Time delay in the reflection of particles by semi-harmonic wells

Oscar Rosas-Ortiz
Physics Department, Cinvestav, A.P. 14-740, México D.F., Mexico
E-mail: orosas@fis.cinvestav.mx

Sara Cruz y Cruz, Nicolás Fernández-García
Sección de Estudios de Posgrado e Investigación, UPIITA-IPN, Av. IPN 2580, C.P. 07340
México D.F., Mexico
E-mail: sgcruzc@ipn, jfernandezg@ipn.mx

Abstract. The phase time of wave reflection from a one-dimensional semi-harmonic well includes a delay term which can be negative according to the incoming energy and the well parameters in a quantum scattering process. The model is a rectangular well which is embedded in an environment composed by a zero potential energy to its right and a harmonic-like potential to its left.

1. Introduction
The time spent by a particle in traversing an spatial region is one of the most striking features of quantum theory [1, 2]. For instance, the time taken by a particle in the tunneling of a potential barrier is independent of the barrier thickness [3]. This result has stimulated the designing of high-speed devices based on the tunneling properties of semiconductors [1]. Similar effects have been predicted for potential wells [4], where negative phase times \( \tau_W = \hbar \frac{d}{dE} \delta \) should be observable for electromagnetic propagation [5].

We recently proposed a one-dimensional well which reduces the scattering process to the case of purely wave reflection [6]. This is a rectangular well with a parabolic potential to its left and zero potential energy to its right. In dimensionless form it reads:

\[
V(x; a) = \begin{cases} 
  x^2 & x \leq -a \\
  -V_0 & |x| < a \\
  0 & a \leq x 
\end{cases}
\]  

(1)

The purpose of the semi-harmonic environment is to ensure that all particles coming from \(+\infty\) are reflected by the well. As a byproduct, the number \(N\) of bound states \((E_0, E_1, \ldots, E_{N-1})\) which are admitted by a given square well is preserved when the semi-harmonic background is added. Yet, these two systems are distinguishable because the corresponding energies are displaced towards the positive threshold in the semi-harmonic case. The effect is also present in the resonances \(\epsilon = \epsilon - i\Gamma/2\) by displacing the semi-harmonic resonance positions \(\epsilon\) to the right with respect to their partners of the rectangular well. In our previous work [6], we have
shown that the phase time (group delay) associated to the reflection of particles from a semi-harmonic delta well leads to negative time delays (see also [7]). Similar results can be found for reflectionless potentials (see e.g. [8] for the broadening of wave packets which are scattered by a Pöschl-Teller potential). In the present contribution we make a classification of the time delays associated to the semi-harmonic potentials \( V(x; a) \).

The organization of the paper is as follows. In Section 2 we present the generalities of the quantum problem associated to the semi-harmonic well. Section 3 is devoted to the analysis of the scattering states. The Jost function is used to construct a pair of physical solutions associated to the semi-harmonic potentials \( \psi(x; E) \). In the present contribution we make a classification of the time delays associated to the semi-harmonic potentials \( V(x; a) \).

3. The scattering problem

For scattering states \( E > 0 \), the Jost function \( \mathcal{J} \) is useful to transform the \( \psi \) functions (5) into the so called physical wave solutions

\[
\psi^+(x; E) = \sqrt{\frac{2}{\pi}} \frac{k \psi(x; E)}{\mathcal{J}(k, a)}, \quad \psi^-(x; E) = \sqrt{\frac{2}{\pi}} \frac{k \psi(x; E)}{\mathcal{J}(k, a)}.
\]

These functions are proportional to each other \( \psi^+(x; E) = S(k, a) \psi^-(x; E) \), with

\[
S(k, a) = \frac{\mathcal{J}^*(k, a)}{\mathcal{J}(k, a)}.
\]
the $S$-matrix (reflection amplitude) of the problem [9, 10]. Thus, the physical wave solutions (6) are eigenfunctions of $H$ belonging to the eigenvalue $E = k^2$ and fulfilling the boundary conditions

$$\lim_{x \to -\infty} \psi(x; E) = 0,$$

$$\psi^+(x; E) = \frac{i}{\sqrt{2\pi}} \left[ e^{-ikx} - S(k, a)e^{ikx} \right], \quad x > a,$$

$$\psi^-(x; E) = -\frac{i}{\sqrt{2\pi}} \left[ e^{ikx} - S^*(k, a)e^{-ikx} \right], \quad x > a. \quad (8)$$

