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Quantum dynamics of a particle interacting with a double barrier

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Abstract

Following a previously developed method, the problem of a particle scattered by a double barrier is studied. Instead of the simple transmission or reflection, the more difficult case of the arrival in the region between the barriers is considered and solved explicitly by using matrix methods.

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1. Introduction

It is well known that the integral Schrödinger equation for the propagator takes, after a Laplace transformation, the form of a Fredholm integral equation of the second kind [1]. Recently, in a one-dimensional scheme, a method has been developed in order to obtain the solution in zero potential regions, taking into account boundary conditions in a suitable way [2]. Typical applications are those of transmission and reflection by barriers, and in general of scattering [3]; an extension to a wider kind of kernels is possible, too [4].

We would like to recall that the quantum-mechanical propagator is a fundamental object in physics. It satisfies the Schrödinger equation with a fixed initial condition and so it is therefore an intrinsic feature of the physical system [5], independent of the wavefunction for $t = 0$. Among the various non-standard applications of the propagator, we point out a satisfactory definition of tunnelling time [3, 6], the study of the interaction of a metastable system with a thermal bath [7], the overcoming of perturbative expansions in the study of coupling effects in quantum field theory [8]. We refer to the literature for a complete discussion about this subject [9, 10].

In short, it is not necessary to solve the equation inside the potential, in order to fulfil boundary conditions; in contrast, only a formal expression of this solution is needed. To show this, a large use of the matrix theory is made, such as partitioning techniques and properties of rank-one matrices, among which a theorem previously established by authors [3] plays a basic role. Therefore a great simplification arises, and the solution is found in terms of infinite determinants, which admit a kind expression as an entire power series.

In the following, the theory is extended to obtain the wavefunction in the region between two potential barriers. This is an important improvement with respect to the pure transmission or reflection, allowing the application to problems of trapping and localization of a particle, as well as the decay and evolution of a metastable state; moreover, tunnelling times and scattering characteristics are important parameters in designing a large class of recently developed optoelectronic devices [11, 12].

In section 2, the method of obtaining the integral equation is discussed. In section 3, the full calculation is developed for our model, and in section 4 the evaluation of infinite determinants is outlined. In section 5 limiting cases are considered, and in section 6 an application is shown when the barriers are approximated by delta functions.

2. The integral equation

Let H_0 be a Hamiltonian for which the propagator G_0 is known, and V a general potential. The Schrödinger equation for the system with Hamiltonian $H = H_0 + V$ is

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle \tag{1}$$

where $|\psi(t)\rangle$ is the vector representing the dynamical state of our system. A standard procedure leads to

$$|\psi(t)\rangle = \mathrm{e}^{-\frac{i}{\hbar}H_0 t}|\psi(0)\rangle - \frac{i}{\hbar}\int_0^t \mathrm{d}\tau\, \mathrm{e}^{-\frac{i}{\hbar}H_0(t-\tau)}V|\psi(\tau)\rangle \tag{2}$$

that is the Schrödinger equation in an integral form. By using the representation where the position variables are diagonal [13] (namely, passing from the state vectors $|\psi(t)\rangle$ to the wavefunctions $\psi(x,t)$), this equation is easily written in terms of the propagators G and G_0:

$$\int \mathrm{d}\eta\, \psi_0(\eta)G(x,t;\eta) = \int \mathrm{d}\eta\, \psi_0(\eta)G_0(x,t;\eta) - \frac{i}{\hbar}\int \mathrm{d}\eta\, \psi_0(\eta) \times \left[\int_0^t \mathrm{d}\tau \int_{-\infty}^{\infty} \mathrm{d}\xi\, G_0(x,t-\tau;\xi)V(\xi)G(\xi,\tau;\eta)\right] \tag{3}$$

where

$$G(x,t;\eta) = \langle x|\mathrm{e}^{-\frac{i}{\hbar}Ht}|\eta\rangle, \qquad G_0(x,t;\eta) = \langle x|\mathrm{e}^{-\frac{i}{\hbar}H_0 t}|\eta\rangle \tag{4}$$

and ψ_0 is the wavefunction for $t = 0$. In view of the future use of the Laplace transform, it is better to perform Wick rotation to imaginary time $t \to -it$ [14], and the following equation for the propagator G arises:

$$G(x,t;\eta) = G_0(x,t;\eta) - \frac{1}{\hbar}\int_0^t \mathrm{d}\tau \int_{-\infty}^{\infty} \mathrm{d}\xi\, G_0(x,t-\tau;\xi)V(\xi)G(\xi,\tau;\eta). \tag{5}$$

After a Laplace transform [15]

$$\mathcal{L}\{\psi(x,t)\} = \int_0^{\infty} \mathrm{d}t\, \psi(x,t)\exp(-st) = \psi(x,s) \tag{6}$$

a Fredholm equation of the second kind is obtained [16]:

$$G(x,s;\eta) = G_0(x,s;\eta) - \frac{1}{\hbar}\int_{-\infty}^{\infty} \mathrm{d}\xi\, G_0(x,s;\xi)V(\xi)G(\xi,s;\eta). \tag{7}$$

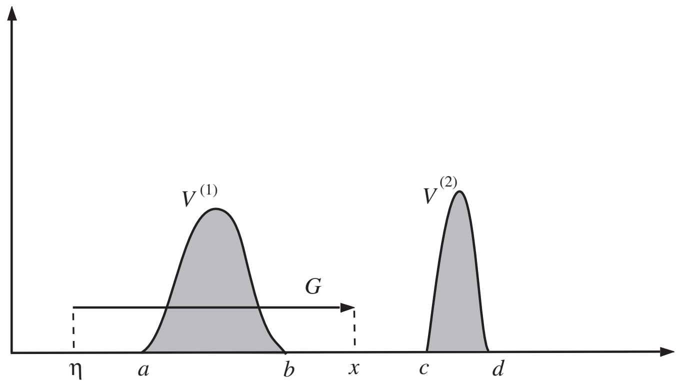

Figure 1. The double barrier.

