Infinite plane wave evolution in a 1-D square quantum barrier

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Abstract. We analytically compute the time evolution of an initial infinite plane wave in the presence of a 1-dimensional square quantum barrier. This calculation generalizes the analysis of the shutter problem and sets the basis for the calculation of the transmission of general wave packets, aiming to work out the explicit contribution of the resonant (Gamow) states. The method relies mainly on the analytical properties of the Green function. The role of separate boundary conditions on the Green function and on the evolution equation is highlighted. As in previous works on related problems, only the determination of the resonant momenta requires numerical methods.

PACS numbers: 11.10.Ef, 11.10.Lm, 04.60

Submitted to: Journal of Physics A: Mathematical and General
1. Introduction

Seemingly simple quantum mechanical problems like the traversal of potential barriers by wave packets are surprisingly rich of mathematical, technical and physical details. The 1-dimensional case is interesting in its own: electron transport through barrier junctions, the physics of light and wave guides, particularly of the transmission through Photonic Band Gaps, the time of arrival of wave packets and the ensuing paradoxes of non-locality and super-luminal tunnelling are examples.

Because of its strong overlapping with the standard theory of 3-D scattering, usually the s-wave radial problem for the spherical shell potential is studied in the literature as an example of the role of the potential barriers in connection with the evolution of decaying states. These states obey specific boundary conditions (BCs), namely the vanishing of the wave function at the origin and a purely outgoing BC outside the barrier. However the corresponding BCs adopted in the 1-D scattering make it different also from a mathematical point of view, providing a different setting for the related resonant (Gamow) states.

On the other hand, practical calculations face important limitations and the effort of pushing the analytical calculation as far as possible is always rewarding. Significant progress has been accomplished [1] for a Gaussian packet impinging on a square barrier, where the Gaussian structure was exploited, and [2] for the shutter problem, where the contribution of the resonant states in a double square barrier was worked out. Relevant resonances are mostly expected in systems of two or more barriers separated by a gap. Actually they generally occur in any simple barrier, and the plain square barrier is most tractable, fully representative for many theoretical purposes and devoid of bound states or other unessential features.

In this paper we consider the time evolution, in the presence of a square barrier, of an initial plane wave with support on the whole 1-D space, aiming to work out the contribution of the resonant states. These states have a central role, as long as they correspond to complex momenta (or energies) which are poles of the S-matrix, and dictate the most convenient type of BCs to be used in the problem.

Our calculation extends the results of shutter problem, where the initial plane wave occupied the space axis at one side of the barrier and was specially suited to study details of the propagation of the wave front. We provide a comprehensive result containing also the evolution of the segments of the initial plane wave lying inside and at the other side of the barrier.

Our main goal however, is to pave the way for further uses since superpositions of infinite plane waves build up any desired initial wave packet. In particular, the compact result obtained for the Gaussian wave packet [1] could be re-derived pinpointing the contribution of each single Fourier component.

A byproduct of our calculation is to provide an explicit example where we can study the properties of completeness of the resonant states in different regions of the square potential, an issue properly dealt with [3] in the frame of Rigged Hilbert Spaces, which
will be addressed elsewhere.

In this paper we follow the approach used by Peierls and García-Calderón [4], namely Laplace-transforming the time evolution equation into a second order linear differential equation (SOLDE) in one variable, expressing its solutions in terms of the Green function (GF) with resonant boundary conditions (RBCs) and then undoing the Laplace transform.

The first step is done in Section 2, where a brief discussion is made of the use of the Green’s method for the solution of SOLDEs when the BCs required for the GF and for the solution are different. This point is relevant for the issue of the completeness of the Gamow states. The GF with RBCs features a simple structure of isolated (resonance) poles, in terms of which the \((p\text{-dependent})\) Laplace-transformed wave function is worked out in Section 3 previously to the second step. Then the explicit calculation of the inverse Laplace transform leading to the sought after \(t\text{-dependent}\) solution is carried out in Section 4.

As a check of this cumbersome analytical calculation, the \(t = 0\) (Section 5 of the paper) and the \(t = \infty\) (Section 6) limits of the time-dependent solution \(\psi(x, t)\) are calculated: at \(t = 0\) one must recover the initial plane wave and at \(t = \infty\) a suitable stationary solution must be reached. Then the conclusions are drawn in Section 7.

Some notations and a number of calculations and technical details are deferred to the Appendices in an effort to make the paper more self-contained.

2. The evolution equations

We consider the 1-D time-dependent Schrödinger equation

\[
(i\hbar \frac{\partial}{\partial t} - H)\psi(x, t) = 0
\]

where the Hamiltonian \(H = p^2/2m + V(x)\) corresponds to the square barrier potential \(V(x) = \theta(x)\theta(L - x)V\) and the solution satisfies the initial condition \(\psi(x, 0) \equiv \psi_o(x) = e^{ikx}, k > 0\).

The Laplace transform \(\tilde{\psi}(s) = \int_0^\infty dt \, e^{-st}\psi(t)\) on the time variable, brings the parabolic partial derivative differential equation (1) to the simpler SOLDE

\[
\left[\frac{\partial^2}{\partial x^2} + p^2 - \frac{2m}{\hbar^2}V(x)\right] \tilde{\psi}(x, p) = i\alpha \, e^{ikx}
\]

where \(\alpha \equiv 2m/\hbar\) and \(p^2 = i\alpha \, s\) (Appendix A). The homogeneous equation \(L_x \tilde{\psi} = 0\), namely the time-independent Schrödinger equation for the potential \(V(x)\), has a variety of solutions according to the BCs we choose at \(x = 0\) and \(x = L\) depending on the physical problem. Besides the usual scattering \textit{in} and \textit{out} solutions for continuous and real \(E = p^2/2m > 0\), one has the resonant solutions satisfying the homogeneous outgoing RBCs

\[
\partial_x \tilde{\psi}|_{x=0} = -ip \, \tilde{\psi}(0) , \quad \partial_x \tilde{\psi}|_{x=L} = ip \, \tilde{\psi}(L)
\]
(the ingoing reversed sign of $p$ is not considered here for the reasons outlined later on). These solutions exist only for a denumerable set of isolated values $p_n$ of $p$ lying in the lower half complex plane (Appendix A).

