Time of arrival through a quantum barrier\footnote{Work supported in part by DGESIC PB97-1256.}

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Abstract

We introduce a formalism for the calculation of the time of arrival \( t \) at a detector of particles traveling through interacting environments. We develop a general formulation that employs quantum canonical transformations from the free to the interacting cases to compute \( t \). We interpret our results for the time of arrival operator in terms of a Positive Operator Valued Measure. We then compute the probability distribution in the times of arrival at a detector for those particles that - after their initial preparation - have undergone quantum tunneling or reflection due to the presence of potential barriers. We make a extensive analysis of several cases, the main results being the presence of the expected retardation or advancement for transmission, and of non-foreseen two bump structures for some cases of reflection.
1 Introduction

In this paper we work out a theoretical framework to compute the time in which a particle that moves in an interacting environment arrives at a given point. We apply our results to answer the long pending question: How long does it take for a particle to tunnel across (or through) a quantum barrier? In the construction of this framework we will have to deal with problems of very different kind that we introduce now:

First, there is the nature of time in quantum mechanics. It appears as the external evolution parameter in the Schrödinger and Heisenberg equations, common to both, systems and observers alike. However, time arises in many instances (transitions, decays, arrivals, etc.) as a property of the physical systems. The attempts to promote time to the category of observable run early into the obstruction detected by Pauli [1]: A self adjoint time operator implies an unbounded energy spectrum. This was soon related to the uncertainty relation for time and energy, whose status and physical meaning has been subject of controversies [2, 3, 4, 5], and is still subject of elucidation today (see for instance [6] and [7]). The question remains unsettled for closed quantum systems, specially in the case of quantum gravity, whose formulation is pervaded by the so called problem of time [8].

Second, the definition of the time-of-arrival (toa), which is probably the simplest candidate time to become a property of the (arriving) physical system, rather than a mere external parameter. Due to its conceptual simplicity, it has been used in many cases to illustrate different problems related to the role of time in quantum theory. Allcock analyzed [9] extensively the difficulties met by the toa concluding they were insurmountable. The present situation is ambiguous. On the one side, there are sound theoretical analysis [10, 11] of the toa showing that it can not be precisely defined and measured in quantum mechanics. This contradicts the possibility of devising high efficiency absorbers [12], that could be used as almost ideal detectors for toa [13]. On the other hand, there are explicit constructions of a self-adjoint toa operator for the non-relativistic free particle in one space dimension [14], the relativistic free particle in 3-D [15], both avoiding the Pauli problem. There is also an alternative formulation [16] as a Positive Operator Valued Measure (POV). Finally, the toa has been measured in high precision experiments [17, 18] on the arrival of two entangled photons produced by parametric down-conversion, one of which has undergone tunneling through a photonic band gap (PBG). The experimental results that show superluminal tunneling, neatly identify the Hartman effect [19] and the Wigner time delay [20] (or phase time) as the physically relevant mechanisms for the tunneling time and toa respectively. Whether these results apply only to photons and are due to the specific properties of the PBG used, or can be extended to other particles and barriers, can not be decided in the lack of a satisfactory theory of the toa at a space point through interacting environments.

The third question is thus the tunneling time, for which there are three main proposals. Wigner introduced the phase time in his analysis [20] of the relationship between retardation, interaction range, and scattering phase shifts. Buttiker and Landauer introduced the traversal time [21] in their study of tunneling through a time-dependent barrier. Soon after, Buttiker used the Larmor precession as a clock [22], identifying the dwell [23], traversal, and reflection times as three characteristic times describing the interaction of particles with a barrier. Recent reviews that include these and other approaches, discussing toa and
tunneling times from a modern, unified perspective, can be found in [24] and [25]. The light shed on these questions by the two photon experiments is revised in [26] and [27].

The plan of the work is as follows: In Section 2 we construct the generic toa formalism, generally valid, but still awaiting the necessary connections to each physical situation of interest. The starting point is the case of the free particle. A suitable canonical transformation, similar to that used in scattering theory, gives the toa in interacting environments, (also at points where \( V(x) \neq 0 \)). In Section 3 we specialize to the case of potential barriers, showing the existence of two characteristic times of arrival at each point, one for incoming and other for outgoing particles, in the same way as there are two different kinds of scattering states associated to the free “in” and “out” asymptotic states. In Section 4 we make some calculations and give estimates of interest for the case of the square barrier. Here we give the toa for both, transmitted and reflected particles, and discuss some properties of the associated probability distributions. Finally, we summarize our results in Section 5.

2 Time of arrival formalism

To measure the time of arrival of a free particle at a point \( x \) one would: a) place a detector at \( x \), b) prepare the initial state \( |\psi\rangle \) of the particle at \( t = 0 \), and then, c) record with a clock the time \( t \) when the detector clicks. The value of \( t \) gives the toa of the state \( |\psi\rangle \) at \( x \). Repeating this procedure with identically prepared initial states, one would get the probability distribution in times of arrival at \( x \). Of course, the results would depend on the initial state chosen, which stores all the information regarding the initial distribution in positions and momenta of the particle.

To determine the effect on these times of climbing (or tunneling through) a potential barrier, one would simply put the barrier in between the detector and the initial state, and then record the new times of arrival. With an initial state identical to that prepared for the free case, any difference in the probability distributions should be an effect of the barrier. Several questions can be investigated by changing the properties of the barrier: its height or width if it is rectangular, even its very form. This has been explicitly done in the two photon experiments at Berkeley, by putting alternatively a mirror and an ordinary glass in the path of one of the photons. It would also be of interest to analyze the dependence on \( x \) when \( V(x) > 0 \), i.e. with the detector within the range of the interaction.

In classical mechanics particles move along the trajectories \( H(q, p) = \text{const.} \) as \( t \) increases. This allows to work out \( t_x \), the time of arrival at the point \( q(t) = x \), by identifying the point \( (q, p) \) of phase space where the particle is at (say) \( t = 0 \), and then following the trajectory that passes by it, up to the arrival at \( x \). The mathematical translation of this procedure is given by the equation of time:

\[
t_x(q, p) = \text{sign}(p) \sqrt{\frac{m}{2}} \int_q^x dq' \sqrt{\frac{dq'}{H(q, p) - V(q')}}
\]

that is discussed at length in many textbooks.