Let us suppose that H_0 corresponds to the free particle, so we have, in imaginary time [13],

$$G_0(x,t;\eta) = \sqrt{\frac{m}{2\pi\hbar t}} \exp\left[-\frac{m}{2\hbar}\frac{(x-\eta)^2}{t}\right] \tag{8}$$

and therefore

$$G_0(x,s;\eta) = \frac{c}{2}\frac{\mathrm{e}^{-c|x-\eta|\sqrt{s}}}{\sqrt{s}}, \qquad c = \sqrt{\frac{2m}{\hbar}}. \tag{9}$$

By defining

$$G_0(x,s;\eta) = \phi(x), \qquad G(x,s;\eta) = \psi(x), \qquad \lambda = \frac{c}{2\hbar}\frac{1}{\sqrt{s}}, \qquad k = c\sqrt{s}, \tag{10}$$

equation (7) can be written in short, assuming that V has a finite range (a,d),

$$\psi(x) + \lambda \int_a^d \mathrm{d}\xi\, \mathrm{e}^{-k|x-\xi|} V(\xi)\psi(\xi) = \phi(x) \tag{11}$$

where the variable s, considered as a parameter, is omitted, since now we are mainly interested in the space coordinates.

3. The double barrier

Let us now consider a particular form of the potential V, as shown in figure 1. It consists of two barriers $V^{(1)}$ and $V^{(2)}$ with finite support, being $V^{(1)} \neq 0$ in (a,b) and $V^{(2)} \neq 0$ in (c,d). The particle is initially on the left of the barrier $V^{(1)}$, and we are interested in its transmission into the region between the two barriers: namely,

$$\eta < a, \qquad b < x < c. \tag{12}$$

Equation (11) now reads, for general x,

$$\psi(x) + \lambda \int_a^b \mathrm{d}\xi\, \mathrm{e}^{-k|x-\xi|} V^{(1)}(\xi)\psi(\xi) + \lambda \int_c^d \mathrm{d}\xi'\, \mathrm{e}^{-k|x-\xi'|} V^{(2)}(\xi')\psi(\xi') = \phi(x) \tag{13}$$

and, between the barriers,

$$\psi(x) + \lambda\, \mathrm{e}^{-kx} \int_a^b \mathrm{d}\xi\, \mathrm{e}^{k\xi} V^{(1)}(\xi)\psi(\xi) + \lambda\, \mathrm{e}^{kx} \int_c^d \mathrm{d}\xi'\, \mathrm{e}^{-k\xi'} V^{(2)}(\xi')\psi(\xi') = \phi(x), \tag{14}$$

which is the equation we have to solve.

Our strategy consists in solving equation (13) in (a, b) and (c, d) (formally, and not explicitly), then introducing the results into equation (14). In these intervals, we denote the position variables as y and z, respectively. When $y \in (a, b)$,

$$\psi(y) + \lambda \int_a^b \mathrm{d}\xi\, \mathrm{e}^{-k|y-\xi|} V^{(1)}(\xi)\psi(\xi) + \lambda\, \mathrm{e}^{ky} \int_c^d \mathrm{d}\xi'\, \mathrm{e}^{-k\xi'} V^{(2)}(\xi')\psi(\xi') = \phi(y) \tag{15}$$

and when $z \in (c, d)$,

$$\psi(z) + \lambda\, \mathrm{e}^{-kz} \int_a^b \mathrm{d}\xi\, \mathrm{e}^{k\xi} V^{(1)}(\xi)\psi(\xi) + \lambda \int_c^d \mathrm{d}\xi'\, \mathrm{e}^{-k|z-\xi'|} V^{(2)}(\xi')\psi(\xi') = \phi(z). \tag{16}$$

A discretization procedure, with $i, j = 1, \ldots, N$ in (a, b), $s, l = 1, \ldots, M$ in (c, d), $\mathrm{d}\xi = (b - a)/N$, $\mathrm{d}\xi' = (d - c)/M$, $y_i = a + i\, \mathrm{d}\xi$, $z_s = c + s\, \mathrm{d}\xi'$, $f_i = f(y_i)$, $f_s = f(z_s)$, leads to

$$\psi_j + \sum_{i=1}^{N} \mathrm{d}\lambda_i\, \mathrm{e}^{-ky_{ij}} \psi_i + \mathrm{e}^{ky_j} \sum_{s=1}^{M} \mathrm{d}\lambda_i'\, \mathrm{e}^{-kz_s} \psi_s = \phi_j \tag{17}$$

$$\psi_l + \mathrm{e}^{-kz_l} \sum_{i=1}^{N} \mathrm{d}\lambda_i\, \mathrm{e}^{ky_i} \psi_i + \sum_{s=1}^{M} \mathrm{d}\lambda_i'\, \mathrm{e}^{-kz_{sl}} \psi_s = \phi_l \tag{18}$$

where $\mathrm{d}\lambda_i = \lambda V_i^{(1)}\, \mathrm{d}\xi$, $\mathrm{d}\lambda_s' = \lambda V_s^{(2)} \mathrm{d}\xi'$, $y_{ij} = |y_i - y_j|$, $z_{sl} = |z_s - z_l|$. It is understood that the limits $N \to \infty$, $M \to \infty$ will be performed at the end.

Now we write these equations in vectorial form:

$$\begin{aligned} &\boldsymbol{A}_1\boldsymbol{\psi}_1 + \boldsymbol{\varphi}_1^+(\tilde{\boldsymbol{v}}_2^-\boldsymbol{\psi}_2) = \boldsymbol{\phi}_1 \\ &\boldsymbol{\varphi}_2^-(\tilde{\boldsymbol{v}}_1^+\boldsymbol{\psi}_1) + \boldsymbol{A}_2\boldsymbol{\psi}_2 = \boldsymbol{\phi}_2, \end{aligned} \tag{19}$$

where the bold symbols denote vector or matrix ($\tilde{}$ = transpose), the indices 1 and 2 represent two subspaces N and M-dimensional, $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ the two matrices $(N \times N)$ and $(M \times M)$, respectively,