From (9) and (10) one gets $(\psi^+)^* = \psi^-$, so that $|S(k, a)|^2 = 1$. That is, the reflection amplitude $S(k, a)$ can only represent a phase shift since the process is elastic. Taking the polar form of the Jost function $J(k, a) = |J(k, a)| e^{-i\delta(k, a)}$, the S-matrix becomes $S(k, a) = e^{2i\delta(k, a)}$, and

$$\psi^+(x; E) = \frac{i}{\sqrt{2\pi}} \left[ e^{-ikx} - e^{i(kx+2\delta)} \right], \quad x > a. \quad (11)$$

The time-displacement of $\psi^+(x; E)$ in $(a, +\infty)$ is given by

$$\psi^+(x; E, t) = \frac{i}{\sqrt{2\pi}} \left[ e^{-i(kx+\omega\Delta t)} - e^{i(kx+2\delta-\omega\Delta t)} \right], \quad x > a. \quad (12)$$

Here we have taken $E = k^2 = \omega$ and $\Delta t = t - t_0$, with $t_0 \geq 0$ an arbitrary value of the time-parameter $t$. The function $\psi^+_\text{inc}(x; k, t) = \frac{i}{\sqrt{2\pi}} e^{-i(kx+\Delta t)}$ represents a plane wave propagating towards the left with phase velocity $v_{\phi}(k) = \frac{\omega}{k} = k$. In turn, the function $\psi^+_\text{out}(x; k, t) = -\frac{i}{\sqrt{2\pi}} e^{i(kx+2\delta-\omega\Delta t)}$ includes a phase shift $2\delta$ and it corresponds to a plane wave propagating towards the right with phase velocity $k$. At a given time $t$, we have $\psi^+_\text{inc} \to \phi_-$ and $\psi^+_\text{out} \to \phi_+$ as $x \to +\infty$, where

$$\phi_{\pm}(x; k) = \mp \frac{i}{\sqrt{2\pi}} e^{\pm ikx} \quad (13)$$

are the irregular eigenfunctions which belong to the continuous eigenvalue $E = k^2 > 0$ of the free Hamiltonian $H_0 = -\frac{d^2}{dx^2}$. To get regular wave solutions let us construct the incoming and outgoing wave packets (by simplicity we take $t_0 = 0$):

$$\psi_{\text{inc}}(x, t) = \int_{-\infty}^{+\infty} dk \Lambda_{\text{inc}}(k) \psi^+_\text{inc}(x; k, t) = \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk \Lambda_{\text{inc}}(k) e^{-i(kx+\omega t)}, \quad x > a \quad (14)$$

$$\psi_{\text{out}}(x, t) = \int_{-\infty}^{+\infty} dk \Lambda_{\text{out}}(k) \psi^+_\text{out}(x; k, t) = \frac{i}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk \Lambda_{\text{out}}(k) e^{i(kx+2\delta+\pi-\omega t)}, \quad x > a \quad (15)$$

The expressions $\Lambda_{\text{inc}}(k)$ and $\Lambda_{\text{out}}(k)$ stand for functions of $k$ which are narrowly peaked around $k_0$. For instance, the distribution

$$\Lambda_{\text{inc}}(k) = (2\pi\lambda^2)^{1/4} e^{-\lambda^2(k-k_0)^2}, \quad \lambda \geq 0 \quad (16)$$

has the width $\lambda \Delta k = 1$, and it gives rise to a Gaussian incoming packet of width $2\Delta x = \lambda$. In the limit $\lambda \to +\infty$, we have $\Delta k = 0$. This means $\Lambda_{\text{inc}}(k) \to \delta(k-k_0)$, so that the wave packet $\psi_{\text{inc}}(x, t)$ is very broad ($\Delta x \to +\infty$). Finally, the peak value of the wave packets (14) and (15) propagates with a group velocity which is twice the phase velocity $v_{\phi}(k_0)$:

