Transmission and Reflection of Wave Packets by Asymmetric Semi-Harmonic Potential Barriers

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Abstract. We study the scattering of a particle by a square barrier potential that has a parabolic hole in between. The barrier is parameterized in such a form that the hole can be partially or completely removed. This can be also chosen to be symmetric or asymmetric with respect to the hole. Some expressions for the phase time are given and the time spent by the particle in the interaction zone of the barrier is calculated. It is shown that the related time delay depends on the symmetry operations that one can do on the potential.

1. Introduction
In a previous work we have analyzed the probability of finding a particle in the interaction zone of a scattering process [1]. In particular, we found the intervals of time that are required in order to get a maximum probability in the interaction zone as a lower bound of the duration of the scattering. The simplest example consists of a square barrier (or well) potential as representing the scatterer [2], but this can be also embedded in a semi-harmonic background [3–5]. In this contribution we report our progress in the study of the times involved in scattering under different conditions. To represent the interaction defined by the scatterer we use a square barrier having a parabolic hole in between. This is parameterized such that profiles as symmetry of the potential and the deepness of the hole can be adapted to the necessities of the (possible) experimental setup or to the theoretical approximations. The problem is soundness in areas as solid state physics [6] where the experimental capabilities of manufacturing heterostructures with practically any profile open a wide arena of possible applications (see also [7, 8]). As we are going to show, the time delay is maximum for energies that are close to the transparencies of the scatterer. Evidence of the Hartman effect [9] must be expected for low energies of the incoming particle. The system is sensitive to symmetry transformations so that the time delay of the reflected particles must increase after a change in the configuration of the potential.

The organization of the paper is as follows. In Section 2 we revisit some generalities of the wave-packets in a scattering process. Then, the stationary phase method is applied to calculate the transmission and reflection time delays. In Section 3 we particularize to the potential described above. Final remarks are given in Section 4.

2. Wave packets and time delay
Consider a particle with definite momentum \( k_0 \) that is sent from a given point \( x_0 \) towards a scatterer at the time \( t = 0 \). For simplicity, let us assume that the interaction is described by
a short-range one-dimensional potential \( V(x) \) centered at the origin of the real line. Thus, the potential is equal to zero everywhere except in \((-a_2, a_1)\), with \(a_{1,2}\) two nonnegative numbers. The initial quantum state of the particle is given by a momentum distribution \( \Lambda(k) \) that is very peaked and centered at \( k = k_0 \). However, the position of the particle is unknown for \( t \geq 0 \), so that its position distribution spreads over all the real line. Considering \( x_0 > 0 \) (i.e., the particle impinges the scatterer from the right), the superposition (proper units assumed)

\[
\psi_{\text{inc}}(x,t) = \int_{-\infty}^{\infty} dk \, \Lambda(k) e^{i(k(x-x_0)+\omega t)}
\]

represents the state of the particle at the right of the interaction zone \((-a_2, a_1)\). The center of the packet moves as a classical particle at the energy \( E = \omega = k^2 \), with a (group) velocity equal to \( v_g(k_0) = d\omega/dk|_{k=k_0} = 2k_0 \). The stationary phase condition gives the dynamical law obeyed by the center of the packet

\[
\frac{d}{dk}(k(x-x_0) + \omega t) \bigg|_{k=k_0} = 0 \quad \Rightarrow \quad x = x_0 - v_g t.
\]

If \( T(k) = |T(k)|e^{-i\gamma(k)} \) and \( R(k) = |R(k)|e^{-i\zeta(k)} \) are the complex transmission and reflection amplitudes respectively, the transmitted wave packet can be written as

\[
\psi_t(x,t) = \int_{-\infty}^{\infty} dk \, \Lambda(k)|T(k)|e^{-i(k(x-x_0)+\omega t+\gamma)} ,
\]

where \( \gamma(k) \) and \( \zeta(k) \) are the corresponding transmission and reflection phase shifts. The center of this new packet obeys the rule \( x = x_0 - v_g(t + \partial\gamma/\partial E|_{E=k_0^2}) \). Finally, it can be shown \([3–5]\) that the transmission and reflection time delays

\[
\Delta\tau_t = -\frac{\partial\gamma}{\partial E} \bigg|_{E=k_0^2}, \quad \Delta\tau_r = -\frac{\partial\zeta}{\partial E} \bigg|_{E=k_0^2},
\]

are in agreement with the notion of phase time introduced by Wigner \([10]\).