For free particles Eq. (1) gives \( t_x^0(q, p) = m(x - q)/p \) that, in spite of its seemingly simple and harmless appearance, presents some problems in its quantization [3, 14, 15].
First of all, it requires symmetrization:

\[
\hat{\rho}^0_x(\hat{q}, \hat{p}) = m \left( \frac{x}{\hat{p}} - \frac{1}{2} \{\hat{q}, \frac{1}{\hat{p}}\}_+ \right) = -e^{-i\hat{p}x} \sqrt{\frac{m}{\hat{p}}} \sqrt{\frac{m}{\hat{p}}} e^{i\hat{p}x}, \tag{2}
\]

As is well known, the eigenstates of this operator \(|txs0\rangle\) in the momentum and energy representations can be given as (\(\hbar = 1\))

\[
\langle p | txs0 \rangle = \theta(sp) \sqrt{\frac{p}{2\pi m}} \exp(i\frac{p^2}{2m}t - ipx) \tag{3}
\]

where we use \(s = r\) for right-movers (\(p > 0\)), and \(s = l\) for left movers (\(p < 0\)). The index label 0 stands for free case. Finally, the argument \(sp\) of the step function that appears in the momentum representation is +\(p\) for \(s = r\), and −\(p\) for \(s = l\). The degeneracy of the energy with respect to the sign of the moment is explicitly shown by means of the label \(s\) in the energy representation

\[
\langle E's'0 | txs0 \rangle = \delta_{s's} \frac{1}{\sqrt{2\pi}} \exp(iEt - is\sqrt{2mEx}) \tag{4}
\]

where the \(s\) in the exponent of the rhs stands for +1 for \(s = r\) and −1 for \(s = l\). These eigenstates are not orthogonal, which in the past gave rise to serious doubts about their physical meaning. The origin of this problem can be traced back to the fact that (2) is not self-adjoint, that is \(\langle \varphi | \hat{\rho}^0_x | \psi \rangle \neq \langle \hat{\rho}^0_x | \varphi | \psi \rangle\). This was proved by Pauli [1] long time ago and is due to the lower bound on the energy spectrum. The problem emerges as soon as one attempts integration by parts in the energy representation. Ref. [25] contains a recent illuminating review of these and other related questions.

A close inspection of (2) reveals that it still needs of some prescription to deal with \(p = 0\), in order to produce a self-adjoint operator with orthogonal eigenfunctions. When \(p \rightarrow 0^+\) the \(\hat{\rho}^0_x\) eigenstates span the subspace \(|E_r\rangle\), that comes abruptly to an end at \(p = 0\), and lacks the continuation to negative values of \(p\) necessary to get orthogonality (in other words, a delta function coming from the integration over \(p\) would require \(p \in (-\infty, +\infty)\), but actually \(p \in (0^+, +\infty)\) alone). The way out [14] is to stretch analytically the interval \(p = (0, \epsilon)\) to \(p = (-\infty, \epsilon)\) in such a way that the new values of \(p\) cover all the real line. The same problem, with the same solution, occurs when \(p \rightarrow 0^-\). Observe that the attempt to “glue” \(|E_r\rangle\) to \(|E_l\rangle\) in a neighbourhood of \(p = 0\) is misleading, because it would connect with continuity states belonging to macroscopically different experimental setups (those moving from the far left to the far right with small but positive momentum, with those moving from the far right to the far left with small but negative momentum). In fact, there is no discontinuity in the eigenstates \(|p\rangle\) at \(p = 0\) while, at the same time, \(|E_r\rangle\) can not be connected continuously to \(|E_l\rangle\). This is a consequence of the different physical meaning of these two classes of states, given mathematically by different kinds of boundary conditions. The correspondence principle maps classical trajectories to energy eigenstates, but does not restrict the momentum eigenstates in the same way.

The measurement problem associated to the toa operator can be solved more simply by the use of a Positive Operator Valued Measure (POV), that only requires the hermiticity.
of $\hat{P}_x^0$ (i.e. $\hat{P}_x^0 = (\hat{P}_x^0)^\dagger$). Here, instead of a Projector Valued spectral decomposition of the identity operator, one has the POV

$$P_x(t_1, t_2) = \sum_s \int_1^2 dt |txs0\rangle \langle txs0|$$

(5)

where $P(1, 2)^2 \neq P(1, 2)$ because $|txs0\rangle \langle txs0|$ is not a projector, as the states are not orthogonal, but where the limit as $t \to \infty$ of $P(-t, +t)$ is the identity. The attained time operator is no longer sharp, but is well suited for measurement. This solution has been implemented in [16], and extensively analyzed in refs. [28, 29] and in the review [25].

In general, Eq.(1) can not be explicitly solved in the presence of interaction. This is not a problem classically, but makes hopeless any attempt to straight quantization. Even for the simple rectangular barrier that looks similar to a piece-wise assembly of free cases, there is no successful way to employ (1) directly. Here, the reason is not the algebraic complexity of that expression, but the fact that it only applies for values of $x$ that are classically within the reach of $(q, p)$, while in quantum mechanics all values of $x$ are possible. Thus, neither quantum tunneling nor quantum reflection have a classical analog in (1), (that gives complex numbers for these cases). Lacking it, this equation is a troublesome starting point for quantization. In spite of these problems, it arises as a critical time for the behaviour of particles in time dependent barriers, in the form of the so-called traversal time $\tau_T$: the time a particle takes to traverse the barrier [21] (which is the absolute value of (1)). As was indicated in the introduction, this time has been compared, giving interesting information [22] about tunneling and related phenomena, with the “dwell time” [23] $\tau_d$, defined as the ratio of the number of particles inside the barrier to the incident flux, and the “phase time” [20] $\tau_\phi$, the time associated to the peak of the propagating wave packet by the stationary phase approximation.

In this work we desist from the attempt of straight quantization of the classical expression. Instead, we will construct the solution to the interacting case in terms of the well known results that apply to the free case. The aim is similar to what has been done in formal scattering theory, where the Lippmann-Schwinger equations give the complete Green function and the scattering amplitude in terms of the free Green function and the potential. This procedure also serves to get the energy eigenstates (stationary scattering states) in terms of plane (or spherical) incoming or outgoing waves. Of particular interest for our problem is the existence of the Möller operators $\Omega_{\pm}$ that connect the free particle Hilbert spaces $\mathcal{H}_{in}$ and $\mathcal{H}_{out}$, to the Hilbert space $\mathcal{H}$ of the scattering and bound states. These operators are only isometric in the presence of bound states, because the correspondence between states in $\mathcal{H}$ and free states can not be one to one. In this paper we will consider only well behaved potentials ($V(q) \geq 0 \forall q$, $V(q)$ vanishes at the spatial infinity, and has no valleys to avoid resonances), for which the operators are unitary because there is one free state for each scattering state. In this case, the intertwining relations $H\Omega_{\pm} = \Omega_{\pm}H_0$ can be put in the form $H = \Omega_{\pm}H_0\Omega_{\pm}^\dagger$. This is an intertwining relation as it stands, but it prompts the following question: Is there a similar relation for obtaining the time of arrival to a in the presence of interactions in terms of $\hat{P}_x^0$? Below, we construct a positive answer, giving explicitly the generic solution for the positive potentials we are considering. In the next section we will apply our results to different cases of interest. There, we will make the appropriate distinctions between incoming (+) and outgoing (−) cases, that are necessary
to predict the probability distributions, but that do not affect the \( t_{oa} \), or its eigenstates, when there is a unique free particle Hilbert space, i.e. when \( \mathcal{H}_{in} = \mathcal{H}_{out} \) as in our case.

