

## **An alternative derivation of the quantum Green's function for a potential presenting a jump**

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### **Abstract**

New derivation of Green's function relative to a moving quantum particle in step potential is derived. This method stands on the resolution of a singular integral equation. With the help of the Wigner-Hopf and Hilbert theorems, we have obtained the Green function of the problem. As an application, we have derived from the Green function, the transmission and reflexion coefficient both for  $E > V_0$  and  $E < V_0$ .

**AMS subject classification:**

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### **1. Introduction**

Green's functions are very useful in the studies of linear partial differential equations and are widely studied from the point of view of fundamental solutions of these equations. They provide a general method for solving the linear differential equations or equivalently the integral equations. They are widely used in quantum mechanics to discover the energy spectra (the eigen values) of physical system and the associated eigen functions. In mathematics the term Green's functions is often attributed to solutions of an initial- or boundary-value problem of a linear differential equation with a  $\delta$ -function as an inhomogeneous term. Some times we encounter, in various fields of mathematics, physics, applied physics, physical chemistry and engineering, the terms: propagator, resolvent, resolvent kernel, signal function, point response function, or transfer function. These terms are nothing but the Green functions spelled differently with respect of the field. Strictly saying, the Green function serves to find the output for a given input. For this reason, one can understand why Green's functions are very useful in many

fields: in electromagnetism, hydrodynamics, acoustics, elasticity, quantum mechanics, elementary-particle physics, etc.... Their usefulness is still growing ascendentely today, as various numerical techniques increase to develop the calculations of Green's functions. Recall that there are usually several Green's functions associated with the same equation. These difference is related to the boundary conditions. Therefore it is important, when we search the Green function associated to the linear differential equation, to specify the boundary conditions. In quantum mechanics, it exist an alternative method to compute the Green's function. It is based on the well known propagator theory or the path integrals techniques [1].

Before starting to give the outlook of our paper, it is better to mention some works that use these techniques to calculate Green's functions: the exact Green's function for the delta-function potential problem [2], for the non-relativistic Coulomb system [3]. Also these techniques were successfully used for deriving the Green's function for the inverse square potential [4]. At this stage we mention that [5], [6] have derived Green function and the propagator for the step potential by solving the Schroedinger equation directly; [7] also derived Green function of the same potential but by using the  $\delta$ -perturbation method on the Wood–Saxon potential and passing in the limit  $R \rightarrow 0$  and also [8] using the combinatorial approach derived Green function of the problem.

In this work we shall present, an explicit calculation of the Green's function, for a piecewise continuous potential presenting a jump. The new here, is the use of the singular integral equations, to calculate the Green's function. The singularity of the integral equations comes from the fact that the Schroedinger operator has a jump. In our work, we address the problem of a time-independant Schroedinger equation in one dimension with a piecewise continuous potential presenting a jump: zero constant for  $x < 0$ , and positive constant  $V_0$  for  $x > 0$ . In quantum mechanics, if the potential has a such jump, the solution of the time-independant Schroedinger equation is continuous and its derivative is discontinuous on the boundary (the edge located at  $x = 0$ ). Specify one more thing in our problem: the time-independant Schroedinger equation takes two different forms depending on whether it is at left or right of  $x = 0$ . This kind of problem matches in quantum mechanics to the study of a particle subject to a potential which is a piecewise continuous possessing a jump: a step potential.

In Section 2, we present a theoretical framework in which our work is focused. In particular we show how the Schroedinger equation transforms to an integral equation and how the latter can be solved using the the theorem of Hilbert and Wigner-Hopf and therefore the bi-sided Laplace transform. In section 3, we calculate Green's functions corresponding to the potential zero for  $x < 0$  and equal to  $V_0$  for  $x > 0$ . At the end, we finish this work by conclusions in Section 4.

## 2. Analytic functions sectionally continuous

In this section we will use the theory related to the analytic functions from Ref. [9] and those related to the singular integral equation from Ref. [10].

Definition: A function  $\Phi$  on  $R^2$  is called sectionally continuous, (s.continuous) with

respect an arc or a contour  $L$ , if it is continuous at any point  $\mathbf{z}$ ,  $z \in \mathbb{R}^2 - L$ , and if it is continuous to the edge on either side of the arc or the contour  $L$  (excepting eventually the two ends of the arc).