3. Scattering by asymmetric semi-harmonic potential barriers

The potential, see Figure 1(a), and the wave functions we are dealing with are defined as follows

\[
V(x) = \begin{cases} 
0, & x \leq -a_2, \\
V_2, & -a_2 < x < -b_2, \\
x^2, & -b_2 \leq x \leq b_1, \\
V_1, & b_1 < x < a_1, \\
0, & x \geq a_1,
\end{cases}
\]

\[
\psi(x) = \begin{cases} 
A_5e^{ikx} + B_5e^{-ikx}, & x \leq -a_2 \\
A_4e^{iq_2x} + B_4e^{-iq_2x}, & -a_2 < x < -b_2 \\
A_3u_e(x) + B_3u_o(x), & -b_2 \leq x \leq b_1 \\
A_2e^{iq_1x} + B_2e^{-iq_1x}, & b_1 < x < a_1 \\
A_1e^{ikx} + B_1e^{-ikx}, & x \geq a_1
\end{cases}
\]

where \(a_i, b_i > 0, \ i = 1, 2; \ A_j, B_j \in \mathbb{C}, \ j = 1, 2, 3, 4, 5; \ k^2 = E > 0, \ q_1^2 = k^2 - V_1, \ q_2^2 = k^2 - V_2, \) and \( V_1, V_2 > 0 \), while \( u_e(x) = e^{-x^2/2}F_1(a, \frac{1}{2}; x^2) \) and \( u_o(x) = e^{-x^2/2}F_1(a + \frac{1}{2}, \frac{3}{2}; x^2) \) are defined in terms of the confluent hypergeometric function with \( a = \frac{1}{4}(1 - k^2) \) \([11]\).
After solving the related Schrödinger equation, the scattering amplitudes are of the form

\[
T = \frac{-4ikq_1q_2 \text{W}(u_e, u_o)|_{x=b_1} e^{-i(k(a_2+a_1)}}}{t_2 + it_1}, \quad R = \frac{r_2 + ir_1 e^{-2ika_1}}{t_2 + it_1},
\]

where

\[
t_1 = k(q_2 + q_1 + \xi(q_2 - q_1)), \quad t_2 = \alpha(k^2 + q_1q_2) - \beta(k^2 - q_1q_2),
\]

\[
r_1 = k(\xi(q_2 + q_1) + \eta(q_2 - q_1)), \quad r_2 = \alpha(k^2 - q_1q_2) - \beta(k^2 + q_1q_2),
\]

\[
\alpha = (y - q_1q_2) \cos \varphi_1 + (q_2v_2 + q_1v_1 \sin \varphi_1, \quad \beta = (y + q_1q_2) \cos \varphi_2 + (v_2q_2 - v_1q_1) \sin \varphi_2,
\]

\[
\eta = (y - q_1q_2) \sin \varphi_1 - (v_2q_2 + v_1q_1) \cos \varphi_1, \quad \xi = -(y + q_1q_2) \sin \varphi_2 + (v_2q_2 - v_1q_1) \cos \varphi_2,
\]

\[
z = u_e(b_1)u_o(b_2) + u_e(b_2)u_o(b_1), \quad y = \left. \frac{du_e(x) dx}{x=b_1} \right|_{x=b_2} + \left. \frac{du_o(x) dx}{x=b_2} \right|_{x=b_1},
\]

\[
v_1 = u_e(b_1) \left. \frac{du_o(x) dx}{x=b_1} \right|_{x=b_2} + u_o(b_1) \left. \frac{du_e(x) dx}{x=b_2} \right|_{x=b_1}, \quad v_2 = u_e(b_2) \left. \frac{du_o(x) dx}{x=b_2} \right|_{x=b_1} + u_o(b_2) \left. \frac{du_e(x) dx}{x=b_2} \right|_{x=b_1},
\]

\[
\varphi_1 = q_2(b_2 - a_2) + q_1(b_1 - a_1), \quad \varphi_2 = q_2(b_2 - a_2) - q_1(b_1 - a_1).
\]

Here \(W(u_e, u_o)\) denotes the Wronskian of \(u_e\) and \(u_o\). The above expressions are valid in the cases \(E \geq V_j (q_j \in \mathbb{R})\), and \(E < V_j\), for \(j = 1, 2\), where in the latter ones it is necessary to write \(q_j = \pm iq_j^0\), where \(q_j^0 = \sqrt{V_j - k^2}\), being indistinct the choice of the sign. Both of the scattering coefficients are invariant under a specular reflection. Indeed, the expressions \(\alpha, \beta, \eta, \varphi_1, z, y, v_1, v_2, \) and \(W(u_e, u_o)|_{x=b_1}\), are invariant under such a transformation, while \(\xi \rightarrow -\xi, \varphi_2 \rightarrow -\varphi_2\). That is, under specular reflection

\[
t_1, t_2, r_2, \text{ remain invariant, while } r_2 \rightarrow -r_2.
\]
In Figure 1(b–d) we show the transmission and reflection by a semi-harmonic potential barrier. In the symmetric case, Fig. 1(b), it is clear that the peaks of the transmission are narrower for the transparencies ($|T|^2 = 1$) in the regime of classical confinement ($E < \min(V_1, V_2)$). In turn, the asymmetric case, Figure 1(d), is such that the narrower peaks of the transmission coefficient do not correspond to transparencies ($|T|^2 \neq 1$).

