Scattering and delay time for 1D asymmetric potentials:
The step-linear and the step-exponential case
Espalhamento e tempo de retardo para potenciais unidimensionais assimétricos:
Casos linear e exponencial por partes

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We analyze the quantum-mechanical behavior of a system described by a one-dimensional asymmetric potential constituted by a step plus (i) a linear barrier or (ii) an exponential barrier. We solve the energy eigenvalue equation by means of the integral representation method, classifying the independent solutions as equivalence classes of homotopic paths in the complex plane. We discuss the structure of the bound states as function of the height \( U_0 \) of the step and we study the propagation of a sharp-peaked wave packet reflected by the barrier. For both the linear and the exponential barrier we provide an explicit formula for the delay time \( \tau(E) \) as a function of the peak energy \( E \). We display the resonant behavior of \( \tau(E) \) at energies close to \( U_0 \). By analyzing the asymptotic behavior for large energies of the eigenfunctions of the continuous spectrum we also show that, as expected, \( \tau(E) \) approaches the classical value for \( E \to \infty \), thus diverging for the step-linear case and vanishing for the step-exponential one.

Keywords: integral transforms, special functions, solutions of wave equations: bound states, scattering theory.

Analisamos o comportamento quântico de um sistema descrito por um potencial assimétrico unidimensional constituído por um degrau junto a (i) uma barreira linear ou (ii) uma barreira exponencial. Resolvemos a equação dos valores próprios da energia por meio do método da representação integral, classificando as soluções independentes como classes de equivalência de caminhos homotôpicos no plano complexo. Discutimos a estrutura dos estados ligados como função da altura \( U_0 \) do degrau e estudamos a propagação de um pacote de onda pontiagudo refletido pela barreira. Para ambos os casos linear e exponencial fornecemos uma fórmula explícita para para o retardo \( \tau(E) \) como função da energia de pico \( E \). Exibimos o comportamento ressonante de \( \tau(E) \) para energias próximas de \( U_0 \). Ao analisar o comportamento assintótico para grandes energias das funções próprias do espectro contínuo, mostramos também que, como esperado, \( \tau(E) \) se aproxima do valor clássico para \( E \to \infty \), divergindo assim para o caso linear e zerando para o caso exponencial.

Palavras-chave: transformações integrais, funções especiais, solução das equações de onda: estados ligados, teoria do espalhamento.

1. Introdução

In Ref. [1], we have analyzed the quantum-mechanical behavior of a system described by a one-dimensional asymmetric potential formed by a step plus a harmonic barrier (the “step-harmonic” potential), by using the integral representation method [2]. We investigated the behavior of the discrete energy levels (as a function of the height of the step) and of the delay time \( \tau \) of a wave packet coming from...
infinity and bouncing back on the harmonic barrier, as a function of the packet’s peak energy and of the height $U_0$ of the step.

Among the convex or concave locally bounded symmetric and confining potentials the harmonic oscillator is a threshold, in that it gives rise to classical isochronous oscillations and evenly spaced quantum energy levels [3,4].

In our quantum mechanical step variant of the problem we recover both these features in the limit in which $U_0 \to \infty$, and the potential reduces to the half-space harmonic oscillator. Then, it is conceivable that the harmonic one is the only confining barrier which displays a constant nonvanishing delay $\tau$ which allows us to recast Eq. (3) as

$$x_0 = 6.$$  

This, for mass, the time-independent Schrödinger equation is

$$\text{If } E \text{ denotes the energy of the particle and } m \text{ its mass, the time-independent Schrödinger equation is}$$

$$- \frac{\hbar^2}{2m} \frac{d^2 u(x)}{dx^2} + U(x)u(x) = Eu(x).$$  

This, for $x < 0$, can be rewritten as

$$\frac{d^2 u(x)}{dx^2} + \left( \frac{2mM}{\hbar^2} x + \frac{2mE}{\hbar^2} \right) u(x) = 0.$$  

It is convenient to define

$$\alpha := \left( \frac{2mM}{\hbar^2} \right)^{1/3}, \quad \beta := \frac{\alpha E}{M}, \quad y := \alpha x,$$  

which allows us to recast Eq. (4) as

$$\frac{d^2 u(y)}{dy^2} + (y + \beta) u(y) = 0,$$  

which is the Airy equation (see Refs. [5,6]). The general solution of Eq. (5) is

$$u(y) = C \text{Ai}(-y - \beta) + DBi(-y - \beta),$$  

where $C$ and $D$ are arbitrary integration constants, and the two linearly independent solutions $\text{Ai}$ and $\text{Bi}$ are expressed in section 5.1 in terms of the integral representation method.