We now come back to phase space and recall that the classical canonical transformations \( \bar{q} = \bar{q}(q,p) \), \( \bar{p} = \bar{p}(q,p) \) can be defined implicitly by the use of auxiliary functions \( F, G, \bar{F}, \bar{G} \) in the following way:

\[
\begin{align*}
\bar{F}(\bar{q}, \bar{p}) &= F(q,p) \\
\bar{G}(\bar{q}, \bar{p}) &= G(q,p).
\end{align*}
\]

(6) (7)

It is easy to work out the following relation among Poisson brackets:

\[
\{ \bar{F}, \bar{G} \}_{\bar{q}, \bar{p}} \{ \bar{q}, \bar{p} \}_{q,p} = \{ F, G \}_{q,p}
\]

(8)

In these conditions, the transformation is canonical (i.e. \( \{ \bar{q}, \bar{p} \}_{q,p} = 1 \)) if and only if

\[
\{ \bar{F}, \bar{G} \}_{\bar{q}, \bar{p}} = \{ F, G \}_{q,p}.
\]

(9)

This relation has the additional property of fixing one of the four functions \( F, G, \bar{F}, \bar{G} \), once the other three are given. We can choose \( F \) and \( G \) as the free particle Hamiltonian and time of arrival respectively. Then, if \( \bar{F} \) is the complete Hamiltonian \( H \), \( \bar{G} \) will be the corresponding \( t_{oa} \), and the above equation gives: \( \{ t_{oa}, H \} = 1 \), whose solution along the classical trajectories is (4).

Canonical transformations were introduced by Dirac in quantum mechanics by the use of unitary transformations \( U \) \( (U U^\dagger = U^\dagger U = 1) \). If the operators \( \hat{q}, \hat{p} \) are canonically transformed from \( \hat{q}, \hat{p} \), then there is a unitary transformation \( U \) such that

\[
\begin{align*}
\bar{q} &= U \hat{q} U^\dagger \\
\bar{p} &= U \hat{p} U^\dagger.
\end{align*}
\]

(10)

Then we can define implicitly quantum canonical transformations, like the classical ones, by \[30\]

\[
\begin{align*}
\bar{F}(\bar{q}, \bar{p}) &= U \hat{F}(\hat{q}, \hat{p}) U^\dagger = F(\hat{q}, \hat{p}) \\
\bar{G}(\bar{q}, \bar{p}) &= U \hat{G}(\hat{q}, \hat{p}) U^\dagger = G(\hat{q}, \hat{p})
\end{align*}
\]

(11)

where the last equality in each row is the definition of the barred operators in terms of the unbarred ones, while the first equality comes from the straight application of (10) to the l.h.s. Being \( U \) a unitary transformation, the spectra of the canonically transformed operators have to coincide, that is:

\[
\begin{align*}
\sigma(\bar{q}) &= \sigma(\hat{q}) = \mathcal{R}, \quad \sigma(\bar{p}) &= \sigma(\hat{p}) = \mathcal{R} \\
\sigma(\bar{F}) &= \sigma(\hat{F}), \quad \sigma(\bar{G}) = \sigma(\hat{G})
\end{align*}
\]

(12)

where the second row stands because \( F \) and \( \bar{F} \), \( G \) and \( \bar{G} \) are also unitarily related operators. We will now show how to use the above relations to build the operator \( \hat{G} \) once \( \bar{F}, \bar{G} \) and
\(\tilde{F}\) are given. The only restriction to our solution is that the operators \(\hat{F}\) and \(\tilde{F}\) are self-adjoint, so that their eigenstates are orthogonal and form a complete basis. The eigenstates of these operators corresponding to the same eigenvalue \(\lambda_f\) are:

\[
\tilde{F}|\tilde{f}\rangle = \lambda_f|\tilde{f}\rangle, \quad \hat{F}|f\rangle = \lambda_f|f\rangle
\]

They form orthogonal and complete bases, i.e. they satisfy

\[
\langle f|s\rangle\langle s'|f\rangle = \delta_{ss'} \delta(\lambda_f - \lambda_{f'}), \quad \sum_s \int_{\sigma(\lambda)} d\lambda_f |f\rangle\langle \tilde{f}| = \mathbb{I}
\]

where \(\sigma(\lambda)\) is a continuous function. We have also assumed that \(\lambda\) is continuous, while \(s\) is a discrete index. These assumptions could be changed straightforwardly if it were necessary. Now, an operator \(U\) satisfying the first row of Eq.(11) can be given simply as:

\[
U = \sum_s \int_{\sigma(\lambda)} d\lambda_f |f\rangle\langle \tilde{f}|
\]

It is straightforward to verify that it is unitary. We can now proceed to the sought for result: the definition of \(\tilde{G}\) in terms of \(\hat{G}\) using \(U\), that is \(\tilde{G} = U^\dagger \hat{G} U\). The full fledged expression is

\[
\tilde{G}(\hat{q}, \hat{p}) = \sum_{ss'} \int_{\sigma(\lambda)} d\lambda_f d\lambda_{f'} |\tilde{f}\rangle \langle \tilde{f}| \langle f| \hat{G}(\hat{q}, \hat{p}) |f'\rangle \langle f'|\tilde{f}\rangle
\]

that constitutes our main result in the quantum canonical formalism. We will now apply it to the case where \(F\) is the free Hamiltonian \(H_0\), \(\tilde{F}\) the complete Hamiltonian \(H\): \(\tilde{F}(\hat{q}, \hat{p}) = \hat{p}^2/2m + V(\hat{q})\), and \(G\) the time of arrival of the free particle Eq.(2). Then we have

\[
U(\pm) = \sum_s \int_{0}^{\infty} dE |Es0\rangle \langle Es(\pm)|
\]

where the label 0 in \(|Es0\rangle\) indicates that it is an eigenstate of \(H_0\), its absence corresponding to the eigenstates \(|Es\rangle\) of the complete Hamiltonian. For notation simplicity, we defer to Section 4 (Eq. (58)) any reference to the incoming or outgoing (\(\pm\)) character of the time operator and states we are constructing, as it is unnecessary here. After substitution in Eq.(17) we get for the \(toa\) at \(x\) in the presence of the potential \(V\)

\[
\hat{t}_x(\hat{q}, \hat{p}) = \sum_{ss'} \int_{0}^{\infty} dE dE' |Es0\rangle \langle Es| \hat{t}_x^0(\hat{q}, \hat{p}) |E's0\rangle \langle E's|\]

where \(\hat{t}_x^0\) is the \(toa\) for the free problem, as given by (3). The bracket in the above expression involves free quantities only and can be computed to give

\[
\langle Es0| \hat{t}_x^0(\hat{q}, \hat{p}) |E's0\rangle = -\langle Es0| \sqrt{\frac{m}{p}} \hat{q} \sqrt{\frac{m}{p}} |E's0\rangle
\]

where \(\delta_{ss'} \left( \frac{d}{dE} \delta(E - E') \right)\)
where we have used \( \langle p|Es0 \rangle = \sqrt{\frac{m}{p}} \delta(p - s\sqrt{2mE}) \), and put \( x = 0 \) for simplicity (we will restore the \( x \) dependence later on). Using the above expression in (19), we get the operator form

\[
\hat{t}_{x=0}(\hat{q}, \hat{p}) = -\frac{i}{2} \sum_s \int_0^{\infty} dE \langle Es \rangle \left( \frac{d}{dE} \right) \langle Es | \tag{21}
\]

that allows the explicit evaluation of the \( \text{toa} \) for all the cases in which the solutions \( \psi_{Es}(q) = \langle q|Es \rangle \) to the Schrödinger equation are known.

