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Boundary conditions for one-dimensional Feshbach–Villars equation

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Abstract

We solve the one-dimensional Feshbach–Villars equation for spinless particle subjected to a scalar smooth potential. The wave function is given in terms of the hypergeometric function and via a limiting procedure, the wave functions of the step potential are deduced. Then, the appropriate boundary conditions for the step potential are deduced using the two-component form. © 2000 Published by Elsevier Science B.V. All rights reserved.

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Historically, the well-known relativistic wave equations are the second-order Klein–Gordon equation and the first order Dirac equation. They are used for the description of spinless and spin-1/2 particles respectively. Recently, many authors have been interested to others first order relativistic wave equations for the description of spinless, spin-1/2 and spin-1 particles, see [1–6] and [7] for historical notes. Among them, The Hamiltonian form of the Klein–Gordon equation, called the Feshbach–Villars (FV) equation [3,4]. This equation has been constructed in a two-component form for spinless particles [8] and in an eight-component form for spin-1/2 particles [3,4].

In order to linearize the Klein–Gordon equation to a first order equation in time, the following two-component form of the wave function has been introduced [8,9]

$$\psi(x,t) = \begin{pmatrix} \psi_1(x,t) \\ \psi_2(x,t) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \Phi + \frac{i}{m}\left(\frac{\partial}{\partial t} + ieV\right)\Phi \\ \Phi - \frac{i}{m}\left(\frac{\partial}{\partial t} + ieV\right)\Phi \end{pmatrix}, \qquad (1)$$

where $\Phi = \Phi(x,t)$ satisfies the Klein–Gordon equation.

This transformation is not unique [9,10]. The Hamiltonian form of the Klein–Gordon equation obtained by this procedure is the one-dimensional

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Feshbach–Villars equation defined by the Hamiltonian [8,9]

$$H=\frac{(\boldsymbol{P}-e\boldsymbol{A})^2}{2m}(\tau_3+i\tau_2)+m\tau_3+eV(x), \quad (2)$$

where $\boldsymbol{P}$ is the one-dimensional momentum, $(V,\boldsymbol{A})$ is the electromagnetic potential in one dimension and

$$\tau_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \tau_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \tau_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},$$

are the isospin Pauli matrices. The wave function $\psi(x,t)$ satisfy a Schrödinger-type equation

$$H\psi(x,t)=i\frac{\partial\psi(x,t)}{\partial t}. \quad (3)$$

We note that H is not Hermitian but that $H=\tau_3 H^{\dagger}\tau_3$.

The density ρ, the one-dimensional current j and the norm of the wave function are defined as follows

$$\rho=\bar{\psi}\psi,$$

$$j=\frac{1}{2im}\left[\bar{\psi}(\tau_3+i\tau_2)\frac{\partial\psi}{\partial x}-\frac{\partial\bar{\psi}}{\partial x}(\tau_3+i\tau_2)\psi -\frac{e}{m}A\bar{\psi}(\tau_3+i\tau_2)\psi\right],$$

$$(\psi,\psi)=\int\bar{\psi}\psi d^3V \quad \text{with} \quad \bar{\psi}=\psi^{\dagger}\tau_3,$$

ρ and j satisfy the continuity equation and ρ is interpreted as the charge density of the particle if the energy is positive or as the charge density of the anti-particle if the energy is negative. The positive solution ψ, the negative solution ψ_c, the charge density and the current are transformed by the charge conjugation as follows

$$\psi\to\psi_c=\tau_1\psi^{\dagger},\quad \rho\to\rho_c=-\rho \quad \text{and} \quad j\to j_c=j.$$

For example, if ψ describes the meson π then ψ_c describes the antiparticle meson π^+ and if $\psi=\psi_c$, it describes the neutral meson π^0.

In this Letter, we are interested by solving the one-dimensional Feshbach–Villars equation for spinless particle (FV-0) in interaction with the scalar step potential $V(x)=V_0\theta(x)$. If we try to find the exact expressions of the wave function in the two regions using the 'naive' boundary conditions, the continuity of ψ_1 and ψ_2 and their first derivatives at $x=0$, the unique solution found is the trivial one $\psi_1=\psi_2=0$.