Since $\text{Bi}(x) \to +\infty$ for $x \to +\infty$, in order for Eq. (6) to be an eigenfunction, we must set $D = 0$. Hence, we obtain

$$u(x) = C \text{Ai}(-\alpha x - \beta).$$  

For $x > 0$, the solution of Eq. (2) has the following from

$$u(x) = \begin{cases} A e^{ikx} + B e^{-ikx} & E > U_0, \\ F e^{-kx} & E < U_0, \end{cases}$$  

where $A$, $B$ and $F$ are arbitrary integration constants and

$$\hbar k := \sqrt{2m|E - U_0|}.$$  

2. The step-linear potential

Let $M$, $U_0$ be positive parameters, and consider the “step-linear” potential

$$U(x) = \begin{cases} -Mx & x \leq 0, \\ U_0 & x > 0, \end{cases}$$  

If $E$ denotes the energy of the particle and $m$ its mass, the time-independent Schrödinger equation is

$$- \frac{\hbar^2}{2m} \frac{d^2 u(x)}{dx^2} + U(x)u(x) = Eu(x).$$  

This, for $x < 0$, can be rewritten as

$$\frac{d^2 u(x)}{dx^2} + \left( \frac{2mM}{\hbar^2} x + \frac{2mE}{\hbar^2} \right) u(x) = 0.$$  

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For $x > 0$, the solution of Eq. (2) has the following from

$$u(x) = \begin{cases} A e^{ikx} + B e^{-ikx} & E > U_0, \\ F e^{-kx} & E < U_0, \end{cases}$$  

where $A$, $B$ and $F$ are arbitrary integration constants and

$$\hbar k := \sqrt{2m|E - U_0|}.$$  

2.1. The case $E < U_0$: Bound states and level spacing

If $E < U_0$ we obtain

$$u(x) = \begin{cases} C \text{Ai}(-\alpha x - \beta) & x \leq 0, \\ F e^{-kx} & x > 0. \end{cases}$$  

The requirement of continuity of $u(x)$ and of its first derivative in $x = 0$ is expressed by

$$\begin{cases} C \text{Ai}(-\beta) - F = 0, \\ C \alpha \text{Ai}'(-\beta) - F k = 0. \end{cases}$$  

System (11) has a non trivial solution if

$$\text{Ai}'(-\beta) = \frac{\sqrt{\beta_0 - \beta}}{\beta_0 - \beta},$$  

where $\beta_0 := \alpha U_0 / M$. The energy levels are determined graphically by the intersections of the curves at the two sides of Eq. (12). An example is depicted in Fig. 1 for $\beta_0 = 6$. In the limit $U_0 \to \infty$ the step of Eq. (1) becomes an infinite barrier. In this case, the energy levels correspond to the zeros $\beta_n$ of $\text{Ai}(-\beta)$, the denominator of Eq. (12). As expected, these energy levels are the ones of the symmetric confining potential $U(x) = M|x|$ corresponding to the odd eigenfunctions of the latter (Appendix A).

To study the level separation for large energies, consider the asymptotics of $\text{Ai}(-\beta)$ for large values of $\beta$ (see Ref. [7]).
Airy function compared with the corresponding approximate zeros from Eq. (16).

<table>
<thead>
<tr>
<th>n</th>
<th>[n \beta_n \text{(exact)}]</th>
<th>[n \beta_n \text{(approximate)}]</th>
<th>Relative Error</th>
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</tr>
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<td>3</td>
<td>5.52055</td>
<td>5.51716</td>
<td>0.62 x 10^{-3}</td>
</tr>
</tbody>
</table>

2.2. The case \(E > U_0\); Scattering and delay

In this case, the (improper) eigenfunctions have the form

\[
u(x) = \begin{cases} 
CAi(-\alpha x - \beta) & x \leq 0, \\
Be^{ikx} + Ce^{-ikx} & x > 0. 
\end{cases}
\]

The junction conditions in \(x = 0\) are

\[
\begin{cases}
CAi(-\beta) = A + B, \\
-C\alpha Ai'(-\beta) = ik (A - B).
\end{cases}
\]

Solving for the constants, the normalized (with respect to \(k\)) improper eigenfunctions are given by

\[
u_k(x) = \frac{1}{\sqrt{2\pi}} \Pi(\beta(k)) \left| Ai[-\alpha x - \beta(k)] \right|
\left\{ \begin{array}{ll}
e^{-ikx} + e^{ikx+i\delta(k)} & x > 0, \\
e^{-ikx} + e^{ikx-i\delta(k)} & x \leq 0,
\end{array} \right.
\]

where

\[
\Pi(\beta) = 2 \left[ Ai(-\beta) + \frac{\alpha}{ik} Ai'(-\beta) \right]^{-1},
\]

\[
e^{i\delta(k)}\left( \frac{ikAi(-\beta) - \alpha Ai'(-\beta)}{ikAi(-\beta) + \alpha Ai'(-\beta)} \right). \tag{21}
\]

As expected, the continuous part of the spectrum \((E > U_0)\) is simple. Note that

\[
\delta(k) = 2 \arctan \left[ \frac{\alpha Ai'(-\beta)}{k Ai(-\beta)} \right]. \tag{22}
\]

From Eq. (20) a generic wave packet

\[
\psi(x,t) = \int_0^\infty dk e^{-\frac{i}{\hbar}E(k)t} u_k(x).
\]

has the form

\[
\frac{1}{\sqrt{\pi}} \Pi(\beta(k)) \left| Ai[-\alpha x - \beta(k)] \right|
\left\{ \begin{array}{ll}
e^{-ikx} + e^{ikx+i\delta(k)} & x > 0, \\
e^{-ikx} + e^{ikx-i\delta(k)} & x \leq 0,
\end{array} \right.
\]

The spacing behavior \(n^{-1/3}\) is the threshold between concave and convex potentials.