$$\begin{aligned} \boldsymbol{A}_1 &= \begin{pmatrix} 1 + \mathrm{d}\lambda_1 & \mathrm{d}\lambda_2\, \mathrm{e}^{-ky_{12}} & \ldots & \mathrm{d}\lambda_N\, \mathrm{e}^{-ky_{1N}} \\ \mathrm{d}\lambda_1\, \mathrm{e}^{-ky_{12}} & 1 + \mathrm{d}\lambda_2 & \ldots & \mathrm{d}\lambda_N\, \mathrm{e}^{-ky_{2N}} \\ \vdots & \vdots & \vdots & \ddots \\ \mathrm{d}\lambda_1\, \mathrm{e}^{-ky_{1N}} & \mathrm{d}\lambda_2\, \mathrm{e}^{-ky_{2N}} & \ldots & 1 + \mathrm{d}\lambda_N \end{pmatrix}, \\ \boldsymbol{A}_2 &= \begin{pmatrix} 1 + \mathrm{d}\lambda_1' & \mathrm{d}\lambda_2'\, \mathrm{e}^{-kz_{12}} & \ldots & \mathrm{d}\lambda_M'\, \mathrm{e}^{-kz_{1M}} \\ \mathrm{d}\lambda_1'\, \mathrm{e}^{-kz_{12}} & 1 + \mathrm{d}\lambda_2' & \ldots & \mathrm{d}\lambda_M'\, \mathrm{e}^{-kz_{2M}} \\ \vdots & \vdots & \vdots & \ddots \\ \mathrm{d}\lambda_1'\, \mathrm{e}^{-kz_{1M}} & \mathrm{d}\lambda_2'\, \mathrm{e}^{-kz_{2M}} & \ldots & 1 + \mathrm{d}\lambda_M' \end{pmatrix}, \end{aligned} \tag{20}$$

and ψ_1, ψ_2, $\varphi_1^\pm$, $\varphi_2^\pm$, $v_1^\pm$, $v_2^\pm$, ϕ_1, ϕ_2, the vectors

$$\psi_1 = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix}, \qquad \psi_2 = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_M \end{pmatrix}, \qquad \varphi_1^\pm = \begin{pmatrix} e^{\pm k y_1} \\ e^{\pm k y_2} \\ \vdots \\ e^{\pm k y_N} \end{pmatrix}, \qquad \varphi_2^\pm = \begin{pmatrix} e^{\pm k z_1} \\ e^{\pm k z_2} \\ \vdots \\ e^{\pm k z_M} \end{pmatrix},$$
$$v_1^\pm = \begin{pmatrix} d\lambda_1\, e^{\pm k y_1} \\ d\lambda_2\, e^{\pm k y_2} \\ \vdots \\ d\lambda_N\, e^{\pm k y_N} \end{pmatrix}, \qquad v_2^\pm = \begin{pmatrix} d\lambda_1'\, e^{\pm k z_1} \\ d\lambda_2'\, e^{\pm k z_2} \\ \vdots \\ d\lambda_M'\, e^{\pm k z_M} \end{pmatrix}, \qquad \phi_{1,2} = \frac{c}{2}\frac{e^{k\eta}}{\sqrt{s}}\varphi_{1,2}^-. \tag{21}$$

The product between the matrices is intended to be performed in the usual way, row by column. Let us now define the matrices, $(M \times N)$ and $(N \times M)$, respectively,

$$U_{21} = \varphi_2^- \tilde{v}_1^+ = \begin{pmatrix} d\lambda_1\, e^{-k\zeta_{11}} & d\lambda_2\, e^{-k\zeta_{12}} & \dots & d\lambda_N\, e^{-k\zeta_{1N}} \\ d\lambda_1\, e^{-k\zeta_{21}} & d\lambda_2 e^{-k\zeta_{22}} & \dots & d\lambda_N\, e^{-k\zeta_{2N}} \\ \vdots & \vdots & \vdots & \ddots \\ d\lambda_1\, e^{-k\zeta_{M1}} & d\lambda_2\, e^{-k\zeta_{M2}} & \dots & d\lambda_N\, e^{-k\zeta_{MN}} \end{pmatrix}, \tag{22}$$

$$U_{12} = \varphi_1^+ \tilde{v}_2^- = \begin{pmatrix} d\lambda_1'\, e^{-k\zeta_{11}} & d\lambda_2'\, e^{-k\zeta_{21}} & \dots & d\lambda_M'\, e^{-k\zeta_{M1}} \\ d\lambda_1'\, e^{-k\zeta_{12}} & d\lambda_2'\, e^{-k\zeta_{22}} & \dots & d\lambda_M'\, e^{-k\zeta_{M2}} \\ \vdots & \vdots & \vdots & \ddots \\ d\lambda_1'\, e^{-k\zeta_{1N}} & d\lambda_2'\, e^{-k\zeta_{2N}} & \dots & d\lambda_M'\, e^{-k\zeta_{MN}} \end{pmatrix}, \qquad \zeta_{li} = z_l - y_i. \tag{23}$$

In this way, equation (19) becomes

$$\begin{pmatrix} A_1 & U_{12} \\ U_{21} & A_2 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \tag{24}$$

giving

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} A_1 & U_{12} \\ U_{21} & A_2 \end{pmatrix}^{-1} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \tag{25}$$

and α, β, γ, δ can be found by the method of partitioning [17]. The result is

$$\begin{aligned} \alpha &= A_1^{-1} + A_1^{-1} U_{12} D U_{21} A_1^{-1}, & \beta &= -A_1^{-1} U_{12} D, \\ \gamma &= -D U_{21} A_1^{-1}, & \delta &= D, \end{aligned} \tag{26}$$

and, by assuming that the inverses A_1^{-1} and A_2^{-1} exist [2], the matrix D is given by

$$D = (A_2 - U_{21} A_1^{-1} U_{12})^{-1}. \tag{27}$$

Let us return to equation (14), whose discretized form is

$$\psi(x) + e^{-kx} \sum_{i=1}^{N} d\lambda_i\, e^{k y_i} \psi_i + e^{kx} \sum_{s=1}^{M} d\lambda_s'\, e^{-k z_s} \psi_s = \phi(x). \tag{28}$$

By using equation (25) and recalling definitions (9), (10) and (21), we obtain

$$\psi(x) = \phi(x) - \mathrm{e}^{-kx}\big(\tilde{\boldsymbol{v}}_1^+\psi_1\big) - \mathrm{e}^{kx}\big(\tilde{\boldsymbol{v}}_2^-\psi_2\big)$$
$$= \phi(x)\big(1 - \tilde{\boldsymbol{v}}_1^+\boldsymbol{\alpha}\boldsymbol{\varphi}_1^- - \tilde{\boldsymbol{v}}_1^+\boldsymbol{\beta}\boldsymbol{\varphi}_2^-\big) - \frac{c}{2}\frac{\mathrm{e}^{k(x+\eta)}}{\sqrt{s}}\big(\tilde{\boldsymbol{v}}_2^-\boldsymbol{\gamma}\boldsymbol{\varphi}_1^- + \tilde{\boldsymbol{v}}_2^-\boldsymbol{\delta}\boldsymbol{\varphi}_2^-\big). \tag{29}$$