By solving the eigenvalue problem posed by (21), we would get the spectrum and eigenfunctions of the \( \text{toa} \). Instead of using that procedure, we will do it in all generality (within our assumptions about the potential and Hilbert spaces) by using the canonical transformation \( U \) to get the answer from the spectrum and eigenfunctions of the free case. From the positive operator valued decomposition of Eq.(5) we can write

\[
\hat{t}_{x=0} = \sum_s \int_{-\infty}^{\infty} dt t \langle ts0 | \langle ts0 | \tag{22}
\]

where we still keep \( x = 0 \), and the spectrum of \( \hat{t}_{x} \) is \( R \). The states \( |ts0 \rangle \) are the non-orthogonal eigenstates of this operator given in (4). When used in (20), Eq. (22) leads to

\[
\langle Es0|\hat{t}^0_{x=0}|E's0 \rangle = \sum_{s''} \int_{-\infty}^{\infty} dt \langle Es0|ts''0 \rangle \langle ts''0 |E's0 \rangle
\]

\[
= \frac{1}{2\pi} \delta_{ss'} \int_{-\infty}^{\infty} dt \exp(i(E - E')t) \tag{23}
\]

Putting this expression in Eq.(19) we get the spectral decomposition for the \( \text{toa} \) at \( x = 0 \) in the presence of the potential \( V(q) \):

\[
\hat{t}_{x=0}(\hat{q}, \hat{p}) = \sum_s \int_{-\infty}^{\infty} dt t \langle ts | \langle ts | , \tag{24}
\]

where the \( \text{toa} \) eigenstates are defined by

\[
|ts \rangle = \frac{1}{\sqrt{2\pi}} \int_0^{\infty} dE \exp(iEt)|Es \rangle. \tag{25}
\]

These eigenstates are not orthogonal. By direct computation using (23) one gets

\[
\langle ts|t's' \rangle = \frac{1}{2\pi} \delta_{ss'} \int_0^{\infty} dE \exp(-iE(t - t' - i\epsilon)) = \frac{i}{2\pi} \frac{1}{t' - t + i\epsilon}
\]

\[
\sum_s \int_{-\infty}^{\infty} dt \langle ts | ts \rangle = \sum_s \int_0^{\infty} dE |Es \rangle \langle Es | = I \tag{26}
\]

A set of relations defining the same kind of positive operator valued measure that appears in the free case [16]. We can now restore the dependence of the different quantities on the detector position \( x \). Restarting from Eq.(20), but this time keeping the term \( mx/\hat{p} \) in the brackets, we arrive to

\[
\hat{t}_x(\hat{q}, \hat{p}) = \sum_s \int_{-\infty}^{\infty} dt t |txs \rangle \langle txs | , \tag{27}
\]
with the position dependent eigenstates given by

\[ |txs⟩ = \frac{1}{\sqrt{2\pi}} \int_0^{+\infty} dE \exp(iEt - isx\sqrt{2mE})|Es⟩. \]  

(28)

where the s in the exponent of the rhs stands for +1 when \( s = r \), or −1 when \( s = l \). We are now provided with the tools necessary for a physical interpretation. Given an arbitrary state \( \psi \) at \( t = 0 \), its time of arrival at a position \( x \) has to be, according to (27),

\[ \langle ψ|\hat{t}_x|ψ⟩ = \sum_s \int_{-\infty}^{+\infty} dt \ |⟨txs|ψ⟩|^2, \]  

(29)

with the standard interpretation of

\[ \sum_s |⟨txs|ψ⟩|^2 \]  

(30)

as the probability density that the state \( |ψ⟩ \) arrives at the detector placed at \( x \) in a time \( t \).

3 Classical trajectories and energy eigenstates

In three space dimensions, the free particle Hamiltonian \( H_0 \) is independent of the position and of the direction of motion as a consequence of the homogeneity and isotropy of space. In the one dimensional case we are considering in this paper, \( H_0 \) continues to be independent of the position, while the only remainder of isotropy is the degeneracy of the Hamiltonian in the sign of the momentum. For a given energy, the particle can move to the right or to the left, and occupy any position in space. With the passage of time (from \( −∞ \) to \( +∞ \)), the particle will successively pass by all the positions in configuration space. A steady flow of (say) one particle of energy \( E \) per unit time coming from the left - and necessarily going to the right at the same rate - will correspond to a properly normalized right mover stationary state. This applies classically in phase space, as well as quantum mechanically in the Hilbert space, and is also valid for left movers.

In the presence of interaction, given by a potential energy \( V(q) \), space is no longer homogeneous, and the removal of degeneracies is more involved. This is the case for the potential barriers we are interested in. To simplify the analysis, avoiding bound states and resonances whose effect we study elsewhere, we will only consider here barriers with positive potential that vanishes sufficiently fast at the spatial infinity. In addition, these barriers will have at most a maximum of value \( V \), and no minima. Two textbook barriers of this kind are the square barrier \( V(q) = V \) if \( 0 < q < a \), else \( V(q) = 0 \), and the well behaved barrier \( V(q) = V/\cosh^2(q/d) \), whose energy spectrum and eigenstates are well known. They can be used to exemplify the material discussed in this section.

The classical trajectories associated to these barriers are simple to compute, they are sketched in the phase space plane \((q,p)\) in Fig.1, where the arrows on the trajectories indicate the direction of motion. A main feature clear in both, the upper and lower drawings, is the symmetry \((q,p) \leftrightarrow (q,-p)\), which comes from the degeneracy in \( \text{sign}(p) \). The symmetry under \((q,p) \leftrightarrow (-q,p)\) is due to the spatial symmetry of the potential
chosen, and is largely irrelevant for the present analysis. Another remarkable feature is given by the two symmetric curves crossing the origin. Consider first in the upper figure the curve that we call $p_V$ of equation $p = p_V(q)$, where $p_V(q) = \text{sign}(q) \sqrt{2m(V - V(q))}$. It divides the plane into two regions. All the trajectories incoming to the barrier from the left, and only them, are above $p_V$. These trajectories share the property that as $t \to -\infty, (q,p) \to (-\infty, \sqrt{2mE})$, and split into transmitted trajectories in the case when $E > V$ and reflected trajectories when $E < V$. Below $p_V$, we have the physically equivalent set of the trajectories incoming to the barrier from the right and only them, verifying that as $t \to -\infty, (q,p) \to (\infty, -\sqrt{2mE})$. As above, there are also transmission or reflection in this region. The important thing is that the curve $p = p_V(q)$ serves to separate the phase space into two distinct (physically equivalent) regions in terms of the asymptotic initial condition at $t \to -\infty$. That is, above $p_V$ there are incoming right-movers and incoming left-movers below it.

We could also make a partition of the phase space as shown in the lower part of Fig.1, using the curve $p = -p_V(q)$. Above it, we find all the outgoing right-movers; below it, all the outgoing left-movers. There is also transmission or reflection depending on whether $E > V$ or not. The partition of phase space is here in terms of the final asymptotic condition for $t \to +\infty$: above $-p_V$ there are right-movers $((q,p) \to (\infty, \sqrt{2mE}))$, and left-movers $((q,p) \to (-\infty, -\sqrt{2mE}))$ below it. Finally, we can count particle trajectories in two alternative ways, as incoming or as outgoing trajectories, according to the value of the asymptotic momentum at $t \to -\infty$ or at $t \to +\infty$ respectively. For each way there will be right and left movers according to the asymptotic sign of $p$. The usefulness of a specific counting procedure will be dictated by the objective pursued. For instance, to investigate properties of the outgoing particles collected to the right (left) of the barrier, we have to select from the set of trajectories above (below) $-p_V$, a selection in terms of $p_V$ being useless to this end.