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\[
\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{0}^{\infty} dk c(k) \Pi(|\beta(k)|) Ai[-\alpha x - \beta(k)] e^{-\frac{i}{\hbar}kE(k)t} \quad x < 0,
\]

(24)

Then, writing \( c(k) = |c(k)| e^{i\gamma(k)} \), \( \psi_{\text{in}} \) and \( \psi_{\text{refl}} \) take the following form

\[
\psi_{\text{in}}(x, t) = \frac{1}{\sqrt{2\pi}} \int_{0}^{\infty} dk |c(k)| e^{-i(kx + \Omega(k))t - \gamma(k)},
\]

(25)

\[
\psi_{\text{refl}}(x, t) = \frac{1}{\sqrt{2\pi}} \int_{0}^{\infty} dk |c(k)| e^{i(kx - \Omega(k))t + \delta(k) + \gamma(k)},
\]

(26)

where

\[
\Omega(k) := \frac{E(k)}{\hbar} = \frac{U_{0}}{\hbar} + \frac{\hbar k^{2}}{2m}.
\]

(27)

If \( c(k) \) is sufficiently regular and non-vanishing only in a small neighborhood of some \( \tilde{k} \), then \( \psi_{\text{in}} \) and \( \psi_{\text{refl}} \) represent wave packets which move according to the following equations of motion [8,9]

\[
x_{\text{in}} = -\frac{d\Omega}{dk} \bigg|_{k=\tilde{k}} t + \frac{d\gamma}{dk} \bigg|_{k=\tilde{k}} = -\frac{\hbar \tilde{k}}{m} (t - t_{0}) = -\tilde{p}_{m}(t - t_{0}),
\]

(28)

for the “incoming” wave packet, and

\[
x_{\text{refl}} = \frac{d\Omega}{dk} \bigg|_{k=\tilde{k}} t - \frac{d\gamma}{dk} \bigg|_{k=\tilde{k}} - \frac{d\delta}{dk} \bigg|_{k=\tilde{k}} = \tilde{p}_{m} \left[ (t - t_{0}) - \frac{m}{\tilde{p}_{m}} \frac{d\delta}{dk} \bigg|_{k=\tilde{k}} \right],
\]

(29)

for the reflected “outgoing” one.

The solution thus built represents a particle of well defined momentum \( \tilde{p} = \hbar \tilde{k} \) which approaches the origin from the right, interacts with the linear potential (at \( t = t_{0} \)), and is totally reflected. Note that the argument of the complex valued function \( c(k) \) determines \( t_{0} \). The phase shift results in a delay \( \tau \) in the rebound, caused by the interaction with the confining linear barrier. The delay is calculated with respect to the case of instantaneous reflection, which takes place in presence of an infinite barrier and for which \( \delta(k) = \pi \). From Eqs. (4) and (5) it follows that

\[
\tau(\tilde{\beta}) = \frac{\alpha h}{M} \frac{d\delta}{d\beta} \bigg|_{\beta=\tilde{\beta}},
\]

(30)

where \( \tilde{\beta} := \beta(\tilde{k}) \). We compute \( \tau \) from Eq. (22). Using the Airy equation \( Ai''(-\beta) = -\beta Ai(-\beta) \), we obtain

\[
\tau(\beta) = \frac{2}{M \sqrt{\beta - \beta_{0}}} \frac{Ai(-\beta)}{Ai'(-\beta)} + \frac{1}{\sqrt{\beta - \beta_{0}}} \left[ \frac{1}{2(\beta - \beta_{0})} + \frac{1}{\beta Ai(-\beta) + Ai'(-\beta)} \right],
\]

(31)

where we have suppressed the tilde on the packet peak energy \( \tilde{\beta} \).

