{ eV}$ and $\alpha = 1 \times 10^9 \text{ nm}^{-1}$.

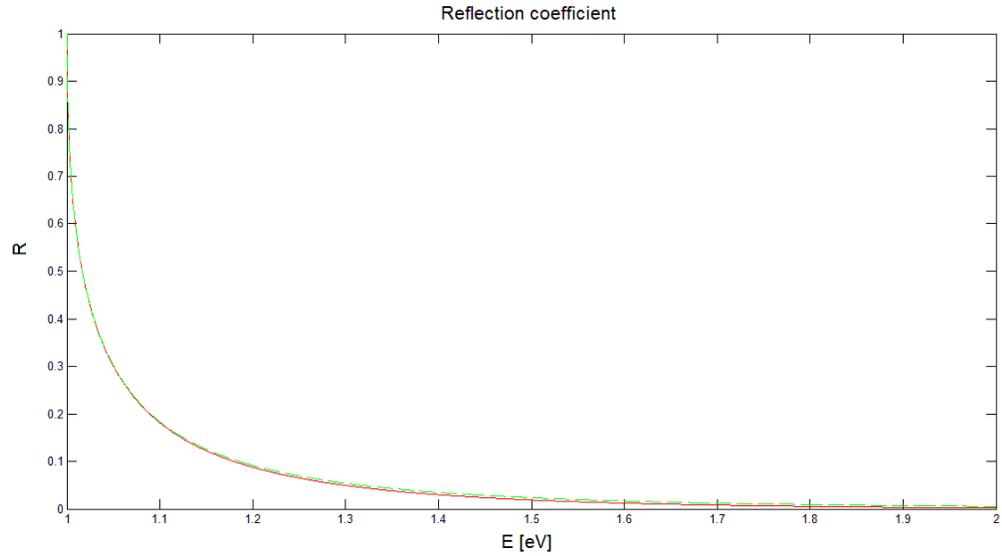


Figure 8. Comparison of the results for the reflection coefficient R for the potential $V_0(x) = \frac{U_0}{1+e^{-\alpha x}}$ where $U_0 = 1 \text{ eV}$ and $\alpha = 1 \times 10^9 \text{ nm}^{-1}$ obtained analytically and with SPPS.

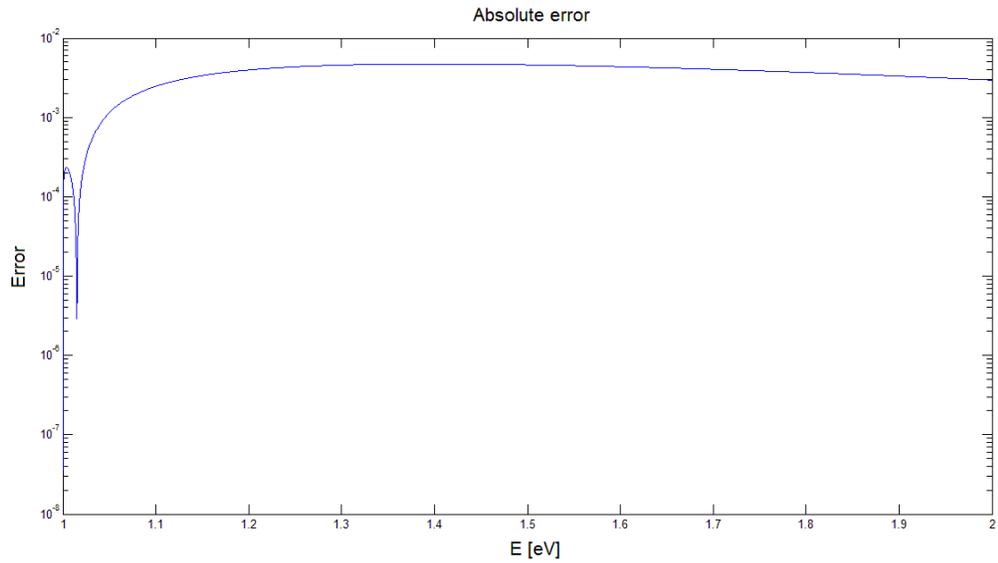


Figure 9. Absolute error of analytical and SPPS results for reflection coefficient R of the potential $V_0(x) = \frac{U_0}{1+e^{-\alpha x}}$ where $U_0 = 1 \text{ eV}$ and $\alpha = 1 \times 10^9 \text{ nm}^{-1}$.