A solution to the inhomogeneous equation (2) for $p^2 \in R_+$ can be explicitly written down for each region of $V(x)$:

$$
\tilde{\psi}_I(x,p) = B e^{-i p x} + \frac{i \alpha}{p^2 - k^2} e^{i k x} \quad (x < 0)
$$

$$
\tilde{\psi}_{II}(x,p) = M e^{i p' x} + N e^{-i p' x} + \frac{i \alpha}{p'^2 - k^2} e^{i k x} \quad (0 \leq x \leq L) \quad (4)
$$

$$
\tilde{\psi}_{III}(x,p) = A e^{i p x} + \frac{i \alpha}{p^2 - k^2} e^{i k x} \quad (x > L)
$$

where the amplitudes $A$, $B$, $M$ and $N$ are functions of $p$ completely determined by the matching conditions at $x = 0$ and $x = L$ and have a common denominator of the form $D(p) \equiv \odot^2 e^{ip'L} - \odot^2 e^{-ip'L}$ (notation in Appendix A). Out of all the terms of the general homogeneous solution, the choice of $e^{ip x}$ (for $x > L$) or $e^{-ip x}$ (for $x < 0$) is dictated by the behaviour of the solution for $x \to \pm \infty$, since a small positive imaginary part in $p$ is supposed when performing the inverse Laplace transform leading to $\psi(x,t), t > 0$ (Appendix D).

However, this expression of the solution is not suited to perform the inverse Laplace transform back to $\psi(x,t)$ because of the nontrivial analytical form of the amplitudes above. Instead the GF approach lets us to express $\tilde{\psi}(x,p)$ as a sum of isolated pole terms plus other simple terms easier to deal with. To this end, (2) together with the Green equation for $G(x,x',p)$ can be written in the form

$$
L_x \tilde{\psi}(x,p) - i \alpha e^{i k x} = 0 \quad (5)
$$

$$
L_x G(x,x',p) - \delta(x-x') = 0 \quad (6)
$$

where $G(x,x',p)$ is required to obey RBCs, namely

$$
\frac{\partial_x G(x,x',p)|_{x=0}}{-ip G(0,x',p) + \partial_x G(x,x',p)|_{x=L} = ip G(L,x',p)} \quad (7)
$$

It is expected that $G(x,x',p) = L_x^{-1}$ will have poles at $p = p_n$, where the homogeneous equation $L_x \tilde{\psi} = 0$ with RBCs has non-trivial solutions.

The equations (5) and (6) may conveniently be given the short-hand notation

$$
\Psi = 0 \quad \Gamma = 0 \quad \text{respectively. Then the Green method uses the integral equation}
$$

$$
\int_0^L dx \left[ \tilde{\psi} \Gamma - G \Psi \right] = 0 \quad \text{to obtain } \tilde{\psi}(x,p) \text{ in terms of } G(x,x',p). \quad \text{Only if } \tilde{\psi} \text{ and } G \text{ obey the same homogeneous BCs, the surface terms in this integral cancel out and one obtains the familiar result}
$$

$$
\tilde{\psi}_{II}(x,p) = \int_0^L dx' i \alpha G(x',x,p) e^{ik x'}.
$$

However the BCs for $\tilde{\psi}(x,p)$ (involving $\tilde{\psi}$ and $\partial_x \tilde{\psi}$ both at $x = 0$ and at $x = L$) stemming from (4) are different from (3) and non-homogeneous. In that case one obtains
a modified expression for the Region II, namely
\[ \bar{\psi}_{II}(x,p) = \int_0^L dx' i\alpha G(x',x,p) e^{ikx'} - \frac{\alpha}{p+k} G(L,x,p)e^{ikL} - \frac{\alpha}{p-k} G(0,x,p) \] (8)

For the external regions I and III, the matching of \( \bar{\psi} \) at \( x=0 \) and \( x=L \) determine the coefficients \( B \) and \( A \) respectively, so that
\[ \bar{\psi}_{I}(x,p) = i\alpha e^{-ipx} \int_0^L dx' i\alpha G(x',0,p) e^{ikx'} - \frac{\alpha}{p+k} G(L,0,p)e^{ikL}e^{-ipx} - \frac{\alpha}{p-k} G(0,0,p)e^{-ipx} \]
\[ - \frac{i\alpha}{p^2-k^2} e^{-ipx} + \frac{i\alpha}{p^2-k^2} e^{ikx} \] (9)

and
\[ \bar{\psi}_{III}(x,p) = i\alpha e^{ip(x-L)} \int_0^L dx' i\alpha G(x',L,p) e^{ikx'} - \frac{\alpha}{p+k} G(L,L,p)e^{ip(x-L)}e^{-ipx} - \frac{\alpha}{p-k} G(0,L,p)e^{ip(x-L)} \]
\[ - \frac{i\alpha}{p^2-k^2} e^{ip(x-L)} e^{ikL} + \frac{i\alpha}{p^2-k^2} e^{ikx} \] (10)

For comparison, only the last term in the r.h.s. of (8), the last three ones in (9) and the third one in (10) appear in the shutter problem.

The crucial advantage of the method is that almost all the Green functions involved in the equations above can be expanded as a sum of terms which are simple poles in \( p_n \).