In quantum mechanics one finds energy eigenstates in the Hilbert space instead of the classical trajectories in phase space. A particle will be described by a wave packet $\psi$, a suitable superposition of energy eigenstates, that evolves according to the Schrödinger equation. If at some instant $t = 0$ the state of the particle is $|\psi\rangle$, the state at an arbitrary time can be written, using completeness of the energy eigenstates, as

$$|\psi(t)\rangle = \exp(-iHt)|\psi\rangle = \sum_s \int dE \exp(-iEt)|E s (\pm)\rangle\langle E s (\pm)|\psi\rangle$$

(31)

where $s = r,l$ gives the (asymptotic) sign of the momentum, necessary to remove the degeneracy of the energy eigenstates, that appears because $E$ is independent of $s$. The signs ($+$) or ($-$) indicate that the decomposition of the identity has been made in terms of the corresponding energy eigenstates: $|E s (\pm)\rangle = \Omega_{\pm}|E s 0\rangle$. These are the quantum analogs of the classical trajectories.

We now analyze in more detail the two mathematically equivalent ways for counting the energy eigenstates. As we said, the ($+$) states represent a steady flow of particles going into the barrier, corresponding to the partition of classical trajectories according to $p_V$. These states can be expanded in terms of the energy eigenstates $|E s (+)\rangle$. The label $s = r,l$ would correspond to the sign of the momentum in the free case. Here, the states with $s = r$ ($s = l$) are initial right-movers (left-movers). Observe that in the presence of the
potential the condition $E > V$ no longer guarantees transmission, nor $E < V$ reflection. The $|E_s(+)\rangle$ states are widely used tools for studying the effects of quantum barriers. The usual procedure is to prepare an incoming right mover $\langle q|Er 0 \rangle = e^{ipq}$, and determine the coefficients of transmission and reflection with the help of the matching conditions. For each particle in the scattering state $|Er(+)\rangle$, these coefficients give its probability amplitude of finally being transmitted to the other side of the barrier, or alternatively, of being reflected, bouncing back to the left. Consider the case of a barrier contained in the range $(0,a)$. The $(+) \rangle$ states can be written in configuration space representation as:

\begin{align}
\langle q|Er(+)\rangle &= \theta(-q)(e^{ipq} + R(p)e^{-ipq}) + \theta(q)\theta(a-q)\chi_r(p,q) + \theta(q-a)T(p)e^{ipq} (32) \\
\langle q|El(+)\rangle &= \theta(-q)T(p)e^{-ipq} + \theta(q)\theta(a-q)\chi_l(p,q) + \theta(q-a)(e^{-ipq} + R(p)e^{ipq})(33)
\end{align}

where $p = \sqrt{2mE}$, the $\chi_{r,l}$ solve the Schrödinger equation in the barrier region, and $R$ and $T$ are given by the matching conditions at $q = 0$ and $q = a$. A (not displayed) overall normalization factor $\sqrt{m/2\pi p}$ will insure a steady incoming flux of one particle per unit time.

The alternative way of counting energy eigenstates is in terms of the $(-)$ states. These are the energy eigenstates that emerge from the interaction region towards the spatial infinity. The $|E_s(-)\rangle$ are states going out from the barrier towards the right ($r$), or towards the left ($l$). They correspond to the classical partition according to $-pq$. They describe a post selection: that of the states that will be recorded with certainty by the appropriate detectors placed to the right ($r$ case), or to the left ($l$ case), of the barrier. By normalizing like the $(+)$ states, there will be one record, i.e. one outgoing particle per unit time in the steady flow corresponding to each of these states. We can give them with the same notation as before:

\begin{align}
\langle q|Er(-)\rangle &= \theta(-q)T(p)e^{ipq} + \theta(q)\theta(a-q)\chi_r(p,q) + \theta(q-a)(e^{ipq} + R(p)e^{-ipq}) (34) \\
\langle q|El(-)\rangle &= \theta(-q)(e^{-ipq} + R(p)e^{ipq}) + \theta(q)\theta(a-q)\chi_l(p,q) + \theta(q-a)T(p)e^{-ipq}(35)
\end{align}

We said above that the $(+)$ and $(-)$ states give mathematically equivalent decompositions of the unity $I$ in terms of the energy eigenstates and their degeneracies. In fact:

\begin{equation}
\sum_{s=r,l} \int dE|E_s(+))\rangle\langle E_s(+)\rangle = \sum_{s=r,l} \int dE|E_s(-))\rangle\langle E_s(-)\rangle = I (36)
\end{equation}

that was used in (31). As already noted, the physical meaning of these states is very different. It is well known the form in which the $(+)$ states are used in three space dimensions to describe the stationary scattering states, and to get the scattering cross sections from its asymptotic form at $|q| \rightarrow \infty$. There, $\langle \vec{q}|p\vec{q}(+))\rangle \sim e^{i\vec{p}\cdot\vec{q}} + f(p,\Omega)i\frac{d\sigma}{d\Omega}$ and $(d\sigma/d\Omega) = |f(p,\Omega)|^2$, with $\vec{q}$ the asymptotic incoming momentum and $\Omega$ the angle $(\vec{p},\vec{q})$. In one dimension, the direction given by $\Omega$ reduces to $r$ or $l$, and the scattering amplitude $f(p,\Omega)$ to the appropriate transmission $T$ and reflection $R$ coefficients. Less used, but also well known is the association of the $(-)$ states to a post selection of the final states. For instance, $|p\vec{q}(-))\rangle$ is the state that comes out from the interaction region becoming asymptotically (at $t \rightarrow \infty$) the free state $|\vec{p}\rangle$. There are several different cases possible.
They can be described by means of projectors, a formulation that we will use later on. Define

\[ \Pi(Es(+)) = |Es(+))\langle Es(+) | \]  
\[ \Pi(Es(-)) = |Es(-))\langle Es(-) | \]

the projector \( \Pi(Es(+)) \) selects the states approaching the barrier from the left (\( s = r \)), or from the right (\( s = l \)), with energy \( E \). In the same form, \( \Pi(Es(-)) \) selects the states coming out from the right of the barrier (\( s = r \)), or from the left (\( s = l \)), with energy \( E \).

Let \( V \) be the maximum value of the potential energy. Classically, there will be full transmission through the barrier for \( E > V \), and complete reflection for \( E < V \). As already said, this is not so in the quantum case in which partial reflection and transmission will take place for values of \( k \) at which they can not occur classically. In general, the wave packets will occupy regions of space that are classically forbidden, giving rise to pure quantum phenomena like tunneling, etc. It is the use of the above projectors that will give us the control of these situations in the Hilbert space, so that we can properly address the time of arrival at a space point in the presence of barriers, mirrors, etc.