$$v_g(k_0) = \left. \frac{d\omega}{dk} \right|_{k=k_0} = 2k_0. \quad (17)$$
Hereafter $\psi_{inc}(x,t)$ will represent the quantum state of a particle with energy $E_0 = k_0^2 > 0$, arriving from $+\infty$ towards the effective zone of the potential ($-\infty, a$). To represent the quantum state of the reflected particle we shall use $\psi_{out}(x,t)$. Remember that the wave packets $\psi_{inc}$ and $\psi_{out}$ are assumed to have very narrow widths so that they are very broad in coordinate representation. Henceforth, before the center of $\psi_{inc}(x,t)$ arrives at $x = a$, the action of the potential makes the packet wavefront of $\psi_{inc}(x,t)$ turn back. This effect produces the wavefront of $\psi_{out}(x,t)$ to appear in $x \geq a$. Hence, close to the cutoff $x = a$, important interference effects between the incident and reflected wave packets are expected.

4. Phase time and delay time

Applying the stationary phase condition\(^1\) on $\psi_{inc}(x,t)$, one gets the classical kinematical rule for particles moving with constant velocity: $x = -v_g t$. This expression defines the time-dependence of the incoming wave packet center $x_{inc}$. In a similar form, $x = v_g(t + \tau_W)$ defines the time-dependence of the outgoing wave packet center $x_{out}$ with

$$\tau_W = -2 \frac{d}{dE} \delta(E,a)$$ \hspace{1cm} (18)

the Wigner phase time \([11]\), and $\delta(E,a)$ the reflection phase shift defined in (A.7).

Though the time-dependence of the wave packet centers $x_{inc}$ and $x_{out}$ seems to be classical, their motion is clearly different from that of the classical particles. The predictions of classical mechanics are as follows: when the particle has the energy $E \geq 0$ and arrives from the right, it undergoes an abrupt acceleration at $x = a$, then an abrupt deceleration at $x = -a$, and then continues towards the left by decelerating its movement until it reaches the turning point $x_0$ defined by $E = x_0^2$. The momentum of the particle is instantly reversed at $x_0$ and the process is repeated in reverse order. In contrast, the motion of $x_{inc}$ does not obey the classical mechanical laws. The center of the incoming wave packet retraces its steps before reaching the classical turning point $x_0$. As it was explained above, the action of the potential on the $\psi_{inc}$ wavefront is sufficient to make this wave packet turn back before its center $x_{inc}$ arrives at the classical turning point $x_0$. To verify our statement let us apply the time-dependence rules derived above and (A.7) to write the explicit form of the phase time

$$\tau_W = \tau_f - \tau \equiv \frac{2a}{v_g} - 2 \frac{d}{dE} \arctan(\alpha).$$ \hspace{1cm} (19)

Here $\alpha(k,a) = \frac{J_r(k,a)}{J_i(k,a)}$, with $J_r(k,a)$ and $J_i(k,a)$ defined in (A.6). Equation (19) shows that $\tau_W$ consists on the time $\tau_f = 2a/v_g$ spent by $x_{inc}$ to traverse the distance $2a$ with constant speed $v_g = 2k$, minus the reflection time delay

$$\tau = 2 \frac{d}{dE} \arctan(\alpha) = \left[ \frac{1}{1 + \alpha^2(k,a)} \right] \frac{d}{dk} \alpha(k,a).$$ \hspace{1cm} (20)

The distance $2a$ corresponds to the trajectory described by a classical free particle in its transit from $x = a$ to the origin of the straight-line $x = 0$, and from $x = 0$ to $a$. Since $0 \neq x_0$ for any scattering energy $E > 0$, there is a clear difference between the motion of $x_{inc}$ and the motion of a classical particle, both of them subjected to the same initial conditions.

According to these last results, the delay contribution $\tau$ to the phase time (18) must be due to both the rectangular well and the semi-harmonic environment. This affirmation is clear by writing the ratio $\alpha = J_r/J_i$ explicitly. From (A.6) one gets the following product

$$\alpha(k,a) = \Theta(k,a) \left[ \left( \frac{k^2 + q^2}{2kq} \right) \tan(2qa) \right].$$ \hspace{1cm} (21)

\(^1\) That is, the derivative with respect to $k$ of the phase is zero for $k = k_0$. 