3. Analytical structure of the \( p \)-dependent solution

General theorems \[5\] and the explicit analytical derivation (Appendix B) of \( G(x,x',p) \) show that \( |G(x,x',p)| \sim 1/|p| \to 0 \) as \( |p| \to \infty \) in the complex plane for almost any \( x \in [0,L] \) and \( x' \in [0,L] \). Then the Mittag-Leffler theorem tells that
\[ G(x,x',p) = \sum_n \frac{C_n(x,x')}{p-p_n} \] (11)

The exception is for \( G(0,0,p) \) and \( G(L,L,p) \), the modulus of which grows as \( |p| \) for \( |p| \to \infty \) in the lower half complex plane \( p \) and requires some special care (Appendix C).

The residues in the r.h.s of (11) can be easily computed \[4\] and one finds \( C_n(x,x') = u_n(x)u_n(x')/N_n \), where the functions \( u_n(x) \) belong to the denumerable set of the resonant solutions satisfying \( L_x u_n(x) = 0 \) with RBCs
\[ \partial_x u_n(x)|_{x=0} = -ip_n u_n(0) , \quad \partial_x u_n(x)|_{x=L} = ip_n u_n(L) \]
and \( N_n \) are suitable normalization factors (Appendix A).

The inverse Laplace transform

\[
\psi(x, t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \ e^{st} \tilde{\psi}(x, p(s)) = \frac{1}{2\pi m} \int_{-\infty}^{+\infty} dp \ p \ e^{-i\frac{p^2}{2m}t} \tilde{\psi}(x, p),
\]

written as an integral over the real momentum variable \( p \) (Appendix D), leads one to consider the pole expansion of \( p \tilde{\psi}(x, p) \) in the integrand, which can be worked out for each sector \( I, II \) and \( III \). We report here only the result (Appendix E) for the sectors \( II \) and \( III \) (sector \( I \) is similar to sector \( III \) because of the symmetry of both the potential and the initial condition):

\[
p \tilde{\psi}_{II}(x, p) = i\alpha \sum_n \frac{p}{p-p_n} \frac{u_n(x)}{N_n} \int_0^L dx' \ u_n(x') \ e^{ikx'}
+ \alpha \sum_n \frac{1}{p-p_n} \frac{1}{k+p_n} \ \frac{u_n(L)u_n(x)}{N_n}
- \alpha \sum_n \frac{1}{p-p_n} \frac{1}{k-p_n} \ \frac{u_n(0)u_n(x)}{N_n}
\]

(13)

\[
p \tilde{\psi}_{III}(x, p) = i\alpha \ e^{ip(x-L)} \sum_n \frac{p}{p-p_n} \frac{u_n(L)}{N_n} \int_0^L dx' \ u_n(x') \ e^{ikx'}
- \alpha \sum_n \frac{p}{p-p_n} \frac{1}{k+p_n} \ \frac{u_n^2(L)}{N_n} \ e^{ip(x-L)} \ e^{ikL}
- \alpha \sum_n \frac{p}{p-p_n} \frac{1}{k-p_n} \ \frac{u_n(0)u_n(L)}{N_n} \ e^{ip(x-L)}
+ \alpha \frac{1}{k-p} \ \frac{kG(0, L, k)e^{ip(x-L)}}{N_n}
+ \frac{i\alpha}{2} \left( \frac{1}{p+k} + \frac{1}{p-k} \right) (e^{ikx} - e^{ip(x-L)} \ e^{ikL})
\]

(14)

One recognizes the terms of the shutter problem in the third row of (13) and in the fourth row of (14).

4. The time-dependent solution

For each of the terms above, the integrals stemming from (12) can be brought to the form of an integral representation of the (complementary) error function \( \text{erfc}(z) \) so that their inverse Laplace transform can be carried out thoroughly (Appendix F). We obtain:

\[
\psi_{II}(x, t) = -\sum_n \frac{u_n(x)}{N_n} \left( \int_0^L dx' \ u_n(x') \ e^{ikx'} \right) [A_n^{II}]
+ ikG(L, x, -k) e^{ikL} [B_{II}] - i\epsilon^{ikL} \sum_n \frac{p_n}{k+p_n} \ \frac{u_n(L)u_n(x)}{N_n} [B_n^{II}]
\]
where the factors in square brackets embody the time \((\tau = t/2m)\) dependence of the solution and are the result of the integrations over the momentum \(p\). Explicitly

\[
\begin{align*}
A_n^{III} &= -p_n e^{-irp_0^2} \text{erfc}(i\sqrt{\tau}) - \frac{e^{-irp_0^2}}{\sqrt{\pi \tau}} \\
B_0^{III} &= -e^{-irkx} \text{erfc}(i\sqrt{\tau}k) \\
B_n^{III} &= -e^{-irp_n^2} \text{erfc}(i\sqrt{\tau}p_n) \\
S_n^{III} &= -e^{-irp_n^2} \text{erfc}(i\sqrt{\tau}p_n)
\end{align*}
\]