### 2.1. Hilbert problem

Let  $L$  be a contour or an arc (or an infinite line). Hilbert's problem consists of the search for an s.analytic function  $\Phi$  with respect to the curve  $L$ . We also require it to have a growth at the most polynomial at infinity and to verify the following equation:

$$\Phi_i(z) = A(z)\Phi_e(z) + B(z), \quad z \in L, \quad (2.1)$$

where  $A(z)$  and  $B(z)$  are given functions operating on the curve  $L$ . The functions  $\Phi_i(z)$  and  $\Phi_e(z)$  are the external and internal limits at the edge  $L$ . The Hilbert problem is called to be homogeneous if  $B(z) \equiv 0$ . We will assume throughout this paragraph that  $A$  has no zeros on curve  $L$ .

### 2.2. Hilbert problem in the case of line

We examine the solution of the Hilbert problem (2.1) in the case of the line  $L$  whose equation is  $Re(z) = b$ . The solutions of the homogeneous problem are given via the following proposition:

**Proposition 2.1.** Let  $A(z)$  holderian on the line  $Re(z) = b$ , not vanishes on that line and verifies:

$$A(z) = 1 + o\left(\frac{1}{|z|^\gamma}\right), \quad \gamma > 0, \quad \text{pour } |z| \rightarrow \infty; \quad (2.2)$$

and let the integer  $p$  (the index) defined by:

$$p = \frac{1}{2\pi} \left[ \lim_{\text{Im } z \rightarrow +\infty} \arg A(z) - \lim_{\text{Im } z \rightarrow -\infty} \arg A(z) \right], \text{ avec } z \in C \text{ et } Re(z) = b \quad (2.3)$$

A s. analytic solution with respect the line of the Hilbert homogeneous problem is given by ( $Re(\alpha) > b$  and  $Re(\beta) < b$ ):

$$\Phi(z) = \begin{cases} (z - \beta)^{-p} \exp\left(\frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} \log\left(A(s) \left(\frac{s - \beta}{s - \alpha}\right)^p\right) (s - z)^{-1} ds\right) \\ (z - \alpha)^{-p} \exp\left(\frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} \log\left(A(s) \left(\frac{s - \beta}{s - \alpha}\right)^p\right) (s - z)^{-1} ds\right) \end{cases} \quad (2.4)$$

for  $Re(z) > b$  and  $Re(z) < b$  respectively. All others s. analytic solutions has the form

$$\Theta(z) = \mathbf{P}(z) \Phi(z), \quad (2.5)$$

where  $\mathbf{P}(z)$  is any polynomial.

**Theorem 2.2.** Let  $A$  hölderian on the line  $L$  whose equation is  $Re(z) = b$ , not vanishes on  $L$  and verifies

$$|A(z) - 1| \leq \frac{C}{|z|^\gamma}, \quad \gamma > 0, \quad z \in L, \quad (2.6)$$

and let  $B(z)$  hölderian on  $L$  such that:

$$|B(z) - B(\infty)| \leq \frac{C}{|z|^\gamma}, \quad \gamma > 0, \quad z \in L. \quad (2.7)$$

then, the only s.analytic solutions with respect the line  $L$  of Hilbert problem (2.1) are given by:

$$\varphi(z) = \frac{\Phi(z)}{2\pi i} \int_{b-i\infty}^{b+i\infty} \frac{B(s)}{\Phi_i(s)(s-z)} ds + \mathbf{P}(z)\Phi(z), \quad z \notin L \quad (2.8)$$

where  $\Phi$  is given by (2.4) and  $\Phi_i$  is given (for any  $z \in L$ ) by:

$$\begin{aligned} \Phi_i(z) = & \frac{1}{(z-\beta)^p} \exp \left[ \frac{1}{2} \log A(z) \left( \frac{z-\beta}{z-\alpha} \right)^p \right. \\ & \left. + \frac{1}{2\pi i} \oint_{b-i\infty}^{b+i\infty} \log \left( A(s) \left( \frac{s-\beta}{s-\alpha} \right)^p \right) \frac{ds}{s-z} \right]. \end{aligned} \quad (2.9)$$

where  $\mathbf{P}(z)$  is any polynomial,  $\alpha$  and  $\beta$  are complex numbers verifying  $Re(\alpha) > b$  and  $Re(\beta) < b$ .