Then, another method is used to find the wave functions of the step potential without using boundary conditions. We solve the one-dimensional Feshbach–Villars equation for spinless particle (FV-0) in interaction with the scalar smooth potential [11–13]

$$V(x)=\frac{V_0}{2}\left(1+\tanh\frac{x}{2r}\right), \quad (4)$$

where V_0 and r are positive constants.

In the limiting case $r\to 0$, $V(x)\to V_0\theta(x)$. The smooth potential is a good approximation for the step potential and it is used in many physical applications [12,13]. It increases from the value $V=0$ for $x=-\infty$ to the value $V=V_0$ for $x=+\infty$, the main rise occurring in the interval $-2r<x<+2r$: $V(-2r)=0.1192V_0$, $V_0(2r)=0.8807V_0$.

We find that the solution of FV equation for the smooth potential is given in terms of the hypergeometric function and the wave functions for the step potential in each region are deduced via a limiting procedure. Then, the appropriate boundary conditions for the step potential are calculated using the definition of the two-component form (1) and the continuity of the Klein–Gordon wave function and its first derivative at $x=0$. At the end, we use the wave functions of the step potential to test the validity of these boundary conditions. On the other hand, we note that the problem of boundary conditions is avoided if the step potential is treated via path integral method in relativistic two-component theory (FV-0) [14].

The one-dimensional Feshbach-villars Hamiltonian for spinless particle subjected to the scalar smooth potential (4) is

$$H=\frac{P^2}{2m}(\tau_3+i\tau_2)+m\tau_3+eV(x). \quad (5)$$

The stationary solution has the form $\psi(x,t)=e^{-iEt}\psi(x)$ and Eq. (3) is equivalent to the following coupled differential equations

$$E\psi_1 = -\frac{1}{2m}\frac{d^2}{dx^2}(\psi_1+\psi_2) + m\psi_1 + eV(x)\psi_1, \tag{6}$$

$$E\psi_2 = +\frac{1}{2m}\frac{d^2}{dx^2}(\psi_1+\psi_2) - m\psi_2 + eV(x)\psi_2. \tag{7}$$

Putting $\varphi_s = \psi_1+\psi_2$ and $\varphi_d = \psi_1-\psi_2$ we deduce $\psi_1=\frac{1}{2}(\varphi_s+\varphi_d)$, $\psi_2=\frac{1}{2}(\varphi_s-\varphi_d)$.

The sum of Eqs. (6), (7) gives

$$\varphi_d(x) = \left[\frac{E-eV(x)}{m}\right]\varphi_s(x). \tag{8}$$

For the difference of Eqs. (6), (7) and using Eq. (8), we have

$$\frac{d^2\varphi_s(x)}{dx^2} + \left[[E-eV(x)]^2 - m^2\right]\varphi_s(x) = 0. \tag{9}$$

In order to find the solution of the differential equation (9), we make the change of variable

$$y = \frac{1}{2}\left(1-\tanh\frac{x}{2r}\right), \tag{10}$$

which maps the interval $x\in]-\infty,+\infty[$ to $y\in]0,1[$. The new form of Eq. (9) is

$$\frac{1}{r^2}y^2(1-y)^2\frac{d^2\varphi_s(y)}{dy^2} + \frac{1}{r^2}y(1-y)(1-2y)\frac{d\varphi_s(y)}{dt} + \left[(E+eV_0y-eV_0)^2 - m^2\right]\varphi_s(y) = 0.$$

The singularities of this differential equation are $y=0,1,\infty$. Let us introduce the change $\varphi_s(y)=y^\nu\times(1-y)^\mu f(y)$, the last equation is reduced to the Hypergeometric equation form

$$y(1-y)\frac{d^2f(y)}{dy^2} + [(2\nu+1) - y(2\nu+2\mu+2)]\frac{df(y)}{dt} - \left[\left(\mu+\nu+\tfrac{1}{2}\right)^2 - \frac{\upsilon_0^2}{4}\right]f(y) = 0. \tag{11}$$

where $\nu^2 = r^2[m^2-(E-eV_0)^2]$, $\mu^2 = r^2(m^2-E^2)$, $\upsilon_0 = \sqrt{(1-2reV_0)(1+2reV_0)}$.