It is easy to show that one has, for any suitable matrix $\boldsymbol{S}$ (Tr = trace),

$$\tilde{\boldsymbol{v}}\boldsymbol{S}\boldsymbol{\varphi} = \mathrm{Tr}[\boldsymbol{S}\boldsymbol{R}], \qquad \text{with} \quad \boldsymbol{R} = \boldsymbol{\varphi}\tilde{\boldsymbol{v}} \tag{30}$$

and therefore

$$\tilde{\boldsymbol{v}}_1^+\boldsymbol{\alpha}\boldsymbol{\varphi}_1^- = \mathrm{Tr}\big[\boldsymbol{\alpha}\big(\boldsymbol{\varphi}_1^-\tilde{\boldsymbol{v}}_1^+\big)\big] = \mathrm{Tr}[\boldsymbol{\alpha}\boldsymbol{V}_1] \tag{31}$$

where

$$\boldsymbol{V}_1 = \boldsymbol{\varphi}_1^-\tilde{\boldsymbol{v}}_1^+ = \begin{pmatrix} \mathrm{d}\lambda_1 & \mathrm{d}\lambda_2\,\mathrm{e}^{ky_{12}} & \dots & \mathrm{d}\lambda_N\,\mathrm{e}^{ky_{1N}} \\ \mathrm{d}\lambda_1\,\mathrm{e}^{-ky_{12}} & \mathrm{d}\lambda_2 & \dots & \mathrm{d}\lambda_N\,\mathrm{e}^{ky_{2N}} \\ \vdots & \vdots & \vdots & \ddots \\ \mathrm{d}\lambda_1\,\mathrm{e}^{-ky_{1N}} & \mathrm{d}\lambda_2\,\mathrm{e}^{-ky_{2N}} & \dots & \mathrm{d}\lambda_N \end{pmatrix}. \tag{32}$$

Then,

$$\tilde{\boldsymbol{v}}_1^+\boldsymbol{\beta}\boldsymbol{\varphi}_2^- = \mathrm{Tr}\big[\boldsymbol{\beta}\big(\boldsymbol{\varphi}_2^-\tilde{\boldsymbol{v}}_1^+\big)\big] = \mathrm{Tr}[\boldsymbol{\beta}\boldsymbol{U}_{21}] \tag{33}$$

with $\boldsymbol{U}_{21}$ being defined by equation (22);

$$\tilde{\boldsymbol{v}}_2^-\boldsymbol{\gamma}\boldsymbol{\varphi}_1^- = \mathrm{Tr}\big[\boldsymbol{\gamma}\big(\boldsymbol{\varphi}_1^-\tilde{\boldsymbol{v}}_2^-\big)\big] = \mathrm{Tr}[\boldsymbol{\gamma}\boldsymbol{W}_{12}] \tag{34}$$

where

$$\boldsymbol{W}_{12} = \boldsymbol{\varphi}_1^-\tilde{\boldsymbol{v}}_2^- = \begin{pmatrix} \mathrm{d}\lambda_1'\,\mathrm{e}^{-k\zeta_{11}^+} & \mathrm{d}\lambda_2'\,\mathrm{e}^{-k\zeta_{21}^+} & \dots & \mathrm{d}\lambda_M'\,\mathrm{e}^{-k\zeta_{M1}^+} \\ \mathrm{d}\lambda_1'\,\mathrm{e}^{-k\zeta_{12}^+} & \mathrm{d}\lambda_2'\,\mathrm{e}^{-k\zeta_{22}^+} & \dots & \mathrm{d}\lambda_M'\,\mathrm{e}^{-k\zeta_{M2}^+} \\ \vdots & \vdots & \vdots & \ddots \\ \mathrm{d}\lambda_1'\,\mathrm{e}^{-k\zeta_{1N}^+} & \mathrm{d}\lambda_2'\,\mathrm{e}^{-k\zeta_{2N}^+} & \dots & \mathrm{d}\lambda_M'\,\mathrm{e}^{-k\zeta_{MN}^+} \end{pmatrix}, \qquad \zeta_{li}^+ = y_i + z_l, \tag{35}$$

and, at last,

$$\tilde{\boldsymbol{v}}_2^-\boldsymbol{\delta}\boldsymbol{\varphi}_2^- = \mathrm{Tr}\big[\boldsymbol{\delta}\big(\boldsymbol{\varphi}_2^-\tilde{\boldsymbol{v}}_2^-\big)\big] = \mathrm{Tr}[\boldsymbol{\delta}\boldsymbol{U}_2] \tag{36}$$

where

$$\boldsymbol{U}_2 = \boldsymbol{\varphi}_2^-\tilde{\boldsymbol{v}}_2^- = \begin{pmatrix} \mathrm{d}\lambda_1'\,\mathrm{e}^{-2kz_1} & \mathrm{d}\lambda_2'\,\mathrm{e}^{-kz_{12}^+} & \dots & \mathrm{d}\lambda_M'\,\mathrm{e}^{-kz_{1M}^+} \\ \mathrm{d}\lambda_1'\,\mathrm{e}^{-kz_{12}^+} & \mathrm{d}\lambda_2'\,\mathrm{e}^{-2kz_2} & \dots & \mathrm{d}\lambda_M'\,\mathrm{e}^{-kz_{2M}^+} \\ \vdots & \vdots & \vdots & \ddots \\ \mathrm{d}\lambda_1'\,\mathrm{e}^{-kz_{1M}^+} & \mathrm{d}\lambda_2'\,\mathrm{e}^{-kz_{2M}^+} & \dots & \mathrm{d}\lambda_M'\,\mathrm{e}^{-2kz_M} \end{pmatrix}, \qquad z_{ls}^+ = z_l + z_s. \tag{37}$$