### 2.2.1 Integral equation of Wiener-Hopf of second kind

Let the integral equation of Wiener-Hopf of the second kind

$$f(t) = \int_0^\infty k(t-t_0)f(t_0)dt_0 + g(t), \quad -\infty < t < \infty, \quad (2.10)$$

where  $g(t)$  et  $k(t)$  are given functions of any real  $t$ . We assume that exist a real  $b > 0$  such that:

$$k(t) \exp(-bt) \text{ and } g(t) \exp(-bt) \text{ are integrable on the real axis} \quad (2.11)$$

We resume here this study by the method of the Hilbert problem, which weakens the hypotheses. We seek a solution  $f(t)$  such that  $f(t) \exp(-bt)$  is integrable on the real axis. To apply the convolution theorem to the two-sided Laplace transform we must have for interval of integration the interval  $-\infty < t < +\infty$  and define new functions as the following

$$f_+(t) = \begin{cases} 0 & \text{if } t > 0 \\ f(t) & \text{if } t < 0 \end{cases}, \quad f_-(t) = \begin{cases} -f(t) & \text{if } t > 0 \\ 0 & \text{if } t < 0 \end{cases} \quad (2.12)$$

and their two-sided Laplace transforms

$$F_+(s) = \int_{-\infty}^{+\infty} f_+(t)e^{-st} dt = \int_{-\infty}^0 f(t)e^{-st} dt, \quad \text{Re}(s) = b \quad (2.13)$$

$$F_-(s) = \int_{-\infty}^{+\infty} f_-(t)e^{-st} dt = \int_0^{+\infty} -f(t)e^{-st} dt, \quad \text{Re}(s) = b \quad (2.14)$$

$$K(s) = \int_{-\infty}^{+\infty} k(t)e^{-st} dt, \quad \text{Re}(s) = b \quad (2.15)$$

$$F(s) = \int_{-\infty}^{+\infty} f(t)e^{-st} dt = F_+(s) - F_-(s) \quad \text{Re}(s) = b \quad (2.16)$$

$$G(s) = \int_{-\infty}^{+\infty} g(t)e^{-st} dt, \quad \text{Re}(s) = b \quad (2.17)$$

These transformations are defined for any  $s$  on the line  $\text{Re}(s) = b$ . Furthermore  $F_+$  and  $F_-$  are analytic for  $\text{Re}(s) < b$  and  $\text{Re}(s) > b$  respectively. We reminder that (2.12) ensure that all the bi-sided Laplace transforms go to zero at the infinity. In particular

$$K(s) \rightarrow 0 \quad \text{when } |\text{Im}(s)| \rightarrow \infty, \quad \text{Re}(s) = b \quad (2.18)$$

The equation (2.11) gives

$$F_+(s) = [1 - K(s)]F_-(s) + G(s), \quad \text{Re}(s) = b \quad (2.19)$$

By considering the function  $\varphi$  s.analytic with respect the line  $L$  (of equation  $\text{Re}(s) = b$ ), it is defined by

$$\begin{cases} F_+(s), & \text{if } \text{Re}(s) < b, \\ F_-(s), & \text{if } \text{Re}(s) > b. \end{cases} \quad (2.20)$$

the equation (2.19) can be considered as a Hilbert problem for this function  $\varphi$ . By putting (taking in mind that the line  $L$  is oriented from the left to the right)

$$\begin{cases} \varphi_i(s) = F_-(s) \\ \varphi_e(s) = F_+(s) \end{cases}, \quad s \in C, \quad \text{Re}(s) = b, \quad (2.21)$$

this problem transforms as

$$\varphi_i(s) = \frac{1}{(1 - K(s))} \varphi_e(s) + \frac{1}{(K(s) - 1)} G(s), \quad \text{Re}(s) = b. \quad (2.22)$$

All s.analytic solutions of the last equation are given by the above theorem.