Likewise

\[
\psi_{III}(x, t) = -\sum_n \frac{u_n(L)}{N_n} \left( \int_0^L dx' u_n(x') e^{ikx'} \right) [A_n^{III}] \\
- iG(L, L, 0) \frac{e^{ikL}}{k} [B_0^{III}] + iG(L, L, -k) \frac{e^{ikL}}{k} [B_{-k}^{III}] \\
- ie^{ikL} \sum_n \frac{1}{p_n} \frac{1}{k + p_n} \frac{u_n^2(L)}{N_n} [B_n^{III}] \\
- iG(0, L, k) [S_n^{III}] + i \sum_n \frac{p_n}{k - p_n} \frac{u_n(0)u_n(L)}{N_n} [S_n^{III}] \\
- 2e^{ikx} [C_1^{III}] - 2e^{ikx} [C_2^{III}] + \frac{1}{2}e^{ikL} [C_3^{III}] + \frac{1}{2}e^{ikL} [C_4^{III}]
\]

where

\[
\begin{align*}
A_n^{III} &= -e^{\frac{i(2-L)^2}{4\tau}}(p_n e^{g_n^2} \text{erfc}(y_n) + \frac{e^{i\pi/4}}{\sqrt{\pi \tau}}) \\
B_0^{III} &= -\frac{e^{i\pi/4}}{\sqrt{\pi \tau}} \frac{x-L}{2\tau} e^{\frac{i(x-L)^2}{4\tau}} \\
B_{-k}^{III} &= -e^{\frac{i(2-L)^2}{4\tau}}(k^2 e^{g_k^2} \text{erfc}(y_{-k}) + \frac{e^{i\pi/4}}{\sqrt{\pi \tau}}(-k + \frac{x-L}{2\tau})) \\
B_n^{III} &= -e^{\frac{i(2-L)^2}{4\tau}}(p_n^2 e^{g_n^2} \text{erfc}(y_n) + \frac{e^{i\pi/4}}{\sqrt{\pi \tau}}(p_n + \frac{x-L}{2\tau})) \\
S_n^{III} &= -e^{\frac{i(2-L)^2}{4\tau}} e^{g_k^2} \text{erfc}(y_k) \\
S_{-k}^{III} &= -e^{\frac{i(2-L)^2}{4\tau}} e^{g_k^2} \text{erfc}(y_{-k}) \\
C_1^{III} &= -e^{-irk^2} \text{erfc}(i\sqrt{\tau}k) \\
C_2^{III} &= -e^{-irk^2} \text{erfc}(i\sqrt{\tau}k) \\
C_3^{III} &= -e^{\frac{i(2-L)^2}{4\tau}} e^{g_{-k}^2} \text{erfc}(y_{-k})
\end{align*}
\]
We have introduced the variables \( y_q = e^{-i\pi/4} (4\tau)^{-1/2} (x - L - 2\tau q) \) for \( q = p_n, k, -k \). In both equations the terms \([S]\) are the ones arising in the shutter problem. The particular values of the Green function involved in eqs.(15) and (17) are calculated in Appendix B.

5. The short time limit

The \( t \to 0 \) limit is interesting both as a check of the calculation above and for the study of the scattered wave at short times. Here we aim only to recover the initial wave function \( \psi(x,0) = e^{ikx} \) at \( t = 0 \), which must happen in each of the sectors I, II and III. The sector I similar to III, so we refrain from calculating it.

Careful use of the limiting values of \( \text{erfc}(z) \) and/or \( w(z) = e^{-z^2} \text{erfc}(-iz) \) for \( z \to 0 \) and for \( z \to \infty \) in different directions of the complex \( z \) plane must be made. Notice that \( y_q \) tends to \( \infty \) in different directions for different \( q \). Also the properties of the set of resonant functions \( u_n(x) \) as a basis of the space of solutions are crucial (Appendix G).

5.1. Region II

For \( \tau \to 0 \) the factors \([B^I]\), \([B^I_n]\), \([S^I]\) and \([S^I_n]\) tend to the value \(-1\), so that the \([B]\) terms in (15) yield

\[
\begin{align*}
   ikG(L, x, -k)e^{ikL} - ie^{ikL} \sum_{n} \frac{p_n}{k + p_n} \frac{u_n(L)u_n(x)}{N_n} &
   = ik e^{ikL} \sum_{n} \frac{1}{-k - p_n} \frac{u_n(L)u_n(x)}{N_n}
   - i e^{ikL} \sum_{n} \frac{p_n}{k + p_n} \frac{u_n(L)u_n(x)}{N_n}
   = -ie^{ikL} \sum_{n} \frac{u_n(L)u_n(x)}{N_n} = 0
\end{align*}
\]

and likewise for the \([S]\) terms:

\[
\begin{align*}
   ikG(0, x, k) - i \sum_{n} \frac{p_n}{k - p_n} \frac{u_n(0)u_n(x)}{N_n} &
   = ik \sum_{n} \frac{1}{k - p_n} \frac{u_n(0)u_n(x)}{N_n}
   - i \sum_{n} \frac{p_n}{k - p_n} \frac{u_n(0)u_n(x)}{N_n}
   = i \sum_{n} \frac{u_n(0)u_n(x)}{N_n} = 0
\end{align*}
\]

The limit of the factor \([A^I_n]\) is not readable in (16) since it seemingly blows up for \( \tau \to 0 \). Actually, the changes of variables done to perform the integration leading to this form of \([A^I_n]\) become singular in this limit. The right result can be reached by the
following reasoning: For $\tau \to 0$, an increasingly large range of values of $p$ (as compared to $\text{Re} \, p_n$) does contribute to the integral $\int_{-\infty}^{+\infty} dp \, e^{-i\tau p^2} p/(p - p_n)$. Therefore its limiting value $(\pi/\tau)^{1/2}$ does not depend on $p_n$ and becomes a common factor outside the first sum in (15). Then one recovers the sum $\sum u_n(x)u_n(x')/N_n = \delta(x - x')$, as expected from the $t \to 0$ limit of the Green function $G(x, x', t)$.

Therefore, for $0 \leq x \leq L$,

$$\lim_{t \to 0} \psi_{I I}(x, t) = e^{ikx} \equiv \psi_o(x)$$

as required.

Asymptotic expressions for $\text{erfc}(z)$ and $w(z)$ can be used to obtain approximations to the form of $\psi_{I I}(x, t)$ for small values of $t$, a task that will be faced elsewhere.