Then, to sum up, we are led to the result

$$\psi(x) = \phi(x)\,\{1 - \mathrm{Tr}[\boldsymbol{\alpha}\boldsymbol{V}_1] - \mathrm{Tr}[\boldsymbol{\beta}\boldsymbol{U}_{21}]\} - \frac{c}{2}\frac{\mathrm{e}^{k(x+\eta)}}{\sqrt{s}}\,\{\mathrm{Tr}[\boldsymbol{\gamma}\boldsymbol{W}_{12}] + \mathrm{Tr}[\boldsymbol{\delta}\boldsymbol{U}_2]\}\,. \tag{38}$$

In order to calculate the traces, we first observe that all the matrices constructed by product of vectors are of rank 1 [17]; then, denoting by $|\boldsymbol{M}|$ the determinant of a matrix $\boldsymbol{M}$, we use the following theorem [3]:

If $\boldsymbol{S}$ is a non-singular matrix and $\boldsymbol{R}$ is a matrix of rank 1, then

$$\mathrm{Tr}[\boldsymbol{S}^{-1}\boldsymbol{R}] = 1 - \frac{|\boldsymbol{S}-\boldsymbol{R}|}{|\boldsymbol{S}|}. \tag{39}$$

So, we are allowed to write, recalling equations (26) and (27),

$$\mathrm{Tr}[\boldsymbol{\delta U}_2] = 1 - \frac{\left|\boldsymbol{A}_2 - \boldsymbol{U}_{21}\boldsymbol{A}_1^{-1}\boldsymbol{U}_{12} - \boldsymbol{U}_2\right|}{\left|\boldsymbol{A}_2 - \boldsymbol{U}_{21}\boldsymbol{A}_1^{-1}\boldsymbol{U}_{12}\right|}, \tag{40}$$

and since

$$\boldsymbol{U}_{21}\boldsymbol{A}_1^{-1}\boldsymbol{U}_{12} = \varphi_2^-\left(\tilde{\boldsymbol{v}}_1^+\boldsymbol{A}_1^{-1}\varphi_1^+\right)\tilde{\boldsymbol{v}}_2^- = \mathrm{Tr}\left[\boldsymbol{A}_1^{-1}\left(\varphi_1^+\tilde{\boldsymbol{v}}_1^+\right)\right]\varphi_2^-\tilde{\boldsymbol{v}}_2^- = \mathrm{Tr}\left[\boldsymbol{A}_1^{-1}\boldsymbol{W}_1\right]\boldsymbol{U}_2, \tag{41}$$

where

$$\boldsymbol{W}_1 = \varphi_1^+\tilde{\boldsymbol{v}}_1^+ = \begin{pmatrix} \mathrm{d}\lambda_1\,\mathrm{e}^{2ky_1} & \mathrm{d}\lambda_2\,\mathrm{e}^{ky_{12}^+} & \ldots & \mathrm{d}\lambda_N\,\mathrm{e}^{ky_{1N}^+} \\ \mathrm{d}\lambda_1\,\mathrm{e}^{ky_{12}^+} & \mathrm{d}\lambda_2\,\mathrm{e}^{2ky_2^+} & \ldots & \mathrm{d}\lambda_N\,\mathrm{e}^{ky_{2N}^+} \\ \vdots & \vdots & \vdots & \ddots \\ \mathrm{d}\lambda_1\,\mathrm{e}^{ky_{1N}^+} & \mathrm{d}\lambda_2\,\mathrm{e}^{kx_{2N}^+} & \ldots & \mathrm{d}\lambda_N\,\mathrm{e}^{2ky_N} \end{pmatrix}, \qquad y_{ij}^+ = y_i + y_j, \tag{42}$$

we achieve the result

$$\boldsymbol{U}_{21}\boldsymbol{A}_1^{-1}\boldsymbol{U}_{12} = \left(1 - \frac{|\boldsymbol{A}_1 - \boldsymbol{W}_1|}{|\boldsymbol{A}_1|}\right)\boldsymbol{U}_2 \tag{43}$$

and therefore

$$\mathrm{Tr}[\boldsymbol{\delta U}_2] = 1 - \frac{\left|\boldsymbol{A}_2 - \left(1 - \frac{|\boldsymbol{A}_1 - \boldsymbol{W}_1|}{|\boldsymbol{A}_1|}\right)\boldsymbol{U}_2 - \boldsymbol{U}_2\right|}{\left|\boldsymbol{A}_2 - \left(1 - \frac{|\boldsymbol{A}_1 - \boldsymbol{W}_1|}{|\boldsymbol{A}_1|}\right)\boldsymbol{U}_2\right|}. \tag{44}$$

We follow the same procedure to obtain

$$\mathrm{Tr}[\boldsymbol{\gamma W}_{12}] = -\mathrm{Tr}\left[\boldsymbol{D}\boldsymbol{U}_{21}\boldsymbol{A}_1^{-1}\boldsymbol{W}_{12}\right] \tag{45}$$

and since

$$\begin{aligned}\boldsymbol{U}_{21}\boldsymbol{A}_1^{-1}\boldsymbol{W}_{12} &= \varphi_2^-\left(\tilde{\boldsymbol{v}}_1^+\boldsymbol{A}_1^{-1}\varphi_1^-\right)\tilde{\boldsymbol{v}}_2^- = \mathrm{Tr}\left[\boldsymbol{A}_1^{-1}\left(\varphi_1^-\tilde{\boldsymbol{v}}_1^+\right)\right]\varphi_2^-\tilde{\boldsymbol{v}}_2^- = \mathrm{Tr}\left[\boldsymbol{A}_1^{-1}\boldsymbol{V}_1\right]\boldsymbol{U}_2 \\ &= \left(1 - \frac{|\boldsymbol{A}_1 - \boldsymbol{V}_1|}{|\boldsymbol{A}_1|}\right)\boldsymbol{U}_2\end{aligned} \tag{46}$$

it follows

$$\mathrm{Tr}[\boldsymbol{\gamma W}_{12}] = -\left(1 - \frac{|\boldsymbol{A}_1 - \boldsymbol{V}_1|}{|\boldsymbol{A}_1|}\right)\mathrm{Tr}[\boldsymbol{\delta U}_2]. \tag{47}$$