**Proposition 2.3.** Let  $k$  and  $g$  two functions verifying (2.12) such that their bi-sided Laplace transforms  $K(s)$  and  $G(s)$  are holderian on the line  $L$  (of equation  $\text{Re}(s) = b$ ). Assume that

$$|K(s)| \leq \frac{C}{|s|^\gamma}, \quad \gamma > 0, \quad s \in L, \quad (2.23)$$

and  $(1 - K(s))$  not vanishes on the line  $L$ . Then the bi-sided laplace transform  $F(s)$  of any solution  $f(t)$  of the equation (2.10) is given by:

$$F(s) = \varphi_i(s) - \varphi_e(s), \quad s \in L, \quad (2.24)$$

where the s.analytic function  $\varphi$  is the solution of the equation (2.22) given by:

$$\Phi(z) \begin{cases} \frac{1}{(z-\beta)^p} \exp \left( \frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} \log \left( \frac{(s-\beta)^p}{(1-K(s))(s-\alpha)^p} \right) \frac{ds}{s-z} \right); \operatorname{Re}(z) > b \\ \frac{1}{(z-\alpha)^p} \exp \left( \frac{1}{2\pi i} \int_{b-i\infty}^{b+i\infty} \log \left( \frac{(s-\beta)^p}{(1-K(s))(s-\alpha)^p} \right) \frac{ds}{s-z} \right); \operatorname{Re}(z) < b \end{cases} \quad (2.25)$$

where

$$p = \frac{1}{2\pi} \left[ \lim_{\operatorname{Im}(s) \rightarrow +\infty} \arg \left( \frac{1}{1-K(s)} \right) - \lim_{\operatorname{Im}(s) \rightarrow -\infty} \arg \left( \frac{1}{1-K(s)} \right) \right], \quad (2.26)$$

and

$$\begin{aligned} \Phi_i(z) = & \frac{1}{(z-\beta)^p} * \exp \left( \frac{1}{2} \log \left( \frac{1}{1-K(z)} \left( \frac{z-\beta}{z-\alpha} \right)^p \right) \right) \\ & * \exp \left( \frac{1}{2i\pi} \oint_{b-i\infty}^{b+i\infty} \log \left( \left( \frac{s-\beta}{s-\alpha} \right)^p \frac{1}{1-K(s)} \right) \frac{ds}{s-z} \right), \quad z \in L, \end{aligned} \quad (2.27)$$

by

$$\varphi(z) = \frac{\Phi(z)}{2\pi i} \int_{b-i\infty}^{b+i\infty} \frac{G(s) ds}{\Phi_i(s) (1-K(s)) (s-z)} + \mathbf{P}(z) \Phi(z), \quad z \notin L, \quad (2.28)$$

where  $\mathbf{P}(z)$  is a polynomial such that:

- i) if  $p > 0$ , degree  $(\mathbf{P}(z)) \leq p - 1$ ;
- ii)  $p = 0$ ,  $\mathbf{P}(z) \equiv 0$ ;
- iii)  $p < 0$ , no solution only if

$$\int_L \frac{s^m G(s)}{\Phi_i(s) (1-K(s))} ds = 0, \quad 0 \leq m \leq -(p+1), \quad (2.29)$$

### 3. Green's function for the step potential

We consider the following eigen-values problem in one dimension:

$$\left(-\frac{\hbar^2}{2m}\Delta + V(x)\right)\Psi = E\Psi \quad (3.1)$$

where  $V(x)$  is the step function: equal to  $V_0$  for  $x \geq 0$  and zero for  $x < 0$ . The boundary conditions are those of Dirichlet-Neumann (continuity of the solution and its derivative at the edge points). We will demonstrate that the Green kernel for this problem obeys an integral equation in the complex plane  $C$  that we will solve to find the solutions of the problem:

$$G(x, E : y) = G_0(x, E : y) - \int_{-\infty}^{+\infty} d\xi G_0(x, E : \xi) V(\xi) G(\xi, E : y) \quad (3.2)$$

where ( $V_0 > 0$ )

$$V = V_0\theta(x) = V_0 \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x < 0. \end{cases} \quad (3.3)$$

Then (3.2) becomes

$$G(x, E : y) = G_0(x, E : y) - V_0 \int_0^{+\infty} d\xi G_0(x, E : \xi) G(\xi, E : y) \quad (3.4)$$