We are interested in the behavior of the interaction time for large values of \( \beta \), i.e. for incoming packets with high energy. To this end, we need the asymptotic expansion of \( Ai'(-\beta) \) for \( \beta \rightarrow +\infty \) (see Refs. [5,7])

\[
Ai'(-\beta) = -\frac{\beta^{1/4}}{\sqrt{\pi}} \left[ \cos \left( \zeta + \frac{\pi}{4} \right) \sum_{k=0}^{\infty} (-\beta)^{k} \frac{d_{2k}}{2^{2k}} + \sin \left( \zeta + \frac{\pi}{4} \right) \sum_{k=0}^{\infty} (-\beta)^{k} \frac{d_{2k+1}}{2^{2k+1}} \right],
\]

(32)

where \( \zeta := 2\beta^{3/2}/3 \) and the coefficients \( d_{k} \) are

\[
d_{k} = -\frac{6k + 1}{6k - 1} c_{k},
\]

(33)

with \( c_{k} \) given in Eq. (14). Dividing the two asymptotic expansions of \( Ai'(-\beta) \) and \( Ai(-\beta) \) we obtain to leading order in \( \beta \)

\[
\frac{1}{\sqrt{\beta - \beta_{0}}} \frac{Ai'(-\beta)}{Ai(-\beta)} \sim \tan \left( \frac{2}{3} \beta^{3/2} - \frac{\pi}{4} \right), \quad \beta \rightarrow \infty.
\]

(34)
Thus, Eq. (31) becomes
\[ \tau(\beta) \sim 2^{\frac{\alpha_1}{M}} \sqrt{\beta}, \quad \beta \to \infty. \] (35)

Hence, reintroducing the physical variables, the high-energy behavior of the interaction time is
\[ \tau(E) \sim \frac{2\sqrt{2}mE}{M}, \] (36)

which is exactly the time a classical particle arriving from infinity with energy \( E \) would spend in the \( x < 0 \) region.

In Fig. 2 we plot \( \tau(\beta) \) for a choice of different values of \( \beta_0 \). Note the resonances located at the points \( \beta \simeq \eta_n (n = 1, 2, \ldots) \), zeros of \( \text{Ai}(-\beta) \), corresponding to the formation of metastable states at the respective energies \( E_n \simeq M\eta_n/\alpha \). The values \( M\eta_n/\alpha \) are the energies of the excited states of the confining potential \( M|x| \) (see Appendix A), corresponding to even eigenfunctions. The resonances have lifetimes which decrease as the corresponding energies increase and move farther away from the threshold energy \( U_0 \). Conversely, as \( U_0 \) increases, the lifetime of the resonance closest to the height of the step becomes progressively longer and then infinite when the resonance turns into the next bound state. This behavior is evident in Fig. 2, in which the first three plots correspond to values of \( \beta_0 \) for which there is only one bound state. In the successive three plots the resonance at \( \beta \simeq \eta_1 \) has disappeared, having turned into the second bound state.

Comparing Fig. 2 with Fig. 6 of Ref. 1 we note that, whereas in the step-harmonic case the graph of \( \tau(\beta) \) oscillates with decreasing amplitude about the straight line \( \tau = \pi/\omega \) (the half period of the oscillator), in the step-linear case the corresponding graph similarly oscillates about the parabolic line \( \tau(E) = 2\sqrt{2}mE/M \), corresponding to the delay of the classical particle. Furthermore, whereas in the step-harmonic case the resonances are evenly spaced, in the step-linear case their spacing decreases with the energy, corresponding to the behavior as a function of the energy of the eigenvalues of the corresponding (symmetric) potentials \( U(x) = m\omega^2x^2/2 \) and \( U(x) = M|x| \).

### 3. The step-exponential potential

Let \( \kappa, \sigma \) and \( U_0 \) be positive parameters, and consider the “step-exponential” potential
\[ U(x) = \begin{cases} \kappa \left(e^{-x/\sigma} - 1\right) & x \leq 0, \\ U_0 & x > 0, \end{cases} \] (37)

For \( x < 0 \), introduce the following dimensionless quantities
\[ \alpha^2 := \frac{8m\kappa\sigma^2}{\hbar^2}, \]
\[ \beta := \frac{8m(E + \kappa)\sigma^2}{\hbar^2}, \quad z := \alpha e^{-x/2\sigma}, \] (38)
in terms of which the time-independent Schrödinger equation writes as
\[ z^2 \frac{d^2u(z)}{dz^2} + z \frac{du(z)}{dz} + \left( \beta - z^2 \right) u(z) = 0. \] (39)

Setting \( \nu^2 := -\beta \), Eq. (39) can be cast in the form of a modified Bessel equation (see Ref. 5,10)
\[ z^2 \frac{d^2u(z)}{dz^2} + z \frac{du(z)}{dz} - \left( \nu^2 + z^2 \right) u(z) = 0, \] (40)
whose general solution is
\[ u(z) = CK_{\nu}(z) + DI_{\nu}(z), \] (41)
where \( C \) and \( D \) are arbitrary integration constants and \( K_{\nu} \) and \( I_{\nu} \) are the modified Bessel functions of order \( \nu = i\sqrt{\beta} \).

The function \( I_{\nu}(z) \) diverges exponentially for \( z \to +\infty \). For this reason, in order for \( u(x) \) to be a proper (or improper) eigenfunction, we must set \( D = 0 \). Therefore Eq. (41) reduces to
\[ u(x) = CK_{i\sqrt{\beta}}\left(\alpha e^{-x/2\sigma}\right). \] (42)
Also the solutions of Eq. (40) can be studied with the integral representation method (see section 5.2).