The general solution of Eq. (11) is given in terms of the hypergeometric function

$$\varphi_s(y) = Cy^\nu(1-y)^\mu\,{}_2F_1\left(\mu+\nu+\frac{1}{2}-\frac{\upsilon_0}{2}, \nu+\mu+\frac{1}{2}+\frac{\upsilon_0}{2}, 1+2\nu, y\right) + Dy^{-\nu}(1-y)^\mu\,{}_2F_1\left(\mu-\nu+\frac{1}{2}-\frac{\upsilon_0}{2}, \mu-\nu+\frac{1}{2}+\frac{\upsilon_0}{2}, 1-2\nu, y\right),$$

where C and D are constants.

We choose the regular solution at the origin $y=0$

$$\varphi_s(y) = Cy^\nu(1-y)^\mu\,{}_2F_1\left(\nu+\mu+\frac{1}{2}-\frac{\upsilon_0}{2}, \nu+\mu+\frac{1}{2}+\frac{\upsilon_0}{2}, 1+2\nu, y\right). \tag{12}$$

Then, the final form of the two-component wave function solution of the FV-0 equation is

$$\psi(y) = \frac{C}{2m}\begin{pmatrix} m+E-V_0(1-y) \\ m-E+V_0(1-y)\end{pmatrix} y^\nu(1-y)^\mu \times {}_2F_1\left(\nu+\mu-\frac{\upsilon_0}{2}+\frac{1}{2}, \nu+\mu+\frac{\upsilon_0}{2}+\frac{1}{2}, 1+2\nu, y\right). \tag{13}$$

Now, we write the final solution with the initial variable x

$$\psi(x) = \frac{C}{2m}\begin{pmatrix} m+E-\frac{eV_0}{2}\left(1+\tanh\frac{x}{2r}\right) \\ m-E+\frac{eV_0}{2}\left(1+\tanh\frac{x}{2r}\right)\end{pmatrix}$$
$$\times\left[\frac{1}{2}\left(1-\tanh\frac{x}{2r}\right)\right]^{\nu}\left[\frac{1}{2}\left(1+\tanh\frac{x}{2r}\right)\right]^{\mu}$$
$$\times {}_2F_1\left(\nu+\mu-\frac{v_0}{2}+\frac{1}{2}, \nu+\mu+\frac{v_0}{2}+\frac{1}{2},\right.$$
$$\left.1+2\nu, \frac{1}{2}\left(1-\tanh\frac{x}{2r}\right)\right). \tag{14}$$

We study now the asymptotic behavior of the wave function when $x\to\pm\infty$. First, when $x\to-\infty$ or $y\to 1$, we have $(1-y)\approx\exp(x/r)$; we use the property of the hypergeometric function which links the y and $(1-y)$ argument,

$${}_2F_1(a,b,c,y) = A_1\,{}_2F_1(a,b,a+b-c+1,1-y)$$
$$+A_2(1-y)^{c-a-b}$$
$$\times {}_2F_1(c-a,c-b,c-a-b+1,1-y)$$

with

$$A_1 = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)}$$
$$= \frac{\Gamma(2\nu+1)\Gamma(2\mu)}{\Gamma\left(\nu-\mu+\frac{v_0}{2}+\frac{1}{2}\right)\Gamma\left(\nu+\mu-\frac{v_0}{2}+\frac{1}{2}\right)},$$

$$A_2 = \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}$$
$$= \frac{\Gamma(2\nu+1)\Gamma(-2\mu)}{\Gamma\left(\nu+\mu-\frac{v_0}{2}+\frac{1}{2}\right)\Gamma\left(\nu+\mu+\frac{v_0}{2}+\frac{1}{2}\right)}$$

$$\lim_{y\to1} y^{\nu} = 1 \quad \lim_{y\to1}(1-y)^{\mu}$$
$$= \lim_{x\to-\infty}\left(\frac{\exp(x/r)}{1+\exp(x/r)}\right)^{\mu} = e^{\mu x/r}$$

$$\lim_{y\to1}(1-y)^{-\mu} = e^{-\mu x/r} \quad \text{and} \quad {}_2F_1(a,b,c,0) = 0.$$