We note

$$G(x, E : y) = g(x, y) \quad (3.5)$$

then (3.4) becomes

$$g(x, y) = g_0(x, y) - V_0 \int_0^{+\infty} d\xi g_0(x - \xi) g(\xi, y) \quad (3.6)$$

we define [10]

$$g^+(x, y) = \begin{cases} 0 & \text{if } x > 0 \\ g(x, y) & \text{if } x < 0 \end{cases}, \quad g^-(x, y) = \begin{cases} -g(x, y) & \text{if } x > 0 \\ 0 & \text{if } x < 0 \end{cases} \quad (3.7)$$

then (3.6) becomes

$$g^+(x, y) - g^-(x, y) = g_0(x, y) + V_0 \int_{-\infty}^{+\infty} d\xi g_0(x - \xi) g^-(\xi, y) \quad (3.8)$$

where

$$g_0(x, y) = i \int_0^{+\infty} dT K_0(x, t : y, 0) \exp(-iEt)$$

$$= \frac{m}{k} \exp(-k|x-y|) \text{ avec } k^2 = 2mE \quad (3.9)$$

then (37) transforms as

$$g^+(x, y) - g^-(x, y) = \frac{m}{k} \exp(-k|x-y|) - \frac{mV_0}{k} \int_0^{+\infty} d\xi \exp(-k|x-\xi|) g^-(\xi, y) \quad (3.10)$$

Then the bi-sided Laplace transform of the last equation (seen as a function of  $x$ , and  $y$  as parameter:

$$g(s, y) = \int_{-\infty}^{+\infty} g(x, y) \exp(sx) dx$$

$$g^+(s, y) = B(s) + [1 + L(s)] g^-(s, y) \quad (3.11)$$

The equation (3.11) is the same as (2.1) describing the non-homogeneous Hilbert problem. Its solution is given by the formula (2.8). The case where  $L$  is a line ( $\text{Re}(s) = b$ ), and  $\mathbf{P}(z)$  is zero polynomial:

$$\varphi(s) = \frac{\Phi(s)}{2\pi i} \int_{b-i\infty}^{b+i\infty} \frac{B(\tau)}{\Phi_i(\tau)(\tau-s)} d\tau, \quad s \notin L \quad (3.12)$$

such that

$$\varphi(x) = g(x, y) = g_y(x) \quad (3.13)$$

$$B(x) = \frac{m}{k} \exp(-k|x-y|) \quad (3.14)$$

$$k(x) = -\frac{mV_0}{k} \exp(-k|x|) \quad (3.15)$$

Let  $\Phi_i(s)$ ,  $\Phi_e(s)$  the interior and exterior limits of  $\Phi(s)$ , solution of  $t$  homogeneous Hilbert problem,

$$\begin{aligned} B(s) &= \int_{-\infty}^{+\infty} B(x) \exp(-sx) dx = \frac{m}{k} \int_{-\infty}^{+\infty} \exp(-k|x-y|) \exp(-sx) dx \\ &= \frac{m \exp(-sy)}{k} \int_{-\infty}^{+\infty} \exp(-k|u|) \exp(-su) du, \quad \text{et } u = x - y \\ &= \frac{m \exp(-sy)}{k} \left( \int_{-\infty}^0 \exp((k-s)u) du + \int_0^{+\infty} \exp((-k-s)u) du \right) \\ &= 2m \frac{\exp(-sy)}{k^2 - s^2}, \text{ avec } -k < s < k \end{aligned} \quad (3.16)$$

$$L(s) = \int_{-\infty}^{+\infty} k(x) \exp(-sx) dx = -\frac{mV_0}{k} \int_{-\infty}^{+\infty} \exp(-k|x|) \exp(-sx) dx = \frac{2mV_0}{s^2 - k^2} \quad (3.17)$$

$$1 - L(s) = \frac{s^2 - (k^2 + 2mV_0)}{s^2 - k^2}$$



$$= \frac{(s - \lambda_1)(s + \lambda_1)}{(s - k)(s + k)}, \quad \text{où} \quad \lambda_1 = \sqrt{k^2 + 2mV_0} \quad (3.18)$$