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The term in square brackets of this last equation is the kernel to calculate the phase time of a rectangular well \([4, 5, 12]\), so that the factor \(\Theta(k, a)\) is due exclusively to the semi-harmonic environment. This is defined as follows

\[
\Theta(k, a) = \left( \frac{2k^2}{k^2 + q^2} \right) \left[ \frac{\beta(x, k) - a - q \cot(2qa)}{\beta(x, k) - a + q \tan(2qa)} \right].
\]

Let us emphasize that the zeros of \(\Theta(k, a)\) coincide with the singularities of \(\tan(2qa)\) and vice versa, so that the ratio \((21)\) is a regular function of \(k\) and \(a\). The function \(\beta(x, k)\), on the other hand, plays a relevant role in the definition of \(\Theta(k, a)\). That can be zero or even be singular for specific values of \(a\) and \(k\) which are different from the zeros of \(\sin(2qa)\) and \(\cos(2qa)\), as it is shown in Figure 1.

In order to analyze the behavior of \(\tau_W\) and \(\tau\) notice that the reflection phase shift \(\delta = -ka + \arctan(\alpha)\) consists of a negative monotonically decreasing function \(-ak = -a\sqrt{E}\), plus the monotonically increasing function \(\arctan(\alpha)\). Since this last function is bounded between \(-\pi/2\) and \(\pi/2\), the phase shift is a negative decreasing function of \(E \geq 0\). The periodicity of \(\alpha(k, a)\) induces oscillations on the second term, so that a rapid increasing of the phase is expected in the vicinities of the maxima of \(\arctan(\alpha)\). These increases should be balanced by the appropriate decreases of \(\delta(k, a)\) \([11]\). Under these considerations, the phase time \(\tau_W\) defined in \((19)\) is such that the delay contribution \((20)\) can be even negative. The situation is illustrated in Figure 2, where we have depicted the time delay \(\tau\) for two different semi-harmonic wells of unit area \(2aV_0 = 1\). For \(a = 4.6257\) the time delay \(\tau\) is negative in the energy interval \((0, 7.06965 \times 10^{-4})\). However, if \(a = 4.8257\) the time delay is positive for any energy \(E \geq 0\). In general, for unit area semi-harmonic wells, it can be shown that negative time delays appear for a definite set of parameters \(0 \leq a \leq a_0 \approx 4.7257\) \([12]\). Of particular interest, in the limit \(a \to 0\) we obtain the time delay for a semi-harmonic delta well \([6]\) by the substitution of

\[
\lim_{a \to 0} \alpha(k, a) = \frac{\Gamma \left( \frac{1-k^2}{4} \right) k}{2\Gamma \left( \frac{3-k^2}{4} \right) - \Gamma \left( \frac{1-k^2}{4} \right)}
\]

into the equation \((20)\). It should be pointed out that the semi-harmonic delta well induces negative delays in the energy interval \((0, 0.45727096)\). This is the largest interval in which \(\tau\) is negative for any of the unit area semi-harmonic wells \([7]\).

The phenomenon of negative delays in the semi-harmonic wells is not exclusive of the rectangular wells of unit area. Indeed, the identification of intervals in which the parameters \(a\) and \(V_0\) give rise to negative time delays can be done for arbitrary amounts of bound states. Namely, the unit area potentials \((1)\) admit with certainty a single bound state. However, the set
Figure 2. The time delay $\tau$ for a semi-harmonic well of unit area with $a = 4.6257$ (blue curve) and $a = 4.8257$ (red curve). These values of the parameter $a$ are close to the critical value $a_0 \approx 4.7257$ which defines the change of sign in $\tau$ [12]. A detail of the behavior of $\tau$ for low energies is shown at the right.

Figure 3. The time delay $\tau$ for a semi-harmonic well which admits only two bound states for $a = 1, V_0 = 1$ (blue curve), and $a = 1, V_0 = 4$ (red curve). In this last case $\tau$ becomes negative in the energy interval $(0, 0.2813)$.