4 Gaussian wave packets on square barriers

This section is devoted to the theoretical predictions provided by the previous formalism for the results of the experiments with potential barriers. We will analyze the case of transmission through a barrier in the first place, and then will turn our attention to the case of reflection, as both are aspects of the same problem. To fix notations, we will assume in what follows a square barrier of height \( V \) and width \( a \), in the interval \((0,a)\), so that \( |32, 33, 34\rangle \), and \( |35\rangle \) are the energy eigenstates in the coordinate representation. We also assume that the detector is placed to the right of the barrier (that is, \( x > a \)), and that the initial state at \( t = 0 \) is given by a Gaussian wave packet of width \( \Delta q = \delta \), centered at \( q_0 < 0 \), with mean momentum \( p_0 > 0 \). The wave packet in configuration space and its Fourier transform are:

\[ \langle q | \psi \rangle = \left( \frac{1}{2\pi\delta^2} \right)^{(1/4)} e^{-\delta^2 p_0^2} e^{-\left(\frac{q-q_0}{\Delta q}\right)^2 - ipq_0} \]
\[ \langle p | \psi \rangle = \left( \frac{2\delta^2}{\pi} \right)^{(1/4)} e^{-\delta^2(p-p_0)^2 - ipq_0} \]

(39)

For appropriate values of \( q_0, p_0 \) and \( \delta \), such that \( p_0\delta >> 1 \) and \( \delta << |q_0| \), almost all the packet is initially at the left of the origin and moving with positive momentum towards the barrier. We use this simplifying assumption in our qualitative arguments, and in the intuitive description of the process given below (indicated in the formulas by the use of \( \simeq \) instead of \( = \)), while working with the full expression (39) wherever necessary in the numerical calculations.

Our experiment differs from the usual ones in that it involves a post selection. Usually, one prepares a well defined initial state and observes its distribution into the possible final states. This gives the probabilities of these outcomes. Here, we select the final state of the particles coming out from the barrier to the detector. The procedure is to collect all the particles in this state, registering their times of arrival. From these records we
construct the conditional probability \[31\] in time we are interested in (i.e. in the toa's of all the particles gathered at the detector and only of them). Given the state \(|\psi\rangle\), that of a particle placed at the left of the barrier at \(t = 0\) as in (39), it is only the component \(P_{r}^r |\psi\rangle = \int dE \Pi(Er(-)) |\psi\rangle\) that will come out to the right of the barrier (c.f. Eq.(38)), arriving at \(x > a\) in some time \(t\). Our formalism gives for the probability distribution in these times of arrival

\[
P_{r}^r (t|x) = \frac{1}{N_{r}^r} \sum_{s} |\langle txs | P_{r}^r |\psi\rangle|^2 \tag{40}
\]

with the normalization coefficient \(N_{r}^r\) given in the equation (46) below.

We can now work out explicitly the probability amplitude for a particle initially in the state \(\psi\) to arrive at \(x > a\) in a time \(t\). It will be given by:

\[
\langle txs | P_{r}^r |\psi\rangle = \int dE \langle txs | Er(-)\rangle \langle Er(-) |\psi\rangle \tag{41}
\]

There are two factors in the integrand of the rhs. The first one is obtained from the Eq. (59) of section 2:

\[
\langle txs | Er(-)\rangle = \frac{\delta_{sr}}{\sqrt{2\pi}} \exp(-iEt + ix\sqrt{2mE}) \tag{42}
\]

The second factor can be computed using the solution (35) to the Schrödinger equation:

\[
\langle Er(-) |\psi\rangle = \int dq \langle Er(-) | q\rangle \langle q |\psi\rangle \tag{43}
\]

We said before that \(\langle q |\psi\rangle\) practically vanishes for \(q > 0\). Thence, the main contribution to the integral comes from \(q < 0\), where \(\langle q | Er(-)\rangle = \sqrt{m/2\pi p} T(p)e^{ipq},\) with \(p = \sqrt{2mE}\). In these conditions we obtain

\[
\langle Er(-) |\psi\rangle \approx \sqrt{\frac{m}{p}} T^*(p) \tilde{\psi}(p) \tag{44}
\]

where \(\tilde{\psi}(p)\) is the Fourier transform of \(\langle q |\psi\rangle\). Finally, the sought for probability amplitude is

\[
\langle txs | P_{r}^r |\psi\rangle \approx \frac{\delta_{sr}}{\sqrt{2\pi}} \int dE \sqrt{\frac{m}{p}} T^*(p) \tilde{\psi}(p) \exp(-iEt + ipx) \tag{45}
\]

Observe that \(\langle txl | P_{r}^r |\psi\rangle = 0\) as expected on physical grounds. The amplitude is not yet normalized, and has to be divided by the corresponding normalization factor \(N_{r}^r\). In fact

\[
N_{r}^r = \sum_{s} \int dt |\langle txs | P_{r}^r |\psi\rangle|^2 \approx \int_{0}^{\infty} dp |T(p)|^2 |\tilde{\psi}(p)|^2 \tag{46}
\]

i.e. \(N_{r}^r\) is the probability that the particle be transmitted, as corresponds to the case of conditional probabilities we are considering. If the Gaussian chosen as initial state is narrow enough in momentum space, and \(p_0\) not too close to \(p_V = \sqrt{2mV}\), one can approximate it further to the transmission probability

\[
N_{r}^r \approx |T(p_0)|^2 \int_{0}^{\infty} dp |\tilde{\psi}(p)|^2 \approx |T(p_0)|^2 \tag{47}
\]
as if all the transmission were at the mean momentum $p_0$. For particles initially ($t=0$) in the state $\psi$, the average time of arrival at a point $x$ at the other side of the barrier is:

$$t_x(\psi) = \frac{1}{N_{\psi}} \sum_x \int_{-\infty}^{+\infty} dt \, |\langle t x s | P_{\psi}^r | \psi \rangle|^2$$  \hspace{1cm} (48)

Any quantity related to the probability distribution $P^r_{\psi}(t|x)$ can be easily obtained using (45) and (46) or (47). Observe that the restriction to gaussian wave packets is unnecessary for the validity of (45) and (46). It is enough that $\psi(q)$ fulfills the conditions given after (33).

In Fig. 2 we present the most probable $\text{toa}$ for a selected range of barriers of various heights and sizes. To focus on the effect of the barriers, we keep the same initial wave packet and detector position in all the cases. What we obtain can be summarized as retardation for $E > V$, and advancement for $E < V$. We observe a close agreement between our results and the phase time $\tau_\phi$ in the cases shown. This is because the stationary phase method (that yields $\tau_\phi$) is a good mathematical approximation to the true probability distribution in these cases in which $\text{arg}(T(p))$ varies slowly. We have also investigated numerically (but do not show here) the cases $E \approx V$ where the validity of the approximation is uncertain. In fact, the values of $\tau_\phi$ obtained in these cases run away from the true maximum of $P^r_{\psi}(t|x)$, which turns out to be very sensitive to the parameters $(p_0, \delta, V, a)$ involved. In the cases shown, the maxima give excellent approximations to the mean $\text{toa}$ $t_x(\psi)$, even if the coincidence is not exact due to a small amount of skewness present in the distributions.