We note

$$\Phi_i(s) = \Phi^+(s) \quad \text{for} \quad \text{Re}(s) < b, \quad \text{and} \quad \Phi_e(s) = \Phi^-(s) \quad \text{for} \quad \text{Re}(s) > b.$$

$$\Phi^+(s) = \frac{s - \lambda_1}{s - k}, \quad \text{and} \quad \Phi^-(s) = \frac{s + k}{s + \lambda_1} \quad (3.19)$$

In the region  $\text{Re}(s) < b$ , the formula (3.12) is

$$\varphi^+(s) = \frac{\Phi^+(s)}{2i\pi} \int_{b-i\infty}^{b+i\infty} \frac{B(\tau)}{\Phi^+(\tau)(\tau - s)} d\tau \quad (3.20)$$

On the imaginary line ( $\text{Re}(s) = 0$ ), the solution is

$$\begin{aligned} \varphi^+(s) &= \frac{m}{2\pi i k} \frac{s - \lambda_1}{s - k} \int_{-i\infty}^{+i\infty} \frac{2k \exp(-\tau y)}{(k^2 - \tau^2) \frac{\tau - \lambda_1}{\tau - k} (\tau - s)} d\tau \\ &= -\frac{m}{2i\pi k} \left( \frac{s - \lambda_1}{s - k} \right) \int_{-i\infty}^{+i\infty} \frac{2k \exp(-\tau y)}{(k + \tau)(\tau - \lambda_1)(\tau - s)} d\tau \end{aligned} \quad (3.21)$$

We see now the case  $y < 0$ : then the residue theorem gives this integral: the semicircle is on the left of the imaginary axis, so there are two simple poles one for  $\tau = -k$  and the other for  $\tau = s$

$$\begin{aligned} \varphi^+(s) &= \frac{m}{k} \left( \frac{s - \lambda_1}{s - k} \right) \left[ \frac{2k \exp(ky)}{(k + \lambda_1)(k + s)} + \frac{2k \exp(-sy)}{(s + k)(s - \lambda_1)} \right] \\ \varphi^+(s) &= \frac{2m(s - \lambda_1) \exp ky}{(s - k)(k + \lambda_1)(s + k)} + \frac{2im \exp(-sy)}{(s - k)(s + k)} \end{aligned} \quad (3.22)$$

To invert, we put  $k = ik$ :

$$\lambda_1 = \sqrt{(ik)^2 + 2mV_0} = i\mu, \quad \text{where} \quad \mu = \sqrt{k^2 - k_0^2} \quad \text{with} \quad k_0^2 = 2mV_0, \quad k > k_0$$

$$\varphi^+(s) = \frac{2m(s - i\mu) \exp(iky)}{(s - ik)(ik + i\mu)(s + ik)} + \frac{2m \exp(-sy)}{(s - ik)(s + ik)} \quad (3.23)$$

The case  $x < 0$

$$\begin{aligned} \varphi(x) &= \frac{1}{2i\pi} \int_{-i\infty}^{+i\infty} \varphi^+(t) \exp(tx) dt \\ \varphi(x) &= \frac{2im \exp(iky)}{(i\mu + ik)2i\pi} \int_{-i\infty}^{+i\infty} \frac{(t - i\mu) \exp(tx)}{(t + ik)(t - ik)} dt + \frac{2im}{2i\pi} \int_{-i\infty}^{+i\infty} \frac{\exp t(x - y)}{(t - ik)(t + ik)} dt \end{aligned} \quad (3.24)$$

So for  $x < 0$ : the integral of the first term is taken in the right semicircle (the residual is at pole  $t = ik$ ). The integral of the second term, for  $x < y$ , is taken in the semicircle on the right (the residue is at the pole  $t = ik$ ), for  $x > y$  is taken in the semicircle on the left (the residue is at the pole  $t = -ik$ )

$$\varphi(x) = -\frac{m(k-\mu)\exp(ik(x+y))}{ik(k+\mu)} + \frac{m}{ik} \begin{cases} -\exp(ik(x-y)), & x < y \\ -\exp(-ik(x-y)), & x > y \end{cases} \quad (3.25)$$