5.2. Region III

The limit must be studied term by term. The integral $\int_{-\infty}^{+\infty} dp \, e^{-i\tau p^2} e^{ip(x-L)} p/(p - p_n)$ has now an extra exponential factor which has a regularizing effect. As a result, the limit can be taken directly in $[A^{I I I}_n]$ as given in (18): the term $e^{ip_2} \text{erfc}(y_n)$ vanishes and $(\pi\tau)^{-1/2} e^{(y - L)^2/4\tau}$ approaches a distribution concentrated in $x = L$, namely $\delta(x - L)$. Thus it vanishes for $x > L$.

An analogous reasoning shows that $[B^{I I I}_0]$, $[B^{I I I}_{-k}]$ and $[B^{I I I}_n]$ yield derivatives of $\delta(x - L)$ and also vanish for $x > L$.

The factors $[S^{I I I}_n]$, $[S^{I I I}_n]$, $[C^{I I I}_3]$ and $[C^{I I I}_4]$ vanish exactly, whereas $[C^{I I I}_1]$ and $[C^{I I I}_2]$ tend to $-1$. From (17) we then see that the final result is that also

$$\lim_{t \to 0} \psi_{I I I}(x, t) = e^{ikx} \equiv \psi_o(x)$$

for $x > L$, as required.

The solution $\psi_I(x, t)$ at the left of the barrier will have a structure similar to (17) and the same limit above.

6. The large time limit

For $\tau \to \infty$ we see that also $y_q \to \infty$ as before, but in still different directions of the complex plane for the different $q$.

In the internal Region II, the factors $[A^{I I}_n]$, $[B^{I I}_n]$, $[B^{I I}_n]$ and $[S^{I I}_n]$ vanish, whereas $[S^{I I}] \to -2e^{-irk^2}$. Therefore, for $0 \leq x \leq L$,

$$\lim_{t \to \infty} \psi_{I I}(x, t) = 2ik \, G(0, x, k)e^{-irk^2} = \phi^{in}_r(x)e^{-iE_k t}$$

that is the stationary scattering in solution, where $E_k = k^2 / 2m$ (see Appendices B and H). Thus the infinite plane wave evolves into the same final state of the shutter initial condition.
For the external Region III, the only non-vanishing factors are
\[ S_{III} \rightarrow -2 e^{ik(x-L)}e^{-irk^2} \]
\[ C_{II}^{III} \rightarrow -2 e^{-irk^2} \]
\[ C_{IV}^{III} \rightarrow -2 e^{ik(x-L)}e^{-irk^2} \]
\[ (22) \]

Then the terms corresponding to \( C_{II}^{III} \) and \( C_{IV}^{III} \) in (17) cancel each other and, again, one is left with the same asymptotic solution of the shutter
\[ \lim_{t \to \infty} \psi_{III}(x,t) = 2i k G(0,L,k)e^{ik(x-L)}e^{-irk^2} \]
\[ = T(k)e^{ikx}e^{-iE_k t} \]
\[ = \phi_{in}^r(x)e^{-iE_k t} \]
\[ (23) \]

The finite time behaviour is thus made up of transient modes which quickly disappear leaving (for \( k > 0 \)) the scattering asymptotic solution with outgoing BC at \( x = L \).

7. Conclusions

A solution for the time evolution of an infinite plane wave in the presence of a simple square barrier has been worked out for each of the regions of the potential and Section 4 is the main result of this paper. Among other terms, this solution contains a sum of explicit analytical contributions corresponding to each of the (infinitely many) resonance poles. As in previous works in related problems [1] [2], only the location of these poles needs to be obtained by numerical methods.

In the solution obtained the shutter terms have been pinpointed. Similarly, the contributions to the evolved wave function coming from the segments of the initial wave function lying inside and at the right of the barrier can be identified.

As the main application of this knowledge we envisage the possibility of studying the enhancement or the suppression of the transmission of the single Fourier components of any realistic wave packet. This should provide new detailed insight on interesting phenomena like the super-luminal tunnelling [6], the breakdown of energy conservation [7] by transient interference in wave packet collisions with barriers [8] or the rising of forerunners.

Other side results of this work are more mathematical and preliminary for further study. The exact analytic expression for the GF of the square barrier subject to RBCs has been worked out. Some particular values of it are involved in the time-dependent solution obtained above, but its knowledge is also useful for computing in each region the extra terms in general resonance pole expansions of wave functions in order to implement, with an explicit example, the related question of the completeness of the set of the resonant solutions [9]. We have relied on the adoption of different boundary conditions for the GF and for the solutions of the (Laplace transformed) evolution
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equations. The link between this point and the properties of completeness of the solutions will be addressed elsewhere.

On more physical grounds, the explicit solution obtained for finite time is useful for deriving approximations valid for short times, hence for the study of transient structures and forerunners. An immediate result of the work is that the large time limit yields the same stationary solution of the shutter. This again shows that the resonances contribute only to transient structures of the scattered wave.

Acknowledgments

Work supported by MEC projects BFM2002-00834 and FIS2005-05304. The authors are indebted to J. León for suggestions and helpful discussions. J. Julve acknowledges the hospitality of the Dipartimento di Fisica dell’Università di Bologna, Italy, where part of this work was done.