Going on,

$$\mathrm{Tr}\left[\boldsymbol{\beta U}_{21}\right] = -\mathrm{Tr}\left[\boldsymbol{A}_1^{-1}\boldsymbol{U}_{12}\boldsymbol{D}\boldsymbol{U}_{21}\right] = -\mathrm{Tr}\left[\boldsymbol{D}\boldsymbol{U}_{21}\boldsymbol{A}_1^{-1}\boldsymbol{U}_{12}\right], \tag{48}$$

$$\begin{aligned}\boldsymbol{U}_{21}\boldsymbol{A}_1^{-1}\boldsymbol{U}_{12} &= \varphi_2^-\left(\tilde{\boldsymbol{v}}_1^+\boldsymbol{A}_1^{-1}\varphi_1^+\right)\tilde{\boldsymbol{v}}_2^- = \mathrm{Tr}\left[\boldsymbol{A}_1^{-1}\left(\varphi_1^+\tilde{\boldsymbol{v}}_1^+\right)\right]\varphi_2^-\tilde{\boldsymbol{v}}_2^- = \mathrm{Tr}\left[\boldsymbol{A}_1^{-1}\boldsymbol{W}_1\right]\boldsymbol{U}_2 \\ &= \left(1 - \frac{|\boldsymbol{A}_1 - \boldsymbol{W}_1|}{|\boldsymbol{A}_1|}\right)\boldsymbol{U}_2,\end{aligned} \tag{49}$$

so that

$$\mathrm{Tr}[\boldsymbol{\beta U}_{21}] = -\left(1 - \frac{|\boldsymbol{A}_1 - \boldsymbol{W}_1|}{|\boldsymbol{A}_1|}\right)\mathrm{Tr}[\boldsymbol{\delta U}_2]. \tag{50}$$

Eventually,

$$\begin{aligned}\mathrm{Tr}[\boldsymbol{\alpha}\boldsymbol{V}_1] &= \mathrm{Tr}\big[\boldsymbol{A}_1^{-1}\boldsymbol{V}_1\big] + \mathrm{Tr}\big[\boldsymbol{A}_1^{-1}\boldsymbol{U}_{12}\boldsymbol{D}\boldsymbol{U}_{21}\boldsymbol{A}_1^{-1}\boldsymbol{V}_1\big]\\ &= \mathrm{Tr}\big[\boldsymbol{A}_1^{-1}\boldsymbol{V}_1\big] + \mathrm{Tr}\big[\boldsymbol{D}\boldsymbol{U}_{21}\boldsymbol{A}_1^{-1}\boldsymbol{V}_1\boldsymbol{A}_1^{-1}\boldsymbol{U}_{12}\big],\end{aligned} \tag{51}$$

so that, being

$$\begin{aligned}\boldsymbol{U}_{21}\boldsymbol{A}_1^{-1}\boldsymbol{V}_1\boldsymbol{A}_1^{-1}\boldsymbol{U}_{12} &= \varphi_2^-\big(\tilde{\boldsymbol{v}}_1^+\boldsymbol{A}_1^{-1}\varphi_1^-\big)\big(\tilde{\boldsymbol{v}}_1^+\boldsymbol{A}_1^{-1}\varphi_1^+\big)\tilde{\boldsymbol{v}}_2^-\\ &= \mathrm{Tr}\big[\boldsymbol{A}_1^{-1}\big(\varphi_1^-\tilde{\boldsymbol{v}}_1^+\big)\big]\mathrm{Tr}\big[\boldsymbol{A}_1^{-1}\big(\varphi_1^+\tilde{\boldsymbol{v}}_1^+\big)\big]\varphi_2^-\tilde{\boldsymbol{v}}_2^-\\ &= \mathrm{Tr}\big[\boldsymbol{A}_1^{-1}\boldsymbol{V}_1\big]\mathrm{Tr}\big[\boldsymbol{A}_1^{-1}\boldsymbol{W}_1\big]\boldsymbol{U}_2,\end{aligned} \tag{52}$$

we obtain

$$\mathrm{Tr}[\boldsymbol{\alpha}\boldsymbol{V}_1] = \left(1 - \frac{|\boldsymbol{A}_1 - \boldsymbol{V}_1|}{|\boldsymbol{A}_1|}\right)\left\{1 + \left(1 - \frac{|\boldsymbol{A}_1 - \boldsymbol{W}_1|}{|\boldsymbol{A}_1|}\right)\mathrm{Tr}[\boldsymbol{\delta}\boldsymbol{U}_2]\right\}. \tag{53}$$

Therefore we see that, in principle, equations (44), (47), (50) and (53), introduced in equation (38), solve our problem.

4. Calculation of the determinants

We can now proceed to examine the problem of calculating the determinants in the previous equations. An immediate simplification arises, since $|\boldsymbol{A}_1 - \boldsymbol{V}_1| = 1$, as follows from equations (20) and (32). Since the explicit limits $N \to \infty$ and $M \to \infty$ can be performed independently, we can first make $N \to \infty$ and evaluate $|\boldsymbol{A}_1|$ and $|\boldsymbol{A}_1 - \boldsymbol{W}_1|$. $|\boldsymbol{A}_1|$ is nothing but the Fredholm determinant [16] $\Delta_1(\lambda)$ relative to the Fredholm integral equation of the second kind with kernel

$$K(y_i, y_j) = K_{ij} = \mathrm{e}^{-ky_{ij}} V^{(1)}(y_j) \tag{54}$$

and can be written as

$$|\boldsymbol{A}_1| = \Delta_1(\lambda) = \begin{vmatrix} 1 + \lambda K_{11}\,\mathrm{d}\xi & \lambda K_{12}\,\mathrm{d}\xi & \dots & \lambda K_{1N}\,\mathrm{d}\xi \\ \lambda K_{21}\,\mathrm{d}\xi & 1 + \lambda K_{22}\,\mathrm{d}\xi & \dots & \lambda K_{2N}\,\mathrm{d}\xi \\ \vdots & \vdots & \ddots & \vdots \\ \lambda K_{N1}\,\mathrm{d}\xi & \lambda K_{N2}\,\mathrm{d}\xi & \dots & 1 + \lambda K_{NN}\,\mathrm{d}\xi \end{vmatrix} \tag{55}$$

where the following expansion can be used [19, 18]:

$$\begin{aligned}\Delta_1(\lambda) = 1 + \lambda \sum_{p_1=1}^{N} K_{p_1p_1}\mathrm{d}\xi + \frac{\lambda^2}{2}\sum_{p_1,p_2=1}^{N}\begin{vmatrix} K_{p_1p_1} & K_{p_1p_2} \\ K_{p_2p_1} & K_{p_2p_2}\end{vmatrix}\mathrm{d}\xi^2 \\ + \dots + \frac{\lambda^N}{N!}\sum_{p_1,p_2,\dots,p_N=1}^{N}\begin{vmatrix} K_{p_1p_1} & K_{p_1p_2} & \cdots & K_{p_1p_N} \\ K_{p_2p_1} & K_{p_2p_2} & \cdots & K_{p_2p_N} \\ \vdots & \vdots & \ddots & \vdots \\ K_{p_Np_1} & K_{p_Np_1} & \cdots & K_{p_Np_N}\end{vmatrix}\mathrm{d}\xi^N.\end{aligned} \tag{56}$$