Table 1. Absolute errors

$q(x)$	Maximum absolute error
5 eV (Reflection coefficient)	1.4451×10^{-7}
5 eV (Transmission coefficient)	1.4454×10^{-7}
$\frac{U_0}{\cosh^2(ax)}$	7.3972×10^{-6}
$\frac{U_0}{1+e^{-ax}}$	4.7137×10^{-3}

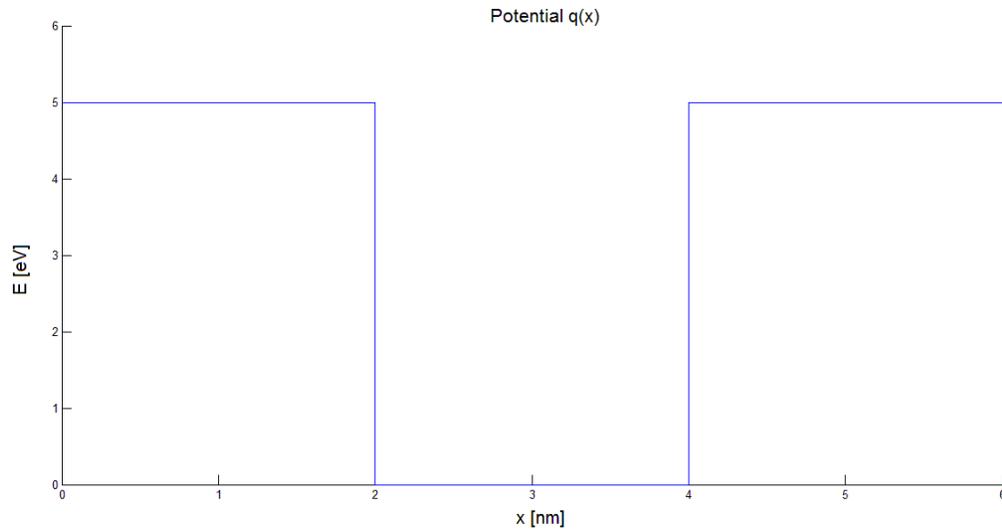


Figure 10. Graph of a double barrier potential with height $V_0 = 5 \text{ eV}$ and width of the every barrier $b = 2 \text{ nm}$.

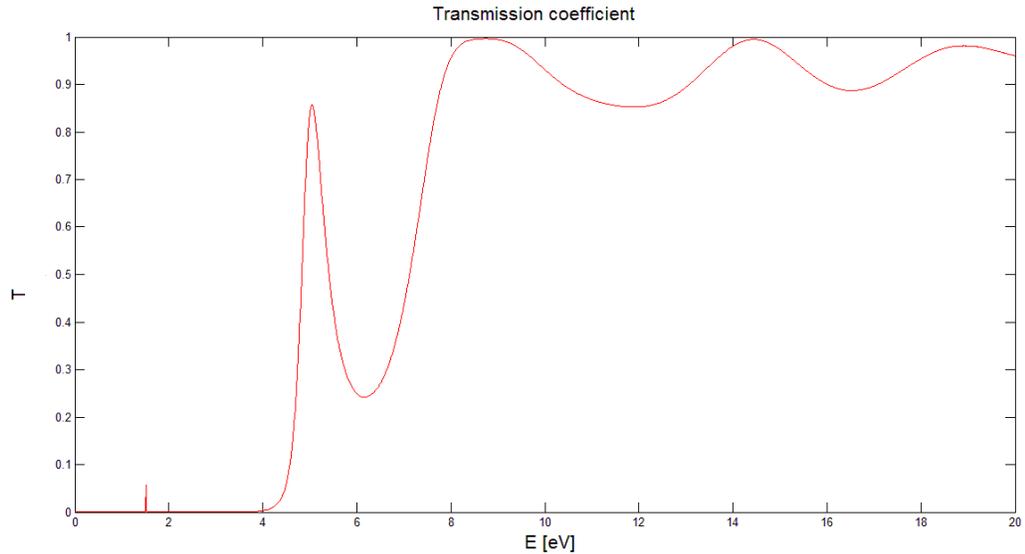


Figure 11. Transmission coefficient T for a double barrier potential obtained by means of SPPS.

5 Conclusions

We obtained the general formulas of transmission and reflection coefficients for a scattering of a particle on a potential barrier applying the SPPS method. We give a comparison of numerical results obtained by SPPS method with numerical results obtained from well known analytical formulas. The comparisons reveals a satisfactory performance of SPPS method for this kind of problems.

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