Appendix A. Resonant solutions

We adopt units such that $\hbar = 1$ and define the differential operator

$$L_x \equiv \left[ \frac{\partial^2}{\partial x^2} + p^2 - 2mV(x) \right].$$

A piece-wise general solution for the homogeneous SOLDE $L_x u(x) = 0$ is

$$u(x, p) = \theta(-x)B e^{-ipx} + \theta(x)\theta(L-x)(M e^{ip'x} + N e^{-ip'x}) + \theta(x-L)A e^{ipx},$$

which has already built-in the RBCs (3). Choosing $B(p)$ arbitrary, the matching conditions at $x = 0$ and at $x = L$ yield the amplitudes

$$M(p) = -\frac{\Theta}{2p'}B(p),$$

$$N(p) = -\frac{\Theta}{2p'}B(p),$$

$$A(p) = -\frac{1}{2p'}(\Theta e^{-i\Theta L} - \Theta e^{-i\Theta L})B(p),$$

(A.1)

where $p' \equiv \sqrt{p^2 - 2mV}$, $\Theta \equiv p + p'$ and $\Theta \equiv p - p'$, plus an extra condition on $p$ which is proportional to

$$\Theta^2 e^{-i\Theta L} - \Theta^2 e^{-i\Theta L} = 0$$

(A.2)

This transcendent equation has a denumerable set of solutions $p_n$ lying in the lower complex plane $p$. The common denominator $D(p) \equiv \Theta^2 e^{ip'L} - \Theta^2 e^{-ip'L}$ in the amplitudes of (4) is just proportional to the l.h.s. of (A.2). One can check that if $p_n$ is a solution, then $-p_n^*$ is too, so that these values are in symmetrical locations with respect to the imaginary axis. We let the label $n$ take integer values ($n \neq 0$), with the growing
positive $n$ indicating the $p_n$ with growing real positive part and $p_{-n} \equiv -p_n^*$. One finds that $-\frac{\pi}{4} < \arg p_n < 0$ and $\pi < \arg p_{-n} < \frac{5\pi}{4}$.

The simplest writing of the solution (24) is obtained for $B(p) = -2p'$, namely

$$u_n(x) = \theta(-x)(-2p'_n)e^{-ip_n x} + \theta(x)\theta(L-x)(\Theta_n e^{ip'_n x} - \Theta_n e^{-ip'_n x}) + \theta(x-L)(\Theta_n e^{-i\Theta_n L} - \Theta_n e^{-i\Theta_n L}) e^{ip_n x}.$$  \hspace{1cm} (A.3)

Notice that the solution (4) should yield the outgoing resonant ones, which exist only for the momenta $p_n$, when we let the terms involving the initial condition $e^{ikx}$ (namely the particular solution of the inhomogeneous equation) vanish. In fact, one sees that for $p \to p_n$, these terms belong to the regular part of (4), with corresponding inhomogeneous BCs, while the pole part yields the resonant solution.

The crucial role of the BCs in solving the Schrödinger equation [10] is behind the fact that different BCs like the RBCs, obeyed by the resonant solutions and by the Gf (causing its resonance poles), on one side, and the ones characterizing the scattering solutions (whose amplitudes display the S-matrix poles) on the other, lead to the same poles.

The residues $C_n(x,x') = u_n(x)u_n(x')/N_n$ obtained in (11) correspond to the following choice of (complex) ”norm” [4]

$$N_n = i(u_n^2(0) + u_n^2(L)) + 2p_n \int_0^L dx \ u_n^2(x)$$  \hspace{1cm} (A.4)

which takes the value $N_n = -8mV(p_n L + 2i)$ for the solutions (A.3). This ”norm” is somehow related to the usual one in Hilbert space: when applied to ordinary square-integrable wave functions $\psi(x) \in \mathcal{L}^2$, replacing the squares by the square modulus and letting 0 and $L$ recede respectively to $-\infty$ and to $+\infty$, equation (A.4) approaches the usual norm (up to a factor). For the resonant solutions however, $N_n$ diverges in this limit.

**Appendix B. Analytical Green function**

The analytical solution to the Green equation $L_\alpha G(x,y,p) = \delta(x-y)$ for $x$ and $y$ in the interval $[0,L]$, and obeying the RBCs (7), can be directly constructed:

$$G(x,y,p) = \frac{i}{2p'} \frac{1}{D(p)} \left\{ 2mV \left( e^{ip'(L-(x+y))} + e^{-ip'(L-(x+y))} \right) \right.$$ \hspace{1cm} (B.1)

$$- \Theta^2 e^{-ip'L}(\theta(y-x)e^{ip'(y-x)} + \theta(x-y)e^{ip'(x-y)})$$

$$- \Theta^2 e^{ip'L}(\theta(y-x)e^{-ip'(y-x)} + \theta(x-y)e^{-ip'(x-y)}) \right\},$$

where the symmetry $x \leftrightarrow y$ is explicit and the zeroes of $D(p)$ give the expected simple poles.
Particular useful values of (B.1) are:

\[
G(0, x, p) = \frac{i}{D(p)}(\oplus e^{ip'(L-x)} - \oplus e^{-ip'(L-x)})
\]

\[
G(L, x, p) = \frac{i}{D(p)}(\oplus e^{ip'x} - \oplus e^{-ip'x})
\]

\[
G(0, L, p) = -i \frac{2p'}{D(p)}
\]

\[
G(0, 0, p) = G(L, L, p) = \frac{i}{D(p)}(\oplus e^{ip'L} - \oplus e^{-ip'L})
\]

\[
G(x, y, 0) = \frac{-1}{2\sqrt{2mV} \sinh[L\sqrt{2mV}]} \{ \cosh[\sqrt{2mV}(L - (x + y))] \\
+ \theta(y - x) \cosh[\sqrt{2mV}(L - (y - x))] \\
+ \theta(x - y) \cosh[\sqrt{2mV}(L - (x - y))] \}
\]

\[
G(0, 0, 0) = G(L, L, 0) = -\frac{1}{\sqrt{2mV}} \coth[L\sqrt{2mV}]
\]

\[
\partial_p G(0, 0, p)|_{p=0} = -\frac{i}{4mV} \frac{3 + \cosh[2L\sqrt{2mV}]}{\sinh[L\sqrt{2mV}]}
\]

The limit \(|p| \to \infty\) can be directly read out in the above expressions. It can be seen that in all the cases the Green function vanishes as \(1/p\) or faster in any direction of the complex plane, with the only exception of \(G(0, 0, p)\) and \(G(L, L, p)\), which grow as \(p\) in the lower half plane, though they still decrease as \(1/p\) in the real axis.