Now we can perform explicitly the limit $N \to \infty$, and obtain the everywhere convergent series [20] (in other terms, $\Delta_1(\lambda)$ is an *entire* function of λ)

$$\Delta_1(\lambda) = 1 + \sum_{n=1}^{\infty} \frac{\lambda^n}{n!} D_n \quad , \tag{57}$$

$$D_n = \int_a^b \mathrm{d}y_n \cdots \int_a^b \mathrm{d}y_2 \int_a^b \mathrm{d}y_1 \begin{vmatrix} K(y_1, y_1) & K(y_1, y_2) & \cdots & K(y_1, y_n) \\ K(y_2, y_1) & K(y_2, y_2) & \cdots & K(y_2, y_n) \\ \vdots & \vdots & \ddots & \vdots \\ K(y_n, y_1) & K(y_n, y_2) & \cdots & K(y_n, y_n) \end{vmatrix}$$
$$= \int_a^b \mathrm{d}y_n \cdots \int_a^b \mathrm{d}y_2 \int_a^b \mathrm{d}y_1 \begin{vmatrix} 1 & \mathrm{e}^{-ky_{12}} & \cdots & \mathrm{e}^{-ky_{1n}} \\ \mathrm{e}^{-ky_{12}} & 1 & \cdots & \mathrm{e}^{-ky_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{e}^{-ky_{1n}} & \mathrm{e}^{-ky_{2n}} & \cdots & 1 \end{vmatrix} V^{(1)}(y_1)V^{(1)}(y_2)\cdots V^{(1)}(y_n). \tag{58}$$

Analogously, $\Lambda_1(\lambda)$ is the companion determinant (but not strictly a 'Fredholm determinant', since it is not directly related to the kernel of an integral equation)

$$|\boldsymbol{A}_1 - \boldsymbol{W}_1| = \Lambda_1(\lambda) = \begin{vmatrix} 1 + \lambda H_{11}\,\mathrm{d}\xi & \lambda H_{12}\,\mathrm{d}\xi & \ldots & \lambda H_{1N}\,\mathrm{d}\xi \\ \lambda H_{21}\,\mathrm{d}\xi & 1 + \lambda H_{22}\,\mathrm{d}\xi & \ldots & \lambda H_{2N}\,\mathrm{d}\xi \\ \vdots & \vdots & \ddots & \vdots \\ \lambda H_{N1}\,\mathrm{d}\xi & \lambda H_{N2}\,\mathrm{d}\xi & \ldots & 1 + \lambda H_{NN}\mathrm{d}\xi \end{vmatrix} \tag{59}$$

where

$$H_{ij} = H(y_i, y_j) = (\mathrm{e}^{-ky_{ij}} - \mathrm{e}^{ky_{ij}^+})V^{(1)}(y_j) \tag{60}$$

and it can be expanded in the same way, as

$$\Lambda_1(\lambda) = 1 + \sum_{n=1}^{\infty} \frac{\lambda^n}{n!} L_n \quad , \tag{61}$$

$$L_n = \int_a^b \mathrm{d}y_n \cdots \int_a^b \mathrm{d}y_2 \int_a^b \mathrm{d}y_1 \begin{vmatrix} 1 - \mathrm{e}^{2ky_1} & \mathrm{e}^{-ky_{12}} - \mathrm{e}^{ky_{12}^+} & \cdots & \mathrm{e}^{-ky_{1n}} - \mathrm{e}^{ky_{1n}^+} \\ \mathrm{e}^{-ky_{12}} - \mathrm{e}^{ky_{12}^+} & 1 - \mathrm{e}^{2ky_2} & \cdots & \mathrm{e}^{-ky_{2n}} - \mathrm{e}^{ky_{2n}^+} \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{e}^{-ky_{1n}} - \mathrm{e}^{ky_{1n}^+} & \mathrm{e}^{-ky_{2n}} - \mathrm{e}^{ky_{2n}^+} & \cdots & 1 - \mathrm{e}^{2ky_n} \end{vmatrix}$$
$$\times V^{(1)}(y_1)V^{(1)}(y_2)\cdots V^{(1)}(y_n). \tag{62}$$

Now, we can define the function

$$h(\lambda) = 1 - \frac{|\boldsymbol{A}_1 - \boldsymbol{W}_1|}{|\boldsymbol{A}_1|} \tag{63}$$

and $\mathrm{Tr}[\boldsymbol{\delta U}_2]$ is calculated by performing the limit $M \to \infty$:

$$\mathrm{Tr}[\boldsymbol{\delta U}_2] = 1 - \frac{|\boldsymbol{A}_2 - g(\lambda)\boldsymbol{U}_2|}{|\boldsymbol{A}_2 - h(\lambda)\boldsymbol{U}_2|}, \qquad \text{with} \quad g(\lambda) = 1 + h(\lambda). \tag{64}$$