In the upper part of Fig. 3, we show the probability distributions in $\text{toa}$ $P^r_{\psi}(t|x)$ for three cases: free propagation, a low $V$ barrier, and transmission by quantum tunneling $E < V$. They look quite similar, apart from the retardation or advancement pointed out in Fig. 2. In fact, almost all of the many cases we have investigated have a similar Gaussian look. Usually it is argued that the higher momentum components are transmitted preferably through the barrier, and that they propagate faster than the lower momentum parts of the packet, being this the cause of advancement. The argument is untenable for two reasons: First, advancement is obtained even in the cases of packets whose spread is within a range of momenta for which the transmission probabilities $|T(p)|^2$ are constant (i.e. no preferred transmission for higher $p$’s). Second, would the higher momenta be transmitted preferably, then the transmitted average momentum should be shifted upwards, and then, the transmitted packet should move faster than the incident one! Of course this is physically untenable and false too.

We now turn to the time of arrival of states reflected from the barrier. First of all, we place the detector at a position $y < 0$ to the left of the barrier. We keep the same barrier and the same initial state. Now, it is $P^f_{\psi} = I - P^r_{\psi} = \int dE \, \Pi(El(-))$ that projects on the subspace of the reflected states in which the particle is detected at $y$ in some time $t$. The corresponding probability amplitude can be given borrowing Eq. (41) from the transmission case,

$$\langle t y s | P^f_{\psi} | \psi \rangle = \int dE \, \langle t y s | E l(-) \rangle \langle E l(-) | \psi \rangle$$  \hspace{1cm} (49)
There are again two factors on the right hand side. The first one is given by the formalism of section 2 as in (42). Note that, according to (59), there will be a change in sign in the second term of the exponent, as now \( r \rightarrow l \). The second factor, written as before, is

\[
\langle El(-)|\psi \rangle = \int dq \langle El(-)|q \rangle \langle q|\psi \rangle
\]  

(50)

In the relevant region \( q < 0 \), one has from (35) that \( \langle q|El(-) \rangle = \sqrt{m/2\pi p} \left( e^{-ipq} + R(p)e^{ipq} \right) \), where \( p = \sqrt{2mE} \). We now obtain the sum of two contributions (coming from 1 and \( R \)), giving

\[
\langle El(-)|\psi \rangle \approx \sqrt{m/p} (\bar{\psi}(-p) + R^*(p) \bar{\psi}(p))
\]  

(51)

As there is no way that a detector can discriminate between these two contributions, they add in the amplitude, and may produce potentially detectable interferences. However, for a properly chosen initial wave packet with positive mean momentum such that \( p_0 \delta >> 1 \) or, in other words, with negligible negative momentum tail, the first term in the sum on the rhs will practically vanish. Dropping this term, we get the probability amplitude as given by:

\[
\langle tys|\mathcal{P}_{(-)}^l|\psi \rangle \approx \frac{\delta_{sl}}{\sqrt{2\pi}} \int dE \sqrt{m/p} \bar{R}(p) \bar{\psi}(p) \exp(-iEt - ipy)
\]  

(52)

which is a look-alike of the transmission case (45). The normalization factor \( N_{l(-)}^2 \) is also similar:

\[
N_{l(-)}^2 = \sum_s \int dt |\langle t, y, s|\mathcal{P}_{(-)}^l|\psi \rangle|^2 \approx \int_0^\infty dp |R(p)|^2 |\bar{\psi}(p)|^2 \approx |R(p_0)|^2
\]  

(53)

where the last approximation is valid only when the initial state \( \psi(q) \) is narrow enough and, as for transmission, \( p_0 \) not too close to \( p_V \). We can now give the average time of arrival at a point \( y \) to the left of the barrier of the outgoing particles that were in the initial state \( \psi \) at \( t = 0 \):

\[
t_y(\psi) = \int_{-\infty}^{+\infty} dt t \mathcal{P}_{(-)}^l(t|y) = \frac{1}{N_{l(-)}^2} \sum_s \int_{-\infty}^{+\infty} dt t |\langle tys|\mathcal{P}_{(-)}^l|\psi \rangle|^2
\]  

(54)

with a probability distribution \( \mathcal{P}_{(-)}^l(t|y) \) that is also normalized to one. In the lower part of Fig. 3 we show the probability distributions for reflection by the same potential barriers of the upper part. When the barrier acts as a classical mirror (the long dashes curve) the distribution is almost the same as that of a free particle that would travel the same distance. However, dramatic differences appear for purely quantum reflection (i.e. when \( E > V \)), whenever the condition \( p_0 a = n\pi, \ n = 1,2,... \) (where \( p_0 = \sqrt{p_0^2 - k_v^2} \) is the momentum inside the barrier) holds. In these cases, a two bump structure with a dip in the middle appears in the distribution. The reason of this behaviour can be found in the value of the reflection coefficient

\[
R(p) = \frac{k_v^2 \sin(p_0 a)}{\sqrt{2p_0^2 p^2 + k_v^4 \sin^2(p_0 a)}} \exp(i\pi - i \arctan(\frac{k_v^2}{4p_0^2 p^2} \tan(p_0 a)))
\]  

(55)
which vanishes whenever the above condition is satisfied. The proportionality between the reflection probability and \( \sin^2(p' a) \), that originates the dip, could also be used to explain the bumps as due to reflection of the components of momenta greater and lesser than \( p_0 \). Were this the case, the bumps should be reflected with different velocities, one above and the other below \( p_0/m! \). Of course, this does not hold. The actual mechanism of the bumps is the spread of the incident wave packet in configuration space (not in momentum space). The centre of the packet (placed initially at \( q = q_0 \)) is reflected with probability zero, while the bumps are composed by the parts ahead and behind it (both carrying main momentum \( p_0 \)). Here, as in the case of tunneling, there is a matching between the real and imaginary exponents in the probability amplitude. Thus, while the participating momenta are in the small range \( p_0 \pm \delta^{-1} \), due to the Gaussian shape of the wave packet, the distances and times involved are macroscopic. Therefore, the phases of the different contributions within this range of \( p \) are rapidly varying and their sum cancels out. The only remaining survivors come from the stationary phases \( p \simeq m(x - q_0 - \text{arg}'(T(p)))/t \) or \( p \simeq m(-y - q_0 - \text{arg}'(R(p)))/t \). These contributions have still to be weighted by the different remaining factors, thus giving rise to the observed probability distributions, in which \( p \) is a function of \( t \), and depends parametrically on \( x, (y) \) and \( q_0 \) according to the above relations. To illustrate the result of this mechanism, it is enough to point out the approximate relation \( P_{t_\rightarrow}(t|y) \propto \sin^2(\sqrt{p_0(t)^2 - k_v^2}) \exp(-2\delta^2(p_0(t) - p_0)^2) \) with \( p_0(t) = m(-y - q_0 - \text{arg}' R(p_0))/t \), as the main responsible of the two bump structure.