The particular cases \(G(0, x, p)\) and \(G(L, x, p)\) are related to the scattering solutions \(\phi_i^n(x)\) (see Appendix H). From the integral formula \(\int_0^L dx [\phi(L_xG - \delta(x-x')) - GL_x\phi] = 0\) and the use of the BCs for \(\phi\) and the RBCs for \(G\), one obtains [11]

\[
G(0, x, p) = \frac{-i}{2p} \sqrt{2\pi} \sqrt{\frac{p}{m}} \phi_i^n(x) \quad (0 < x \leq L) \quad (B.3)
\]

\[
G(L, x, p) = \frac{-i}{2p} \sqrt{2\pi} \sqrt{\frac{p}{m}} \phi_i^n(x) \quad (0 \leq x < L) \quad (B.4)
\]

Appendix C. Pole expansion and subtractions

Whenever the Green function \(G(x, x', p)\) vanishes as \(1/p\) in the limit \(|p| \to \infty\), the Mittag-Leffler theorem applies and the validity of the pole expansion (11) is assured. This is not the case for \(G(0, 0, p)\) and \(G(L, L, p)\), which grow as \(p\) in the lower half plane, and a subtraction technique must be used [5]. This is performed by using the contour integral

\[
0 = \frac{1}{2\pi i} \oint \frac{G(x, x', z)}{z^2} \frac{dz}{z - p} \quad (C.1)
\]
where the contour $\Gamma \equiv \{C_o, C_p, C_n, C_s\}$ consists of small closed paths counterclock-wise encircling the poles of the integrand (namely $C_o$ around the double pole at $z = 0$, $C_p$ around $p$ and $C_n$ around each $p_n$) plus a large circle $C_s$ clock-wise encircling all these poles. The factor $z^{-2}$ has been introduced to assure that the integrand goes as $z^{-2}$ even for $G(0,0,p)$ and $G(L,L,p)$ so that the integral over $C_s$ vanishes when the radius of the circle grows to $\infty$.

From (C.1) one readily obtains (see also [12])

$G(x, x', p) = p^2 \sum_{n} \frac{1}{N_n p_n^2} \frac{u_n(x) u_n(x')}{p - p_n} + [G(x, x', 0) + p \partial_p G(x, x', p)]_{p=0}$  (C.2)

When the pole expansion (11) holds, (C.2) becomes a trivial identity, whereas in the case of $G(0,0,p)$ and $G(L,L,p)$ a holomorphic (linearly growing with $|p|$) part remains.

Appendix D. Inverse Laplace transform

The inverse Laplace transform in the variable $s$ in (12), involves an integration in the complex $s$-plane along a line parallel to the imaginary axis with $Re c > 0$. In the $p$-plane (recall $p = \sqrt{i \sqrt{2m s}}$), this path translates to a hyperbola-like one with asymptotes in the positive real and imaginary axis. For $t > 0$, the factor $e^{-\frac{1}{2m} t^2}$ assures that it can be deformed into an integration from $+\infty$ to $-\infty$ along (and slightly above) the real axis if the integrand has poles only in the lower half plane (and on the real axis). For $t < 0$, the path can be closed along a quarter circle of large radius in the 1st quadrant, thus enclosing a region without poles and giving $\psi(x,t) = 0$, consistently with the Laplace method and causality [5].

Appendix E. Pole expansion of $p \tilde{\psi}(x,p)$

We rewrite (8) as

$\tilde{\psi}_{II}(x,p) = i \alpha \int_0^L dx' f_{1II}(x',x,p) e^{ikx'} - \alpha e^{ikL} f_{2II}(x,p) - \alpha f_{3II}(x,p)$ (E.1)

where

$f_{1II}(x',x,p) = G(x',x,p)$, $f_{2II}(x,p) = \frac{G(L,x,p)}{p + k}$ and $f_{3II}(x,p) = \frac{G(0,x,p)}{p - k}$.

According to the asymptotic behaviour of the $f_{iII}(p)$ $(i = 1,2,3)$ above we consider the contour integrals

$0 = \frac{1}{2\pi i} \oint_{\Gamma_i} dz \frac{z^{n_i}}{z - p} f_{iII}(z)$ (E.2)

where the values $n_1 = 0$, and $n_2 = n_3 = 1$ are assigned so that the integrand of (E.2) behaves as $z^{-2}$ for large $z$. The contours $\Gamma_i$ include circles around the poles in the respective integrand (namely $p$, $p_n$, $k$ or $-k$) plus the large circle $C_s$, as in Appendix C. For $i = 1$, equation (E.2) yields $f_{1II}(p)$, which must be multiplied by $p$ later on,
whereas for $i = 2, 3$ one directly obtains $p f_{II}^{I}(p)$. Collecting these results and using the pole expansion of the Green function, (13) is obtained.

The derivation of (14) follows the same lines. Here we define

$$f_{I}^{I}(p) = G(x', L, p), f_{II}^{I}(p) = \frac{G(L, L, p)}{p + k} \quad \text{and} \quad f_{III}^{I}(p) = \frac{G(0, L, p)}{p - k},$$

and the powers required are $n_{1} = 0$, $n_{2} = -1$ and $n_{3} = 1$. Notice that the negative power $n_{2} = -1$, needed by the asymptotic behaviour of $G(L, L, z)$, introduces an extra pole at $z = 0$ and is related to the discussion of App.C.