Thus, when $x\to-\infty$ or $y\to1$, the wave function has the following behavior

$$\psi(x) \underset{x\to-\infty}{\to} \frac{C}{2m}\left[A_1 e^{\mu x/r} + A_2 e^{-\mu x/r}\right]\begin{pmatrix} m+E \\ m-E\end{pmatrix}. \tag{15}$$

Setting $\mu = -irk_1$, with $k_1^2 = E^2 - m^2$ where k_1 is real

$$\psi(x) \underset{x\to-\infty}{\to} \frac{C}{2m}\left[A_2 e^{ik_1x} + A_1 e^{-ik_1x}\right]\begin{pmatrix} m+E \\ m-E\end{pmatrix}. \tag{16}$$

For the limit when $x\to+\infty$, or $y\to0$, the hypergeometric function is equal to 1,

$$\lim_{y\to0} y^{\nu} = \lim_{x\to+\infty}\left(\frac{1}{1+\exp(x/r)}\right)^{\nu}$$
$$= \lim_{x\to+\infty}\left(e^{-x/r}\right)^{\nu} = e^{-\nu x/r} \quad \text{and}$$

$$\lim_{y\to0}(1-y)^{\mu} = \lim_{x\to+\infty}\left(1-\frac{1}{1+\exp(x/r)}\right)^{\mu}$$
$$= \lim_{x\to+\infty}\left(\frac{\exp(x/r)}{1+\exp(x/r)}\right)^{\mu} = 1.$$

Then the wave function has the following behavior:

$$\psi(x) \underset{x\to+\infty}{\to} \frac{C}{2m}e^{-\nu x/r}\begin{pmatrix} m+E-eV_0 \\ m-E+eV_0\end{pmatrix}. \tag{17}$$

Setting $\nu = -irk_2$, with $k_2^2 = \left[(E-eV_0)^2 - m^2\right]$ while k_2 is real for $E < eV_0 - m$ or $E > eV_0 + m$ and k_2 is imaginary for $eV_0 - m < E < eV_0 + m$. Then, the wave function is

$$\psi(x) \underset{x\to+\infty}{\to} \frac{C}{2m}e^{ik_2x}\begin{pmatrix} m+E-eV_0 \\ m-E+eV_0\end{pmatrix}. \tag{18}$$

The reflection and transmission coefficients can be calculated from the current density in the one-dimensional case

$$j = \frac{1}{2im}\left[\left(\psi_1^{\dagger}+\psi_2^{\dagger}\right)\frac{\partial}{\partial x}(\psi_1+\psi_2)\right.$$
$$\left.-(\psi_1+\psi_2)\frac{\partial}{\partial x}\left(\psi_1^{\dagger}+\psi_2^{\dagger}\right)\right], \tag{19}$$

where $\psi_1^\dagger$ and $\psi_2^\dagger$ are the ordinary complex conjugate of ψ_1 and ψ_2.

Using the last definition (19) of the current and the incident wave, we find that the incident current is

$$j_{\mathrm{inc}} = \frac{k_1}{m} |C|^2 |A_2|^2.$$

The reflected current is evaluated using the reflected wave

$$j_{\mathrm{ref}} = -\frac{k_1}{m} |C|^2 |A_1|^2.$$

Then, the reflection coefficient is

$$R = \frac{|j_{\mathrm{ref}}|}{|j_{\mathrm{inc}}|} = \frac{|A_1|^2}{|A_2|^2}.$$

The transmission coefficient is evaluated in terms of the transmitted wave

$$j_{\mathrm{tr}} = \frac{1}{2m}\left(k_2 + k_2^\dagger\right) |C|^2 \exp ix\left(k_2 - k_2^\dagger\right).$$

If k_2 is real

$$j_{\mathrm{tr}} = \frac{1}{m} k_2 |C|^2$$

and the transmission coefficient T is

$$T = \frac{|j_{\mathrm{tr}}|}{|j_{\mathrm{inc}}|} = \frac{k_2}{k_1 |A_2|^2}.$$

If k_2 is imaginary

$$j_{\mathrm{tr}} = 0, \quad T = 0 \quad \text{and} \quad R = 1.$$

In this case we have a total reflection.