### 3.1. The case \( E < U_0 \): Bound states

If \( E < U_0 \) we obtain
\[ u(x) = \begin{cases} CK_{i\sqrt{\beta}}\left(\alpha e^{-x/2\sigma}\right) & x \leq 0, \\ F e^{-kx} & x > 0. \end{cases} \] (43)

The junction conditions in \( x = 0 \) give
\[ \alpha K_{i\sqrt{\beta}}(\alpha) = 2\pi k K_{i\sqrt{\beta}}(\alpha), \] (44)
which, setting $\beta_0 := 8m(U_0 + \kappa)\sigma^2/\hbar^2$ can be recast in the form

$$\frac{K'_{\sqrt{\beta}}(\alpha)}{K_{\sqrt{\beta}}(\alpha)} = \frac{\sqrt{\beta_0 - \beta}}{\alpha}.$$  \hspace{1cm} (45)

Graphical solutions of Eq. (45) are shown in Fig. 3.

Analogously to what happens in the step-linear case \[12\], in the limit of an infinite barrier ($U_0 \to \infty$) the energy levels are specified by the zeros of $K_{\sqrt{\beta}}(\alpha)$, the denominator of Eq. (44), as a function of $\beta$ and they are the ones of the symmetric confining potential $U(x) = \kappa(e^{2|x|/\sigma} - 1)$, corresponding to the odd eigenfunctions of the latter (Appendix B).

To study how the energy levels behave for large energies, we employ the following formula for the asymptotic behavior of the function $K_{\sqrt{\beta}}(\alpha)$ for large $\beta$ (see Ref. [5])

$$K_{\sqrt{\beta}}(\alpha) \sim \int_{2\pi} \sqrt{\beta} e^{-\pi \sqrt{\beta}/2} \sin \left( \alpha \frac{2}{\sqrt{\beta}} - \frac{\sqrt{\beta}}{\alpha} \log \left( 2\sqrt{\beta} \alpha \right) \right) \left[ 1 + O \left( \frac{1}{\sqrt{\beta}} \right) \right],$$  \hspace{1cm} (46)

for $\beta \to \infty$. Note that expansion (46) can be proved starting from Eq. (76). Therefore, the zeros of $K_{\sqrt{\beta}}(\alpha)$, as a function of $\beta$, are asymptotically the solutions of the following equation

$$-\sqrt{\beta_n} + \sqrt{\beta_n} \log \left( \frac{2\sqrt{\beta_n}}{\alpha} \right) = n\pi.$$  \hspace{1cm} (47)

Solving for $\beta_n$ we obtain

$$\beta_n \sim \frac{\alpha^2 \kappa^2}{4} \exp \left[ 2W \left( \frac{2n\pi \alpha^2}{\kappa} \right) \right],$$  \hspace{1cm} (48)
where \( W(x) \) is the Lambert function \[5\]. Since \( W(x) \sim x - \log x \) for \( x \to \infty \) we have for large \( n \)

\[
\beta_n \sim \frac{n^2 \pi^2}{\left( \log \frac{2n}{\alpha e} \right)^2}.
\]

We see from Eq. (49) that the potential \( U(x) = \kappa \left( e^{x/\sigma} - 1 \right) \) behaves for large \( x \) as an infinite square well whose width, up to inessential factors, grows as \( \log n \), an intuitive fact. Moreover,

\[
\beta_{n+1} - \beta_n \sim \frac{2n \pi^2}{\left( \log \frac{2n}{\alpha e} \right)^2},
\]

for \( n \to \infty \), proving thus that the level spacing diverges.

### 3.2. The case \( E > U_0 \): Scattering and delay

The unbound eigenstates have the form

\[
u(x) = \begin{cases} CK_i \sqrt{\beta} (\alpha e^{-x/2}) & x \leq 0, \\ Ae^{ikx} + Be^{-ikx} & x > 0. \end{cases} \tag{51}
\]

Then, following the same argument adopted for the step-linear case, we obtain the following formula for the delay \( \tau \) of the rebound of an incoming wavepacket with peak energy \( \beta \)

\[
\tau(\beta) = \frac{8m \sigma^2}{\hbar} d \delta = \frac{8m \sigma^2}{\hbar} \frac{2}{\sqrt{\beta - \beta_0} K_i \sqrt{\beta} (\alpha) + \sqrt{\beta - \beta_0} K_i \sqrt{\beta} (\alpha)} \left[ -\frac{1}{2 (\beta - \beta_0)} + \frac{d}{d \beta} \log K_i \sqrt{\beta} (\alpha) \right]. \tag{56}
\]