5. Concluding remarks
It is well known that the quantum mechanical problem of a piecewise constant potential can be always associated with an optical problem [13]. Consider a medium $M$ whose index $n$ has discontinuities of the same type as those of the quantum potential $V$. The propagation of an electromagnetic wave of angular frequency $\Omega$ in $M$ is related to the quantum problem in terms of the identification ([13], pp 36):

$$n(\Omega) = \sqrt{\frac{2mc^2(E - V)}{\hbar^2\Omega^2}}.$$ 

A transparent medium $M$ corresponds to the region where $E > V$, and the light wave is of the form $e^{ipx}$. If $E < V$ the index $n$ is pure imaginary and the light wave is evanescent $e^{-px}$. This optical analog has been used in the study of particles passing through a rectangular well for which negative phase times have been confirmed [4, 5]. The time delay of the semi-harmonic wells can be studied in a similar form in order to look for observable effects which are attainable to the environment. The detailed study of this problem can be found elsewhere [12].
Appendix A

The solutions of the Schrödinger equation (2) which satisfy the boundary conditions (4) are given by

\[ \psi(x; E) = A_1 \varphi(-a, k)e^{-a^2/2} \begin{cases} \frac{\varphi(x,k)}{\varphi(-a,k)} e^{(a^2-x^2)/2} & x < -a \\ C(k, a) \sin(qx) + D(k, a) \cos(qx) & |x| \leq a \\ \frac{1}{2\pi} \left[ J(k, a)e^{-ikx} - J^*(k, a)e^{ikx} \right] & a < x \end{cases} \]  

where the superscript “*” stands for complex conjugation, and

\[ \varphi(x, k) = _1F_1 \left( \frac{1-k^2}{4}, \frac{1}{2}; x^2 \right) + 2x \frac{\Gamma \left( \frac{3-k^2}{4} \right)}{\Gamma \left( \frac{1-k^2}{4} \right)} _1F_1 \left( \frac{3-k^2}{4}, \frac{3}{2}; x^2 \right), \]  

with \(_1F_1(a, c; z)\) and \(\Gamma(z)\) respectively the hypergeometric and Euler gamma functions of \(z \in \mathbb{C}\). Given the energy \(E\), the wavenumber \(k = \sqrt{E}\) and the interaction parameter \(q = \sqrt{V_0 + k^2}\) take definite values so that the coefficients in (A.1) become

\[ C(k, a) = -q \left[ \frac{\sin(qa) + (\beta_{\varphi})(-a, k) - \lambda \cos(qa))}{\lambda} \right], \]

\[ D(k, a) = q \left[ \frac{\cos(qa) - (\beta_{\varphi})(-a, k) - \sin(qa))}{\lambda} \right]. \]  

Here, \(-\beta_{\varphi}(x, k)\) stands for the logarithmic derivative of \(\varphi(x, k)\) with respect to \(x\). The arbitrary integration constant \(A_1\) has been taken as \(A_1 = e^{a^2/2}/\varphi(-a, k)\) in the paper. On the other hand, the Jost function \(J(k, a)\) of the problem we are dealing with is defined by

\[ e^{-ika} J(k, a) = \sin(qa)[-ik + q \cot(qa)]C(k, a) - \cos(qa)[ik + q \tan(qa)]D(k, a). \]  

This last expression can be rewritten in the form

\[ e^{-ika} J(k, a) = J_r(k, a) - iJ_i(k, a), \]  

with

\[ J_r(k, a) = q \left[ C(k, a) \cos(qa) - D(k, a) \sin(qa) \right] \]

\[ = -q \left( \sin(2qa) + (\beta_{\varphi})(-a, k) - \lambda \cos(2qa) \right); \]

\[ J_i(k, a) = k \left[ C(k, a) \sin(qa) + D(k, a) \cos(qa) \right] \]

\[ = q k \left[ \cos(2qa) - (\beta_{\varphi})(-a, k) - \sin(2qa) \right]. \]  

Using \(J(k, a) = |J(k, a)|e^{-i\delta(k, a)}\), we finally get

\[ \delta(k, a) = -ka + \arctan \left( \frac{J_i(k, a)}{J_r(k, a)} \right) \equiv -ka + \arctan[\alpha(k, a)], \]  

where we have made \(\alpha(k, a) = \frac{J_i(k, a)}{J_r(k, a)}\).