We consider now the limiting case when the smooth potential tends to step potential, i.e., when the parameter r tends to 0.

For the first region $x < 0$, the limit of the wave function (16) when $r \to 0^+$ is

$$\psi(x) = \frac{C(k_1 + k_2)}{4mk_1} \theta(-x) \left[\exp(ik_1 x) + \frac{k_1 - k_2}{k_1 + k_2} \exp(-ik_1 x)\right] \begin{pmatrix} m+E \\ m-E \end{pmatrix}, \tag{20}$$

where $\lim_{r \to 0^+} A_1 = \frac{k_1 - k_2}{2k_1}$, $\lim_{r \to 0^+} A_2 = \frac{k_1 + k_2}{2k_1}$.

For the second region $x > 0$, the wave function is the same as Eq. (18)

$$\psi(x) = \frac{C}{2m} e^{ik_2 x} \begin{pmatrix} m + E - eV_0 \\ m - E + eV_0 \end{pmatrix}. \tag{21}$$

Then, the wave function can be written in compact form for the two regions

$$\psi(x) = \frac{C(k_1 + k_2)}{4mk_1} \left\{ \theta(-x) \left[\exp(ik_1 x) + \frac{k_1 - k_2}{k_1 + k_2} \exp(-ik_1 x)\right] + \theta(x) \frac{2k_1}{k_1 + k_2} \exp(ik_2 x) \right\} \times \begin{pmatrix} m + E - eV_0 \theta(x) \\ m - E + eV_0 \theta(x) \end{pmatrix}. \tag{22}$$

At the end, the reflection coefficient R and the transmission coefficient T for the step potential are

- for k_2 real and $E < eV_0 - m$, we have

  $$R = \frac{(k_1 + k_2)^2}{(k_1 - k_2)^2}, \quad T = \frac{4k_1 k_2}{(k_1 - k_2)^2},$$

  and $R - T = 1$,

  which is the well known Klein's Paradox.
- for k_2 real and $E > eV_0 + m$, we have

  $$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}, \quad T = \frac{4k_1 k_2}{(k_1 + k_2)^2},$$

  and $R + T = 1$.

For the special case of free particle $V_0 = 0$, $k_1 = k_2$, the wave function is

$$\psi(x) = \frac{C}{2m} \begin{pmatrix} m+E \\ m-E \end{pmatrix} \exp(ik_1 x).$$

From the waves functions (20) and (21) of the step potential, it's easy to note that the components of the wave function $\psi(x)$ and their first derivatives satisfy the following boundary conditions at $x = 0$

$$\psi_1(0^+) + \psi_2(0^+) = \psi_1(0^-) + \psi_2(0^-),$$

$$\psi_1'(0^+) + \psi_2'(0^+) = \psi_1'(0^-) + \psi_2'(0^-),$$

where $\psi_{1,2}'(0^\pm) = d\psi_{1,2}/dx$ at $x = 0^\pm$.

These boundary conditions seem to be particulars and in the following we are going to look for more general boundary conditions for the step potential using the two-component form, the continuity of the Klein–Gordon wave function and its derivative.

From the definition (1) of the two-component form of the wave function it follows that

$$\Phi = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2), \tag{23}$$

$$\left(i\frac{\partial}{\partial t} - eV\right)\Phi = \frac{m}{\sqrt{2}}(\psi_1 - \psi_2). \tag{24}$$

The stationary Klein–Gordon function $\Phi(x,t)$ has the form $\Phi(x,t) = e^{-iEt}\Phi(x)$ and the last equation is written as

$$(E - eV)\Phi = \frac{m}{\sqrt{2}}(\psi_1 - \psi_2). \tag{25}$$

The continuity of the Klein–Gordon wave function Φ defined in Eq. (23) and its derivative at $x=0$ give

$$\psi_1(0^+) + \psi_2(0^+) = \psi_1(0^-) + \psi_2(0^-), \tag{26}$$

$$\psi_1'(0^+) + \psi_2'(0^+) = \psi_1'(0^-) + \psi_2'(0^-). \tag{27}$$

The continuity of the Klein–Gordon wave function Φ defined in Eq. (25) and its derivative at $x=0$ give

$$\psi_1(0^+) - \psi_2(0^+) = \frac{E - eV_0}{E}(\psi_1(0^-) - \psi_2(0^-)), \tag{28}$$

$$\psi_1'(0^+) - \psi_2'(0^+) = \frac{E - eV_0}{E}(\psi_1'(0^-) - \psi_2'(0^-)). \tag{29}$$