Using Eq. (46), we obtain for large values of \( \beta \)

\[
\frac{K_i' \sqrt{\beta} (\alpha)}{K_i \sqrt{\beta} (\alpha)} \sim \frac{\sqrt{\beta}}{\alpha} \cot \left( -\sqrt{\beta} + \sqrt{\beta} \log \frac{2 \sqrt{\beta}}{\alpha} + \frac{\pi}{4} \right), \tag{57}
\]

from which

\[
\frac{d}{d \beta} \log K_i \sqrt{\beta} (\alpha) \sim \frac{1}{2 \beta} - \frac{1}{2 \sqrt{\beta} - \sqrt{\beta} \log \frac{2 \sqrt{\beta}}{\alpha} + \frac{\pi}{4}} \frac{1}{\sqrt{\beta} \log \frac{2 \sqrt{\beta}}{\alpha}}. \tag{58}
\]

A comment is here in order. In general, taking the derivative of an asymptotic expansion with respect to the variable or a parameter may lead to wrong results. However, in our case this procedure can be justified using the integral representation of Eq. (27) (we leave this as an exercise for the interested reader).

Thus, plugging Eq. (58) into Eq. (56) we obtain the asymptotic behavior of the delay time for large
As expected, in both cases these delays exhibit a behavior for $x \to +\infty$ (see Refs. [8,11]). Since $u_L(x) = a(E)u_R(x) + b(E)v_R(x)$, the energy eigenvalues are the roots $E_n$ of the equation $b(E) = 0$. Since the potential is symmetric, these roots correspond to even and odd eigenfunctions alternatively, the ground state being even. However, in the general case the eigenvectors cannot be found explicitly. Therefore, for example, no explicit formula is available in general for the delay time of the reflected packet in the corresponding step variant potential (61).

5. Airy and modified Bessel functions through the integral representations

In this section we solve the energy eigenvalue equations by means of the integral representation method, classifying the independent solutions as equivalence classes of homotopic paths in the complex plane. For the step-linear case we obtain Airy function, while for the step-exponential case we get modified Bessel functions. This technique is interesting \textit{per se}, as it can be applied to more general cases, provided one is able to guess the correct integral kernel. The Airy case is somehow classical, while the Bessel case is more interesting. We present them both for completeness.

5.1. The step-linear case: Airy functions

We look for a solution of Eq. (5) of the form

\[ E(y) = \int_\gamma dt f(t)e^{yt}, \]

where $\gamma$ is a path in the complex plane and $f$ is an holomorphic function. Plugging Eq. (62) into Eq. (5) we find

\[ \int_\gamma dt \left[ (t^2 + \beta)f(t)e^{yt} + \frac{de^{yt}}{dy} f(t) \right] = 0. \]  

Integrating by parts, we obtain:

\[ \left[ e^{yt}f(t) \right]_{\partial \gamma} + \int_\gamma dt \left[ (t^2 + \beta)f(t) - f(t)' \right] e^{yt} = 0. \]

Therefore, $E(y)$ is a solution of Eq. (5) if

\[ \left[ e^{yt}f(t) \right]_{\partial \gamma} = 0 \quad \text{and} \quad f(t) = \exp \left( \frac{t^3}{3} + \beta t \right). \]
Figure 4: Plots of the delay $\tau$ (in units of $8m\sigma^2/\hbar$) versus the energy $\beta$ of the incoming wave packet (solid red lines) for six values of the step height: $\beta_0 = 10, 11, 12$ (upper panels) $\beta_0 = 22, 24, 25$ (lower panels). The blue dotted lines represent the classical delay.

Hence, a class of solutions of the Airy equation is of the form

$$E_\beta(y) = \int_\gamma dt \exp \left[ \frac{t^3}{3} + (\beta + y)t \right], \quad (66)$$

where $\gamma$ is a suitable path for which the contour term vanishes.

The integrand of Eq. (66) entire. Thus, by Cauchy theorem, every closed path represents the trivial solution $E(y) = 0$.

Consider an unbounded path. In order for $[e^{ty}f(t)]_{\partial\gamma}$ to vanish, we require the leading term in the exponent of $f(t)$ (i.e. $t^3$) to have a negative real part. Therefore, the acceptable unbounded paths are those whose phase $\phi$ is confined to the regions $\frac{\pi}{6} < \phi + \frac{2}{3}n\pi < \frac{\pi}{2} (n = 0, 1, 2)$. These possible paths are showed in Fig. 5, where the allowed sectors $\frac{\pi}{6} < \phi + \frac{2}{3}n\pi < \frac{\pi}{2} (n = 0, 1, 2)$ are shaded.

Paths with both endpoints in the same sector (e.g. $\Gamma_4$ in Fig. 5) can be closed at infinity using Jordan’s Lemma; therefore, they correspond to the trivial solution. The only non-trivial paths are those which link different sectors. There are only 3 non-equivalent classes of such paths which we dub $\Gamma_1$, $\Gamma_2$ and $\Gamma_3$ respectively (see Fig. 5).