The solution in the case  $y < 0$  and  $x < 0$  noted  $g_{-,-}(x, y)$

$$g_{-,-}(x, y) = \frac{im}{k} \left[ \exp(ik|x-y|) + \frac{k-\mu}{k+\mu} \exp(ik(x+y)) \right] \quad (3.26)$$

Region  $y > 0$ : so the theorem of residue gives the integral of (3.21) using the right semi-circle (at the pole  $\tau = \lambda_1$ )

$$\begin{aligned} \varphi^+(s) &= -\frac{m}{k} \left( \frac{s-\lambda_1}{s-k} \right) 2k \left( \frac{\exp(-\lambda_1 y)}{(\lambda_1+k)(s-\lambda_1)} \right) \\ \varphi^+(s) &= \frac{2m \exp(-\lambda_1 y)}{(s-k)(\lambda_1+k)} \end{aligned} \quad (3.27)$$

before performing the inverse, turn back to the valeur of  $k = ik$ .

The case  $x < 0$

$$\begin{aligned} \varphi(x) &= \frac{1}{2i\pi} \int_{-i\infty}^{+i\infty} \varphi^+(t) \exp(tx) dt \\ &= \frac{2m \exp(-i\mu y)}{2i\pi(ik+i\mu)} \int_{-i\infty}^{+i\infty} \frac{\exp tx}{(t-ik)} dt \end{aligned} \quad (3.28)$$

The residue theorem gives (thee semicircle at the right, i.e the pole at  $t = ik$ )

$$\varphi(x) = -\frac{m}{ik} \left[ \frac{2k}{k+\mu} \exp(ikx - i\mu y) \right] \quad (3.29)$$

The solution in the case  $x < 0$  and  $y > 0$  noted  $g_{-,+}(x, y)$  is

$$g_{-,+}(x, y) = \frac{2im \exp(ikx - i\mu y)}{k+\mu} \quad (3.30)$$

The region  $\text{Re}(s) > 0$ : the formula (3.12) can be written as

$$\begin{aligned} \varphi^-(s) &= \frac{\Phi^-(s)}{2i\pi} \int_{-i\infty}^{+i\infty} \frac{B(\tau)}{\Phi^+(\tau)(\tau-s)} d\tau \\ \varphi^-(s) &= -\frac{m}{k} \frac{s+k}{s+\lambda_1} \frac{1}{2i\pi} \int_{-i\infty}^{+i\infty} \frac{2k \exp(-\tau y)}{(k^2-\tau^2) \frac{\tau-\lambda_1}{\tau-k} (\tau-s)} d\tau \end{aligned} \quad (3.31)$$

$$= \frac{m}{k} \frac{s+k}{s+\lambda_1} \frac{2k}{2i\pi} \int_{-i\infty}^{+i\infty} \frac{\exp(-\tau y)}{(\tau+k)(\tau-\lambda_1)(\tau-s)} d\tau \quad (3.32)$$

Consider the case  $y < 0$ : the residue theorem gives (the semicircle at the left, the only pole is at  $\tau = -k$ )

$$\varphi^-(s) = \frac{m}{k} \frac{s+k}{s+\lambda_1} \frac{2k \exp ky}{(k+\lambda_1)(k+s)} \quad (3.33)$$

$$\varphi^-(s) = \frac{m}{k} \left[ \frac{2k \exp ky}{(s+\lambda_1)(k+\lambda_1)} \right] \quad (3.34)$$

Before performing the inverse, turn back to the valeur of  $k = ik$ .

The case  $x > 0$

$$\begin{aligned} \varphi(x) &= -\frac{1}{2i\pi} \int_{-i\infty}^{+i\infty} \varphi^-(s) \exp(sx) ds \\ \varphi(x) &= -\frac{m}{ik} \left[ \frac{2k \exp ik y}{k+\mu} \right] \int_{-i\infty}^{+i\infty} \frac{\exp tx}{(t+i\mu)} dt \end{aligned}$$

The residue theorem gives (the semicircle at the left, the pole is at  $t = -i\mu$ )

$$\varphi(x) = i \frac{m}{k} \left[ \frac{2k \exp(-i\mu x + ik y)}{k+\mu} \right] \quad (3.35)$$