We now recall that the \( \text{toa} \) of incoming states can be described with the same formalism used above. It is now necessary to project on the subspace of incoming states using \( \Pi(Es(+)) \). The physical picture here is a detector placed before the barrier to intercept these states. There are two opposite incoming directions. Mathematically, they are selected by the two projectors \( \Pi(Er(+)) \) (for detecting right movers at the left of the barrier), or \( \Pi(El(+)) \) (for left movers at the right). We choose as an example the first of these cases. The probability amplitude in times of arrival at \( y \) of the incoming states is:

\[
\langle t_{ys}|P_{t_\rightarrow}^E(+)|\psi\rangle = \int dE \langle t_{ys}|Er(+))\langle Er(+)|\psi\rangle
\]

Now, instead of (51), we have

\[
\langle Er(+)|\psi\rangle \simeq \sqrt{\frac{m}{p}} (\psi(p) + R^*(p) \tilde{\psi}(-p))
\]

As occurred for reflection, there are two potentially interfering terms, due to the lack of discrimination between the direct incoming component and the receding part of the reflected component. However, only the first term will give a sizeable contribution when the negative momentum tails are negligible. It is worth noting that the direct component gives the same time of arrival distribution that in the absence of barrier, as it should be on physical grounds. In the stationary phase approximation, the peak of the distribution is on the classical \( \text{toa} \): \( t = m(y - q_0)/p_0 \), as expected. This also gives the meaning of the negative \( \text{toa} \)'s [4]: they are obtained when the detector is placed to the left of the incoming right mover, so that the particle would have arrived at it before \( t = 0 \). Finally, we note that the probability amplitude of incoming states at a point \( x \) to the right of the barrier would be proportional to the receding part of the transmitted state.
We now restore the \((\pm)\) labeling that should be explicitly included in the \(toa\) formulation of Section 2, and that we ignored from Eq. (18) on. By doing it, instead of the equations (27,59) at the end of that section we would arrive to

\[
\hat{t}_x(\pm) = \sum_s \int_{-\infty}^{+\infty} dt \, |txs(\pm)\rangle \langle txs(\pm)|,
\]

with the position dependent eigenstates given by

\[
|txs(\pm)\rangle = \frac{1}{\sqrt{2\pi}} \int_0^{+\infty} dE \exp(iEt - isx\sqrt{2mE})|Es(\pm)\rangle.
\]

We thus see that many of the physical considerations made in this section in order to obtain the probability distributions in \(toa\) are automatically taken into account by the formalism. Instead of Eq. (40) we would get directly

\[
P_r(\pm)(t|x) = \frac{1}{N_r^{\pm}} \left| \langle txr(\pm)|\psi\rangle \right|^2
\]

and similar abridged (but fully equivalent) expressions in analogous cases. We recall from a formal point of view, that there are two possible constructions of \(t(\pm)\) starting from the free \(toa\), as there are two constructions of the stationary scattering states \(|Es(\pm)\rangle\) starting from the free states \(|E_0\rangle\). Even if each of these, \(t(+)\) or \(t(-)\), is associated to a kind of asymptotic state, \(in\) or \(out\) respectively, nowhere in the construction have we imposed or used any asymptotic value for \(x,y,t\) or for any other quantity in the problem. It is the finite extension of the barrier the only responsible for the simple asymptotic looking of our expressions. We used this to discuss the physical questions with a minimum of burden.

5 Conclusions

We have worked out a formalism for obtaining the time of arrival at a space point of particles that move through interacting environments. Our construction follows a circuitous path; we desist from first computing the classical \(toa\) of the problem, and then quantize it, a procedure that leads to a dead end. Instead, we start from the quantum \(toa\) of the free moving particle, and then transform it canonically to the interacting case. This is achieved by the use of the appropriate Möller operators, that we employ in a nonstandard, but orthodox, setting. Usually, they are introduced to connect the values (at \(t = 0\)) of those free and scattering states that will coincide asymptotically (at \(t \to \pm\infty\), depending on the case). Here, we first derive them from the connection between the free and interacting Hamiltonians, and then use them to connect the free and interacting \(toa\)'s, which solves our problem. For simplicity, we have only addressed explicitly the cases in which the transformations are unitary. The well known results from formal scattering theory pave the way to the general cases that require isometric transformations.

We have also performed a quite exhaustive (and a bit heavy) analysis of the relation between classical trajectories and scattering states. We found necessary to delve into the parallelism between the partitions of classical phase space by means of \(in\) or \(out\)
trajectories on the one side, and the spans of the Hilbert space by means of the (+) or
(−) states on the other. The right appreciation of the different issues involved in that
correspondence was necessary for a successful use of the formalism previously developed.
At the end, we reached the conclusion that this formalism did incorporate from the outset
these subtleties. In fact, for the asymptotically vanishing potentials considered here we
obtain two different operators \( t(+) \) and \( t(−) \). They measure the \( t_{oa} \) at a space point of
the incoming and outgoing states respectively.

In the course of our numerical analysis we have detected that the phase time \( \tau_ϕ \) gives
a good approximation to the most probable time of arrival. It provides a first estimate
of the time spent in the transmission or reflection, after subtracting the time of free
flight. We have found advancement of the transmitted wave packet in the case of pure
quantum tunneling. This is a long known phenomenon first predicted by Hartman [13],
and experimentally evinced by the two photon experiments at Berkeley [17, 18]. We have
found an unexpected phenomenon for purely quantum reflection: the two bump structure
that appears when \( \rho'_0 a = n \pi \). We have shown it only in one case in Fig. 3, which by
no means is the most crisp case. Neat double humps appear in all the expected cases,
the lesser the potential barrier the finer the feature. With the insight provided by our
formalism, we have also proposed an explanation to this structure. We think this feature,
even if less spectacular than the superluminal tunneling of photons, deserves experimental
confirmation. A minor modification of the two photon experiment could serve for this
purpose. It would be enough to place a quantum mirror in the path of one of the entangled
photons, and check for the presence (or absence) of a two dip structure in the number of
coincidence counts.

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Figure 1: Alternative partitions of the phase space plane \((q, p)\) in terms of the trajectories of particles with Hamiltonian \(H(q, p) = p^2/2m + V/\cosh^2(q/d)\). The trajectories of incoming right movers \(r(+)\) are above the separatrix \(p = p_V(q)\), and those of incoming left movers \(l(+)\) below it, both in the upper figure. The trajectories of outgoing right movers \(r(-)\), and left movers \(l(-)\) are respectively above and below \(p = -p_V(q)\) in the lower figure. The notation is borrowed from that of the stationary scattering states.
Figure 2: Most probable time of arrival and phase times for transmission through barriers of different heights and widths. Times are represented on the vertical axis against the barrier width ranging from 0 to 10. The initial wave packet (c.f. Eq. (39)) has $q_0 = -50$, $p_0 = 2$, $\delta = 10$ and $m = 1$. The detector is at $x = 50$. These parameters are fixed, so that the classical $toa$ for free propagation is 50 in all cases, (with our packet, we get the most probable $toa$ at $t_0 = 49.9377$ quantum mechanically). We show our results for the most probable $toa$ with triangles, squares, pentagons, and crisscrosses, corresponding to barrier heights of $V = 0.5, 1.125, 3.125, \text{and} 4.5$ respectively. The curves represent “$t_0 + Wigner \text{ time delay}$” for these same heights, (being the solid one for $V = 4.5$, etc). The plots neatly indicate retardation when transmission is classically possible, and advancement for pure quantum tunneling.
Figure 3: Probability distributions in times of arrival for transmission (above) and reflection (below), corresponding to equations (40) and (54). The initial wave packet is in all cases the same of Fig.(3). The total length of the particle’s path is always 100 units, so that the classical free $\text{toa}$ is 50. The width of the barrier is $a = 10$. The solid line represents free transmission, the short dashes the cases with $V = 1.125$, and the long ones those with $V = 4.5$. The two bump structure is a general result in the cases where there is no classical reflection as explained in the text.