Taking into account Cauchy theorem, these paths satisfy the relation $\Gamma_1 + \Gamma_2 = \Gamma_3$ in the sense that the corresponding solutions are not independent. The conventional Airy functions $\text{Ai}(z)$ and $\text{Bi}(z)$ are the independent solutions of $w''(z) - zw(z) = 0$ such that (see Ref. [5])

$$\text{Ai}(0) = \frac{3^{-2/3}}{\Gamma(2/3)}, \quad \text{Ai}'(0) = -\frac{3^{-1/3}}{\Gamma(1/3)}, \quad (67)$$

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and
\[
\text{Bi}(0) = \sqrt{3} \frac{3^{-2/3}}{\Gamma(2/3)}, \quad \text{Bi}'(0) = \sqrt{3} \frac{3^{-1/3}}{\Gamma(1/3)}.
\]

Denoting by \( E^{(i)}_\nu(y) \) the solutions in Eq. (66) corresponding to the paths \( \Gamma_i \) \((i = 1, 2)\), it is not difficult to show that
\[
\begin{align*}
\text{Ai}(-y - \beta) &= \frac{1}{2\pi i} \left[ E^{(1)}_\beta(y) + E^{(2)}_\beta(y) \right], \\
\text{Bi}(-y - \beta) &= \frac{1}{2\pi} \left[ E^{(1)}_\beta(y) - E^{(2)}_\beta(y) \right].
\end{align*}
\] (68)

We leave the details to the interested reader (hint: Check the above expressions and their first derivatives in Eq. (66) for \( y = \beta = 0 \). In this case the integrals \( E^{(j)}_0(0) \) correspond to Euler Gamma functions).

5.2. The step-exponential case: Modified Bessel functions

Consider the modified Bessel equation
\[
z^2u''(z) + zu'(z) - (\nu^2 + z^2)u(z) = 0,
\] (69)
with \( z > 0 \). A convenient kernel for the integral representation is the following:
\[
K(z, t) = z^\nu e^{-z \cosh t}.
\] (70)

We look for solutions of the form
\[
u \int_\gamma t f(t) K(z, t).
\] (71)

Plugging Eq. (71) into Eq. (69), we get
\[
z^{\nu+1} \int_\gamma dt \left[ f(t) \frac{d}{dt} \left( \sinh(t) e^{-z \cosh t} \right) + 2\nu f(t) \cosh(t) e^{-z \cosh t} \right] = 0.
\] (72)

Integrating by parts, Eq. (72) gives
\[
z^{\nu+1} e^{-z \cosh t} f(t) \sinh(t) \bigg|_{\partial\gamma} -
z^{\nu+1} \int_\gamma dt \left[ f'(t) \sinh(t) - 2\nu f(t) \cosh(t) \right] e^{-z \cosh t}
= 0.
\] (73)

Then, the integral on the right hand side of Eq. (71) is a solution of Eq. (69) if
\[
f'(t) \sinh(t) - 2\nu f(t) \cosh(t) = 0, \quad \text{and}
\]
\[
z^{\nu+1} e^{-z \cosh t} f(t) \sinh(t) \bigg|_{\partial\gamma} = 0.
\] (74)

Up to a normalization, the solution is \( f(t) = \sinh(t)^{2\nu} \). If \( \nu \) is integer then \( f(t) \) is either entire \((\nu \geq 0)\) or meromorphic \((\nu < 0)\), otherwise it has infinite branch points located at \( t_n = in\pi \) \((n = 0, \pm 1, \ldots)\), see Fig. 6. In the latter instance, the usual procedure is to define a domain in which the function is holomorphic by cutting the \( t \)-plane and thus forbidding loops around the branch points. In Fig. 6 a convenient choice for the cuts is also shown.

Recalling that \( \text{Re}(z) > 0 \), the contour condition
\[
z^{\nu+1} \left[ e^{-z \cosh(t)} f(t) \sinh(t) \right]_{\partial\gamma} = 0
\]
\[
e^{-z \cosh t} \sinh(t)^{2\nu+1} \big|_{\partial\gamma} = 0.
\] (75)

There are 4 different classes of paths for which Eq. (75) is satisfied and
\[
u \int_\gamma \sinh(t)^{2\nu} e^{-z \cosh t} z^{\nu} dt,
\] (76)
is well defined. The “paths zoology” is more complicated and rich than in the linear and in the harmonic case.

1. Closed paths. For any closed path, the contour condition is trivially satisfied and any integral along a path enclosing a region where the integrand function is holomorphic (i.e. the path does not cross the cuts) vanishes. An example is shown by the thin dashed black line in Fig. 6.

2. Infinite paths. For paths whose endpoints are both at infinity, the function \( \sinh(t)^{2\nu+1} \) is well defined. The “paths zoology” is more complicated and rich than in the linear and in the harmonic case.