Appendix F. erfc(z)-related integrals

In the computation of $\psi_{II}(x, t)$ and $\psi_{III}(x, t)$, the following types of integrals arise:

$$I(x) = \frac{1}{i\pi} \int_{-\infty}^{+\infty} dp \, p \, e^{-i\tau p^{2}} e^{i(x-L)p} \quad (F.1)$$

$$I_{0}(x, q) = \frac{1}{i\pi} \int_{-\infty}^{+\infty} dp \, \frac{1}{p - q} e^{-i\tau p^{2}} e^{i(x-L)p} \equiv -2 \, M(x - L, q, t) \quad (F.2)$$

$$I_{1}(x, q) = \frac{1}{i\pi} \int_{-\infty}^{+\infty} dp \, \frac{p}{p - q} e^{-i\tau p^{2}} e^{i(x-L)p} = -i \frac{\partial}{\partial x} I_{0}(x, q) \quad (F.3)$$

$$I_{2}(x, q) = \frac{1}{i\pi} \int_{-\infty}^{+\infty} dp \, \frac{p^{2}}{p - q} e^{-i\tau p^{2}} e^{i(x-L)p} = -i \left( \frac{\partial}{\partial x} \right)^{2} I_{0}(x, q), \quad (F.4)$$

where

$$M(x, q, t) \equiv \frac{-1}{2\pi i} \int_{-\infty}^{+\infty} dp \, \frac{1}{p - q} e^{-i\tau p^{2}} e^{i\tau p^{2}}$$

is the Moshinsky function, often found in the literature.

They can be related to the integral representation of the error function \[13\]

$$w(z) \equiv e^{-z^{2}} \text{erfc}(-iz) = -\frac{i}{\pi} \int_{-\infty}^{+\infty} du \, \frac{e^{-u^{2}}}{u - z} \quad \text{Im} \, z > 0 \quad (F.5)$$

so that

$$M(x, q, t) = \frac{1}{2} e^{i\frac{\pi}{4} x^{2}} w\left( i e^{-i\frac{\pi}{4}} \sqrt{\frac{m}{2t}} (x - \frac{t}{m} q) \right).$$

When converting the exponent $i\tau p^{2}$ into $u^{2}$, namely $u = \sqrt{i\tau} p$, an integration along a line running between $\pm \sqrt{i} \infty$ results. In the case $q = p_{n}$, rotating this path by an angle $\pi/4$ towards the real axis crosses the pole $\sqrt{i\tau} \, p_{n}$, contributing a residue. For $q = \pm k$, a small negative imaginary part is supposed (see Appendix D). The case $\text{Im} \, z < 0$ can be tackled by using the property $w(z^{*}) = w^{*}(-z)$.

The results of the integrals above, as given in Section 4, are
Appendix G. $t \to 0, \infty$ limits of $e^{y_q^2} \text{erfc}(y_q)$

Being $y_q \equiv e^{i\pi/4} (x - L - 2\tau q)$, where $\tau \equiv \frac{t}{2m}$, we see that, for $t \to 0$, 

$$y_q \sim e^{-i\pi/8} \sqrt{\frac{t}{2m}} (x - L) \to e^{-i\pi/4} \cdot \infty,$$

regardless of $q$ being equal to $\pm k, p_n$ or $p_{-n}$.

For $t \to \infty$ one has

$$y_q \sim e^{i\pi/4} \sqrt{\frac{t}{2m}} q \to e^{i\phi_q} \cdot \infty,$$

where $\frac{\pi}{2} < \phi_n < \frac{3\pi}{4}, -\frac{\pi}{4} < \phi_{-n} < 0$, $\phi_k = \frac{3\pi}{4}$ and $\phi_{-k} = -\frac{\pi}{4}$.

The following asymptotic formulas [13] apply:

$$\lim_{z \to \infty} \text{erfc}(z) = 0 \quad |\text{arg} z| < \frac{\pi}{4}$$

$$\lim_{z \to \infty} e^{z^2} \text{erfc}(z) \sim \frac{1}{\sqrt{\pi} z} (1 + \sum_{m=1}^{\infty} \frac{C_m}{z^{2m}}) \to 0 \quad |\text{arg} z| < \frac{3\pi}{4}$$

Only the case $\phi_k = \frac{3\pi}{4}$ is out of their range, in which case the relationship

$$e^{y_k^2} \text{erfc}(y_k) = 2e^{y_k^2} - e^{-y_k^2} \text{erfc}(-y_k),$$

where $|\text{arg}(-y_k)| = \frac{\pi}{4}$, is helpful.
Appendix H. Scattering solutions

The usual scattering solutions of $L_x \tilde{\psi}(x, p) = 0$ for continuous real energies $E = p^2 / 2m > 0$ may be characterized according to the homogeneous BC they obey. Contrary to the resonant solutions, which are subject to two BCs, each one of the scattering solutions solution is subject to one homogeneous BC, alternatively at $x = 0$ or at $x = L$:

$$
\begin{align*}
\partial_x \phi^\text{in}_r (x)|_L &= ip \phi^\text{in}_r (L) \\
\partial_x \phi^\text{in}_l (x)|_0 &= -ip \phi^\text{in}_l (0) \\
\partial_x \phi^\text{out}_r (x)|_0 &= ip \phi^\text{in}_r (0) \\
\partial_x \phi^\text{out}_l (x)|_L &= -ip \phi^\text{in}_l (L),
\end{align*}
$$

where $r(l)$ labels the right(left)-moving character of the impinging wave. Notice that the reverse notation is often found in the literature, with $r(l)$ indicating the wave coming from the right(left) of the barrier.

These solutions, for instance

$$
\phi^\text{in}_r (x, p) = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{m}{p}} \left[ \theta(-x)(e^{ipx} + Re^{-ipx}) + \theta(x)\theta(L-x) \left( P e^{ip'x} + Q e^{-ip'x} \right) + \theta(x-L) Te^{ipx} \right],
$$

are $\delta$-normalized in energy.

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