From Eqs. (26) and (28) we can write the boundary conditions in the matrix form

$$\begin{pmatrix} \psi_1(0^+) \\ \psi_2(0^+) \end{pmatrix} = \begin{pmatrix} 1 - \frac{eV_0}{2E} & \frac{eV_0}{2E} \\ \frac{eV_0}{2E} & 1 - \frac{eV_0}{2E} \end{pmatrix} \begin{pmatrix} \psi_1(0^-) \\ \psi_2(0^-) \end{pmatrix}, \tag{30}$$

and from Eqs. (27) and (29) we have also the matrix form for the derivatives

$$\begin{pmatrix} \psi_1'(0^+) \\ \psi_2'(0^+) \end{pmatrix} = \begin{pmatrix} 1 - \frac{eV_0}{2E} & \frac{eV_0}{2E} \\ \frac{eV_0}{2E} & 1 - \frac{eV_0}{2E} \end{pmatrix} \begin{pmatrix} \psi_1'(0^-) \\ \psi_2'(0^-) \end{pmatrix}. \tag{31}$$

The two last boundary conditions can be combined in the same equation as

$$\begin{pmatrix} \psi_1(0^+) + i\psi_1'(0^+) \\ \psi_2(0^+) + i\psi_2'(0^+) \end{pmatrix} = \begin{pmatrix} 1 - \frac{eV_0}{2E} & \frac{eV_0}{2E} \\ \frac{eV_0}{2E} & 1 - \frac{eV_0}{2E} \end{pmatrix} \begin{pmatrix} \psi_1(0^-) + i\psi_1'(0^-) \\ \psi_2(0^-) + i\psi_2'(0^-) \end{pmatrix}. \tag{32}$$

We verify that the wave functions (20) and (21) of the step potential satisfy these boundary conditions and the current j is continuous

$$j(0^+) = j(0^-),$$

but the charge density ρ is discontinuous

$$\rho(0^+) \neq \rho(0^-).$$

These boundary conditions can be interpreted by analogy with electromagnetic waves (when they traverse two different regions) as follows: the sum of the two components $\varphi_s = \psi_1 + \psi_2$ and its derivative are continuous like the tangential component of the electric field. On the other hand, the difference of the two components $\varphi_d = \psi_1 - \psi_2$ and its derivative are discontinuous like the normal component of the magnetic field.

In summary, in order to find the wave functions of the step potential without the use of boundary conditions, we introduce the smooth potential as an intermediate stage. Then, we solve the one-dimensional Feshbach–Villars equation for spinless particle subjected to the smooth potential. The two component wave function is given in terms of the hypergeometric function. In the limiting case $r \to 0$, the wave functions of the step potential are deduced in each region. Boundary conditions relative to the step potential are extracted using the two-component form, the continuity of the Klein–Gordon wave function and its derivative at $x = 0$. The main result is that boundary conditions for the step potential are:

- the sum of the two components $\varphi_s = \psi_1 + \psi_2$ and its derivative are continuous

$$\varphi_s(0^+) = \varphi_s(0^-), \quad \varphi_s'(0^+) = \varphi_s'(0^-),$$

- the difference of the two components $\varphi_d = \psi_1 - \psi_2$ and its derivative are discontinuous

$$\varphi_d(0^+) = \frac{E - eV_0}{E} \varphi_d(0^-),$$

$$\varphi_d'(0^+) = \frac{E - eV_0}{E} \varphi_d'(0^-).$$

By the same method, this result can be generalized to the step potential defined in the first region by the constant potential V_1 and in the second region by the constant potential V_2.

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