Figure 6: Cut of the complex \( t \)-plane. The dashed red and the solid blue thick paths represent the only classes of paths which provide independent solutions to the modified Bessel equation.
Taking into account the periodicity of the integrand, the exponential \( e^{-z \cosh t} \) vanishes for \( \text{Re}(\cosh t) \to +\infty \) (recall that \( z > 0 \)). Since \( \text{Re}[\cosh(x+iy)] = \cos(y) \cosh(x) \) then \( \gamma \) must stretch at infinity in one of the sectors defined by \( -\pi/2 + 2n\pi < \text{Im}(t) < \pi/2 + 2n\pi \) \((n = 0, \pm1, \ldots)\), which are represented by the shaded regions in Fig. 6. Incidentally, in these bands, when there are no cuts, one can “close” the paths at infinity, by virtue of Jordan’s Lemma. Examples of this class of paths are the black solid thin lines of Fig. 6.

3. Semi-infinite paths. By “semi-infinite” paths we mean paths starting from a point, say \( t_0 \), and ending at infinity. These paths must go to infinity in the shaded bands \(-\pi/2 + 2n\pi < \text{Im}(t) < \pi/2 + 2n\pi \). For the starting point \( t_0 \), the contour condition demands that \( \sinh(t_0)^{2\nu+1} \) = 0. This means that these paths must start from one of the points \( t_n = in\pi \), which are the zeroes of the hyperbolic sine function. It is easy to prove that the integral of Eq. (76) performed along any two such paths lying in the same band gives the same result (indeed, recall that \( \sinh t \) is periodic). Two examples of this class of paths are the blue solid thin lines in Fig. 6.

4. Finite paths. These are the paths starting and ending in two points say \( t_1 \) and \( t_2 \), with \(|t_1|, |t_2| \to \infty\). The contour condition can be satisfied in two different ways: either the values of the contour part are equal at the endpoints, or the contour part vanishes at the endpoints. The former case accounts for paths which do not cross any cut and start from any point \( t_i \), ending at \( t_f = t_i + 2n\pi \) \((n = 0, \pm1, \ldots)\). Examples of this class of paths are represented by the red dash-dotted thick line in Fig. 6. The latter case is realized by paths connecting the branch points and is represented by the red dashed thick line in Fig. 6.

In conclusion, two linear independent solutions of Eq. (69) are

\[
K_{\nu}(z) = \frac{\pi^{1/2}(z/2)^{\nu}}{\Gamma(\nu + 1/2)} \int_0^\infty dx e^{-z \cosh x} \sinh(2\nu x),
\]

and

\[
I_{\nu}(z) = \frac{(z/2)^{\nu}}{\pi^{1/2}\Gamma(\nu + 1/2)} \int_0^\infty dx e^{-z \cos x} \sin(2\nu x),
\]

where \( K_{\nu} \) and \( I_{\nu} \) correspond, respectively, to the integrals performed along the solid blue and the dashed red thick lines in Fig. 6 (a semi-infinite path and a finite one). It can be shown that both solutions (derived here for \( z > 0 \)) can be analytically continued throughout the whole \( z \)-plane cut along the negative real axis (see Ref. 2).

6. Appendix

A. The confining symmetric linear potential

Consider the confining symmetric potential \( U(x) = M|x| \). The eigenfunctions can be written as

\[
\begin{align*}
\begin{cases}
\quad u(x) = C_1 \text{Ai}(-\alpha x - \beta) & x < 0, \\
\quad u(x) = C_2 \text{Ai}(\alpha x - \beta) & x > 0,
\end{cases}
\end{align*}
\]

where \( C_1 \) and \( C_2 \) are constants fixed by the junction conditions in \( x = 0 \). If \( \text{Ai}(-\beta) \neq 0 \), then the continuity of \( u(x) \) in \( x = 0 \) implies \( C_1 = C_2 \). Moreover, the continuity of the derivative implies \( \text{Ai}'(-\beta) = 0 \). This condition determines the even eigenfunctions and their eigenvalues. If \( \text{Ai}(-\beta) = 0 \), then the continuity of the derivative implies \( C_1 = - C_2 \). This condition determines the odd eigenfunctions and their eigenvalues.

B. The confining symmetric exponential potential

Consider the confining symmetric potential \( U(x) = \kappa (e^{x/\sigma} - 1) \). The eigenfunctions can be written as

\[
\begin{align*}
\begin{cases}
\quad u(x) = C_1 K_i \sqrt{\beta}(\alpha e^{-x/2\sigma}) & x < 0, \\
\quad u(x) = C_2 K_i \sqrt{\beta}(\alpha e^{x/2\sigma}) & x > 0,
\end{cases}
\end{align*}
\]

where \( C_1 \) and \( C_2 \) are constants fixed by the junction conditions in \( x = 0 \). If \( K_i \sqrt{\beta}(\alpha) \neq 0 \), then the continuity of \( u(x) \) in \( x = 0 \) implies \( C_1 = C_2 \). Moreover,
the continuity of the derivative implies \( K'_{i\sqrt{\beta}}(\alpha) = 0 \). This condition determines the even eigenfunctions and their eigenvalues. If \( K'_{i\sqrt{\beta}}(\alpha) = 0 \), then the continuity of the derivative implies \( C_1 = -C_2 \). This condition determines the odd eigenfunctions and their eigenvalues.

References