The condition for the trapping of particles corresponds to make \(J(k, a) = 0\) [6]. That is, the wave functions of either bound states or resonances are written as

\[ \psi(x; E) = \begin{cases} \frac{\varphi(x,k)}{\varphi(-a,k)} e^{(a^2-x^2)/2} & x < -a \\ C(k, a) \sin(qx) + D(k, a) \cos(qx) & |x| \leq a \\ \frac{1}{2\pi k} J^*(k, a)e^{ikx} & a < x \end{cases} \]
The zeros of the Jost function are defined by the roots of the transcendental equation
\[ \beta_\varphi(-a,k) = a - ik + \frac{ik\beta_\varphi(-a,k) - ika - q^2}{q} \tan(2qa). \] (A.9)

In particular, if \( k = i\kappa \) is a root of (A.9) with \( \kappa > 0 \), then \( E = k^2 = -\kappa^2 \) is the energy eigenvalue of a bound state. The number \( N \) of these roots is determined by the area \( A = 2aV_0 \) of the rectangular well. Thereby, the bound states are represented by the square-integrable functions
\[ \psi_n(x;E_n) = \begin{cases} \frac{\varphi_n(x,\kappa_n)}{\varphi_n(-a,\kappa_n)} e^{(a^2-x^2)/2} & x < -a \\ C(\kappa_n,a) \sin(q_n x) + D(\kappa_n,a) \cos(q_n x) & |x| \leq a \\ \frac{1}{2i\kappa_n} J^*(\kappa_n,a)e^{i\kappa_n x} & a < x \end{cases} \] (A.10)

where \( n = 0,1,\ldots,N-1 \). It is important to remark that the number \( N \) of bound energies is the same as that of a rectangular well of the same area. The difference lies on the fact that the energies \( E_0, E_1, \ldots, E_{N-1} \) of the semi-harmonic well are displaced towards the positive threshold with respect to their partners of the rectangular well. This property does not depend on the geometry of the rectangle: the wells having the same area admit the same number of bound states. For instance, the single bound energy of a delta well is \( E_0 = -0.25 \). This becomes less negative \( E_0 = -7.97104 \times 10^{-2} \) in the presence of the semi-harmonic background [6].

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References

[1] Muga JG, Sala R and Egusquiza IL (Eds.) 2008 Time in Quantum Mechanics 2nd Ed. (Springer)
[2] Muga JG, Ruschhaupt A, and del Campo A (Eds.) 2010 Time in Quantum Mechanics Vol. 2 (Springer)
[3] Hartman TE 1962 Tunneling of a Wave Packet J. Appl. Phys. 33 3427
[4] Li CF and Wang Q 2000 Negative phase time for particles passing through a potential well Phys. Lett. A 275 287
[5] Vetter RM, Haibel A, and Nintz G 2001 Negative phase time for scattering at quantum wells: A microwave analogy experiment Phys. Rev. E 63 046701
[6] Fernández-García N and Rosas-Ortiz O 2011 Rectangular Potentials in a Semi-Harmonic Background: Spectrum, Resonances and Dwell Time SIGMA 7 044
[7] Rosas-Ortiz O, Cruz y Cruz S, and Fernández-García N 2012 Negative time delay for wave reflection from a one-dimensional semi-harmonic well, to appear in P Kielanowski et. al. (Eds.) Proc. of the XXX Workshop on Geom. Meth. Phys. (Poland)
[8] Nussbaum IG and Kleber M 1988 Delayed broadening in reflectionless scattering J. Phys. A: Math. Gen 21 2953
[9] García-Calderón G 2011 Transient effects in quantum decay AIP Conf. Proc. 1334 84-122
[10] Muga JG 2008 Characteristic Times in One-Dimensional Scattering Lect. Notes Phys. 734 31-72
[11] Wigner EP 1955 Lower limit for the energy derivative of the scattering phase shift Phys. Rev. 98 145
[12] Alonso L, Cruz y Cruz S, Fernández-García N, and Rosas-Ortiz O 2011 preprint Cinvestav
[13] Cohen-Tannoudji C, Diu B, and Laloe F 1977 Quantum Mechanics Vol. 1 (John Wiley)