The solution for the case  $x > 0$  and  $y < 0$ , noted by  $g_{+,-}(x, y)$  is

$$g_{+,-}(x, y) = \frac{2im \exp(-i\mu x + ik y)}{k+\mu}$$

we consider the case  $y > 0$

$$\varphi^-(s) = \frac{m}{k} \frac{s+k}{s+\lambda_1} \frac{2k}{2i\pi} \int_{-i\infty}^{+i\infty} \frac{\exp(-\tau y)}{(k+\tau)(\tau-\lambda_1)(\tau-s)} d\tau$$

The residue theorem gives (the semicircle is at the right, the poles are at  $\tau = \lambda_1$ , and  $\tau = s$ )

$$\begin{aligned} \varphi^-(s) &= \frac{m}{k} \frac{s+k}{s+\lambda_1} \left[ -\frac{2k \exp(-\lambda_1 y)}{(k+\lambda_1)(\lambda_1-s)} - \frac{2k \exp(-sy)}{(s+k)(s-\lambda_1)} \right] \\ \varphi^-(s) &= \frac{m}{k} \left[ \frac{2k(s+k) \exp(-\lambda_1 y)}{(k+\lambda_1)(s^2-\lambda_1^2)} \right] - \frac{m}{k} \left[ \frac{2k \exp(-sy)}{s^2-\lambda_1^2} \right] \end{aligned}$$

The case  $x > 0$ : before performing the inverse, turn back to the valeur of  $k = ik$

$$\begin{aligned} \varphi(x) &= -\frac{m}{ik} \left[ \frac{2k \exp(-i\mu y)}{2i\pi(k+\mu)} \int_{-i\infty}^{+i\infty} \frac{(t+ik) \exp(tx)}{t^2+\mu^2} dt \right] \\ &\quad + \frac{m}{ik} \left[ \frac{2ik}{2i\pi} \int_{-i\infty}^{+i\infty} \frac{\exp t(x-y)}{t^2+\mu^2} dt \right] \end{aligned}$$

By residue theorem, the first term of the last expression is calculated by using the left semicircle (the pole at  $t = -i\mu$ ). Whereas the second term is calculated, if  $x < y$ , by using the right semicircle (the pole at  $t = i\mu$ ), and if  $x > y$ , by using the left semicircle (the pole at  $t = -i\mu$ ):

$$\begin{aligned} \varphi(x) = & \frac{m}{ik} \frac{k - \mu}{\mu k + \mu} \exp(-i\mu(x + y)) \\ & + \frac{m}{ik} \begin{cases} -\frac{k}{\mu} \exp(i\mu(x - y)) & x < y, \\ -\frac{k}{\mu} \exp(-i\mu(x - y)) & x > y. \end{cases} \end{aligned} \quad (3.36)$$

The solution of the problem in the case  $x > 0$  et  $y > 0$ , noted  $g_{+,+}(x, y)$  is then given by:

$$g_{+,+}(x, y) = \frac{im}{\mu} \left[ \exp(i\mu|x - y|) - \frac{\mu - k}{\mu + k} \exp(-i\mu(x + y)) \right] \quad (3.37a)$$

As application we can write down the reflexion coefficient (using the second term of  $g_{-,-}(x, y)$ )

$$R = \left( \left| \frac{k - \mu}{k + \mu} \right| \right)^2 \quad (3.38)$$

and transmission coefficient (using  $g_{-,+}(x, y)$  and the first term in  $g_{-,-}(x, y)$ )

$$T = \frac{\mu}{k} \left( \frac{2m}{k + \mu} \frac{k}{m} \right)^2 = \frac{4\mu k}{(k + \mu)^2} \quad (3.39)$$

it is straightforward that  $R + T = 1$  as it must be. When  $E < V_0$ ,  $\mu$  becomes a pure imaginary complex number, then, the reflexion coefficient  $R$  becomes equal one and so  $T = 0$ : a well known result in quantum mechanics.

## 4. Conclusion

New derivation of Green's function relative to a moving quantum particle in step potential is derived. This method stands on the resolution of a singular integral equation. With the help of the Wigner-Hopf theorem, we have obtain the Green function of the problem. As an application, we have derived from the Green function, the transmission and reflexion coefficient both for  $E > V_0$  and  $E < V_0$ .

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