3.1. Phase shift and time delay

To determine the time delay we first calculate the transmission $\gamma$ and reflection $\zeta$ phase shifts. Two main cases of parameters are distinguishable: If $\max(V_1, V_2) < E < \min(V_1, V_2)$ then $t_1$ and $t_2$ are real. These last are pure imaginary if $\min(V_1, V_2) < E < \max(V_1, V_2)$. Taking this into account, from (6) we obtain

$$\gamma(k) = k(a_1 + a_2) - \arctan \left( \frac{t_2}{t_1} \right).$$  (15)

On the other hand, for the reflection phase shift, if $E < \min(V_1, V_2)$ then $q_j = \pm iq_j^0$, with $q_j^0 = \sqrt{V_j - k^2}$ and $j = 1, 2$. For $V_i < E < V_j$ ($i = 1, j = 2$ or $i = 2, j = 1$), with $q_i, iq_j \in \mathbb{R}$, it is necessary to write either $q_j = \sqrt{k^2 - V_j}$ for $E > V_j$ or $q_j = i\sqrt{V_j - k^2}$ for $E < V_j, j = 1, 2$. Then, for $k > 0$, we have

$$\zeta = 2ka_1 + \arctan \left( \frac{t_1r_2 - t_2r_1}{t_1r_1 + t_2r_2} \right).$$  (16)

Figure 2. Transmission time delay $\Delta \tau_T$ (a) and reflection time delay $\Delta \tau_R$ (c) as function of the energy with $a_1 = a_2 = 3, b_1 = b_2 = 1.75, V_1 = V_2 = b_1^2$ in the symmetric case (blue) and the same parameters except $b_2 = 2$ and $V_2 = b_2^2$ in the asymmetric case (red). Figures (b) and (d) are details of (a) and (b) respectively.

The introduction of (15) and (16) in (4) gives

$$\Delta \tau_T = \frac{W(t_1, t_2) - a_2 + a_1}{2k}, \quad \Delta \tau_R = \frac{(r_1^2 + r_2^2)W(t_1, t_2) - (t_1^2 + t_2^2)W(r_1, r_2)}{(t_1^2 + t_2^2)(r_1^2 + r_2^2)} - \frac{a_1}{k}.$$  (17)

Notice that $\Delta \tau_R = \Delta \tau_T + \Delta \tau_{asy}$, where

$$\Delta \tau_{asy} = -\frac{W(r_1, r_2)}{r_1^2 + r_2^2} - \frac{a_1 - a_2}{2k}.$$  (18)

accounts for the symmetry breaking in the potential which only depends on $r_1, r_2$. Indeed, if the potential is symmetric then $\Delta \tau_{asy} = 0$. Moreover, under specular reflection the transmission time delay $\Delta \tau_T$ is preserved but $\Delta \tau_R$ is not, the latter because $\Delta \tau_{asy}$ changes its sign.

Figure 2 shows the behaviour of $\Delta \tau_T$ and $\Delta \tau_R$ in both the symmetric and the asymmetric cases. Note that the peaks of these graphs are very close to the ones of the transmission shown in Figure 1. This last means that closer to a transparency the time delay is maximum. Interestingly,
the symmetry breaking enhances the spending of time by the particle in the interaction zone because the peaks of the asymmetric case are higher than the ones in the symmetric case. On the other hand, for low energies we find evidence of the Hartman effect [9] as the time delay is negative.

In Figure 3(a) it is presented the specular reflection of the case shown in Figure 2(c). The change of sign suffered by $\Delta \tau_{\text{asy}}$ produces that the peaks of positive time delay are now peaks of negative time delay. That is, the reflected packet is accelerated with respect to a free packet propagating in the same direction and following the same path. Again, the explanation lies on the asymmetric configuration of the barrier. For low energies the incoming packet faces different barriers previous and after the specular reflection. In the first case such a barrier is lower than in the second case, so that tunnelling is most probable and takes less time before than after the symmetry operation. Once the barriers have been interchanged, it is most probable that the incoming packet be reflected so that the process started even before the center of the packet arrives at the interaction zone. This last produces mainly constructive superposition of waves at the right of the scatterer and so the entire reflected packet is formed much earlier than in the case before the symmetry operation.

4. Concluding remarks

The scattering of a particle by a semi-harmonic potential barrier has been studied. The time spent by the particle in the interaction zone has been calculated in terms of the energy derivatives of the phase shift, this last in coincidence with the phase time of Wigner. Then, the time delay has been shown to be maximum close to the transparency energies of the scatterer. As it would be expected, evidence of the Hartman effect has been found for low energies of the projectile. Of particular interest, the system is sensitive to symmetry transformations. That is, the time delay of reflected particles increases after an specular reflection when the asymmetry is such that the first barrier that they face is lower that the second one. The study of the relation between the transparencies and maximum time delay as well as the physical explanation of the peaks in the symmetry breaking term $\Delta \tau_{\text{asy}}$ are part of work under progress.

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