By using previous considerations it is not difficult to show that $(q = g, h)$

$$|\boldsymbol{A}_2 - q(\lambda)\boldsymbol{U}_2| = \Theta_2(\lambda) = 1 + \sum_{n=1}^{\infty} \frac{\lambda^n}{n!} Q_n \quad , \tag{65}$$

$$Q_n = \int_c^d \mathrm{d}z_n \cdots \int_c^d \mathrm{d}z_2 \int_c^d \mathrm{d}z_1$$
$$\times \begin{vmatrix} 1 - q(\lambda)\,\mathrm{e}^{-2kz_1} & \mathrm{e}^{-kz_{12}} - q(\lambda)\,\mathrm{e}^{-kz_{12}^+} & \cdots & \mathrm{e}^{-kz_{1n}} - q(\lambda)\,\mathrm{e}^{-kz_{1n}^+} \\ \mathrm{e}^{-kz_{12}} - q(\lambda)\,\mathrm{e}^{-kz_{12}^+} & 1 - q(\lambda)\,\mathrm{e}^{-2kz_2} & \cdots & \mathrm{e}^{-kz_{2n}} - q(\lambda)\,\mathrm{e}^{-kz_{2n}^+} \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{e}^{-kz_{1n}} - q(\lambda)\,\mathrm{e}^{-kz_{1n}^+} & \mathrm{e}^{-kz_{2n}} - q(\lambda)\,\mathrm{e}^{-kz_{2n}^+} & \cdots & 1 - q(\lambda)\,\mathrm{e}^{-2kz_n} \end{vmatrix}$$
$$\times V^{(2)}(z_1)V^{(2)}(z_2)\cdots V^{(2)}(z_n). \tag{66}$$

Therefore, all determinants can be evaluated as entire series of λ.

5. Limiting cases

It is simple to show that our formulae, when $V^{(2)} = 0$, or $V^{(1)} = 0$, give the pure transmission and the pure reflection cases, respectively. Let us consider $V^{(2)} = 0$: only the first trace survives in equation (38), and equation (53) gives

$$\mathrm{Tr}[\boldsymbol{\alpha}\boldsymbol{V}_1] = \mathrm{Tr}\big[\boldsymbol{A}_1^{-1}\boldsymbol{V}_1\big] = 1 - \frac{1}{\Delta_1(\lambda)}. \tag{67}$$

The formula for the transmission is therefore obtained [2]:

$$G(x, s; \eta) = \frac{G_0(x, s; \eta)}{\Delta_1(\lambda)}. \tag{68}$$

If $V^{(1)} = 0$, on the other hand, only the last trace in equation (38) is different from zero. Equation (64), where $h(\lambda) = 0$, gives

$$\mathrm{Tr}[\boldsymbol{\delta}\boldsymbol{U}_2] = \mathrm{Tr}\big[\boldsymbol{A}_2^{-1}\boldsymbol{U}_2\big] = 1 - \frac{\Gamma_2(\lambda)}{\Delta_2(\lambda)} \tag{69}$$

where Γ_2 is Θ_2 of equation (65) with $q(\lambda) = 1$, and Δ_2 is the analogous of Δ_1 of equation (55) for the potential $V^{(2)}$. So, we obtain

$$G(x, s; \eta) = G_0(x, s; \eta) - \frac{c}{2}\frac{\mathrm{e}^{k(x+\eta)}}{\sqrt{s}}\left[1 - \frac{\Gamma_2(\lambda)}{\Delta_2(\lambda)}\right] \tag{70}$$

that is the formula for the reflection [3].

6. A simple application

In order to show an example with affordable calculations, let us consider the potentials

$$V^{(1)}(y) = V_1\delta(x_1 - y), \qquad V^{(2)}(z) = V_2\delta(x_2 - z), \qquad x_2 > x_1. \tag{71}$$

In this case, the integrals occurring in calculating determinants are straightforward, and all the expansions stop at $n = 1$ [2], so obtaining ($\lambda_{1,2} = \lambda V_{1,2}$)

$$1 - \frac{1}{|\boldsymbol{A}_1|} = \frac{\lambda_1}{1+\lambda_1}, \qquad h(\lambda) = 1 - \frac{|\boldsymbol{A}_1 - \boldsymbol{W}_1|}{|\boldsymbol{A}_1|} = \frac{\lambda_1}{1+\lambda_1}\,\mathrm{e}^{2kx_1}, \tag{72}$$

from which equations (64) and (65) give

$$\mathrm{Tr}[\boldsymbol{\delta U}_2] = 1 - \frac{1+\lambda_2[1-g(\lambda)\,\mathrm{e}^{-2kx_2}]}{1+\lambda_2[1-h(\lambda)\,\mathrm{e}^{-2kx_2}]} = \frac{(1+\lambda_1)\lambda_2\,\mathrm{e}^{-2kx_2}}{D(\lambda)} \tag{73}$$

and the other terms of equation (38) become

$$\begin{aligned}\mathrm{Tr}[\gamma \boldsymbol{W}_{12}] &= -\frac{\lambda_1\lambda_2\,\mathrm{e}^{-2kx_2}}{D(\lambda)}\\ \mathrm{Tr}[\beta \boldsymbol{U}_{21}] &= -\frac{\lambda_1\lambda_2\,\mathrm{e}^{-2kx_{12}}}{D(\lambda)}\\ \mathrm{Tr}[\alpha \boldsymbol{V}_1] &= \frac{\lambda_1(1+\lambda_2)}{D(\lambda)}\end{aligned} \tag{74}$$

where

$$x_{12} = x_2 - x_1, \qquad D(\lambda) = 1 + \lambda_1 + \lambda_2 + \lambda_1\lambda_2(1-\mathrm{e}^{-2kx_{12}}). \tag{75}$$

The final result is

$$G(x,s;\eta) = \frac{c}{2}\left[\frac{(1+\lambda V_2)\,\mathrm{e}^{-c(x-\eta)\sqrt{s}}}{\sqrt{s}D(\lambda)} - \frac{\lambda V_2\,\mathrm{e}^{-c(2x_2-x-\eta)\sqrt{s}}}{\sqrt{s}D(\lambda)}\right]. \tag{76}$$

The spacetime propagator $G(x,t;\eta)$ is obtained from $G(x,s;\eta)$ by Laplace inversion, using for example the approximation methods shown in [21, 22].

7. Conclusions

We have presented a theory that is suitable to solve the Schrödinger equation for a particle localized between two potential barriers. The main result is that the general solution, although rather complicated, is exact. Only the simple case of two delta barriers has been explicitly solved, but in our opinion the method can be applied also to more realistic barriers, owing to the fast convergence of the series expressing determinants and to the effective techniques of inverting Laplace transforms.

A drawback of this approach is evident: it is applicable only to one-dimensional problems, due to the fact that the kernel for the three-dimensional ones is not separable, even outside the potential [1, 4]. However, our work in this direction is in progress.

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