Characteristic times in one dimensional scattering

J. G. Muga
Departamento de Química-Física, Universidad del País Vasco, Apdo 644, Bilbao, Spain

This chapter reviews several quantities that have been proposed in scattering theory to characterize the temporal aspects of one dimensional collisions: the dwell time, the delay time, the decay time, and times characterizing transient effects or the attainment of stationary conditions. Some aspects of tunnelling times are also discussed.

I. INTRODUCTION

Quantum scattering theory deals with collisions, namely, interactions which are essentially localized in time and space. This means that the interaction potential must vanish rapidly enough in coordinate space, so that the wave packet tends to free-motion incoming and outgoing asymptotic states before and after the interaction is effective. The scope of scattering theory also includes “half-collisions” or “decay processes” where the stage before the collision is ignored, i.e., the evolution of the system is only considered from the interaction region.

This chapter reviews various quantities that have been proposed in scattering theory to characterize the temporal aspects of the collision. A quantum wave packet collision with a potential barrier in one dimension (1D) is fully described by the evolution of the wave function \( \psi(x,t) \) from the incoming to the outgoing asymptotic states. However, the whole information contained in \( \psi(x,t) \) is hardly required. A few well chosen quantities are often enough to provide a fair picture of the dynamics. In particular, one of these elementary parameters is the transmission probability \( P_T \), but to describe the time dependence we also need to quantify the duration of the collision, the arrival time at a detector, the decay time of an unstable state, the asymptotic behaviour at short and large times, or response times, such as the time required to “charge” a well or achieve stationary conditions when a source is turned on.

In spite of the inherent time dependence of collisions, the treatises on quantum mechanics or scattering theory concentrate on solutions of the time-independent Schrödinger equation. This is in part because many scattering experiments to obtain cross sections are performed in quasi-stationary conditions, and also because the stationary scattering states form a basis to analyze the actual time dependent collision. In many cases wave packet scattering is relegated to justify the cavalier obtention by stationary methods of cross section expressions, and occasionally to discuss resonance lifetimes. Another widespread limitation is the exclusive interest in the final results of the collision at asymptotic distances and times, which has been generally justified because “the midst of the collision cannot be observed”. However, while it is true that in many collision experiments only the asymptotic results are observed, modern experiments with femtosecond laser pulses or other techniques known as “spectroscopy of the transition state” do probe the structure and the evolution of the collision complex. Also, in quantum kinetic theory of gases, accurate treatments must abandon the “completed collision” approximation and use a non-asymptotic description, e.g. in terms of Möller wave operators instead of \( S \) matrices, as in the Waldmann-Snider equation and its generalizations for moderately dense gases.

The theory has to adapt to these new trends by paying more attention to the temporal description of the collisions. Even if we restrict ourselves to asymptotic aspects, the cross section does not contain the whole information available in a scattering process, since it is only proportional to the modulus of the \( S \)-matrix elements. Information on the phase is available from delay times with respect to free motion. In fact, the full collision and not just the asymptotic regimes should be understood to control or modify the products. This has motivated a recent trend of theoretical and experimental work to investigate the details of the interaction region and transient phenomena.

In this chapter we restrict ourselves to one dimensional scattering. Many physical systems can be described in one dimension: the application of the effective mass approximation to layered semiconductor structures leads to effective one dimensional systems; some surface phenomena are described by 1D models; and chemical reactions can in certain conditions be modelled by effective one dimensional potentials. The simplicity of 1D models have made them valuable as pedagogical and research tools. They facilitate testing hypothesis, new ideas, approximation methods and theories without unnecessary and costly complications. For the same reasons they are frequently used to examine fundamental questions of quantum mechanics. In particular, the time quantities treated in this book, such as tunneling or arrival times, have in most cases been examined in one dimensional models. Many results for 1D are inspired by results previously obtained in 3D, although the direct translation is not always trivial or possible.

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collisions with spherically symmetric potentials are described, by decomposition into partial waves, on the half line, whereas 1D collisions involve the full line and a doubly degenerate spectrum.

The chapter is organized as follows: Section 2 provides a minimal overview of formal 1D scattering theory. The treatment is “formal” because no mathematically rigorous proofs are given. Instead, we summarize the operator structure of the theory and the results needed to define characteristic times later on. For a more rigorous mathematical presentation see e.g. [6]. Sections 3, 4 and 5 are devoted, respectively, to the dwell time, the delay time, and decay times (the exponential decay and its deviations). Quantities related to the tunneling time conundrum are scattered in several parts of the book. In particular, sections 4.1 and 4.6 discuss the Hartman effect and negative delays, while section 6 discusses the role of the Buttiker-Landauer “traversal time” in the time dependence of evanescent waves. A detailed discussion of the arrival times is left for Chapter ......

II. SCATTERING THEORY IN 1D

A. Basic premises and notation

Let $H = H_0 + V$ be the Hamiltonian operator for a single particle in one dimension, where

$$H_0 = \frac{p^{2}_{\text{op}}}{2m}$$

is the kinetic energy operator in terms of the momentum operator $p_{\text{op}}$, and $V$ is a “local” potential operator with coordinate representation

$$\langle x | V | x' \rangle = \delta(x - x') V(x) .$$

$V(x)$ must vanish for large values of $|x|$ so that the Möller operators, defined below, exist. This may certainly be accomplished by finite range potentials, but spatial decays with infinite tails are also possible.

The plane waves $|p\rangle$, with coordinate representation given by

$$\langle x | p \rangle = \frac{1}{\sqrt{2\pi}} e^{ixp/\hbar},$$

are improper eigenstates of $p_{\text{op}}$ and $H_0$, normalized according to Dirac’s delta function,

$$\langle p | p' \rangle = \delta(p - p').$$

Closure relations (or resolutions of the unit operator $1_{\text{op}}$) may therefore be written in momentum or coordinate representation as

$$1_{\text{op}} = \int_{-\infty}^{\infty} dx |x\rangle \langle x| = \int_{-\infty}^{\infty} dp |p\rangle \langle p| .$$

B. Basic abstract and parameterized operators.

The state vector of the particle at time $t$ is denoted as $|\psi(t)\rangle$ or simply as $\psi(t)$. We shall only deal with potentials such that at large times in the past and future certain states $\psi$, the scattering states, tend (in a strong sense) to freely moving asymptotic states $\phi_{\text{in}}$ and $\phi_{\text{out}}$ respectively,

$$\psi(t) \rightarrow \phi_{\text{in}}(t), \quad t \rightarrow -\infty ,$$

$$\psi(t) \rightarrow \phi_{\text{out}}(t), \quad t \rightarrow \infty .$$

1The subscript “op”, meaning “operator”, is not used for all quantum operators, but only when confusion is possible with ordinary numbers or functions.

2i.e., not in the Hilbert space of square integrable states.
The central objects in scattering theory are the abstract Möller operators. They link the asymptotic states with \( \psi, \)

\[
\psi(t) = \Omega_+ \phi_{in}(t) , \\
\psi(t) = \Omega_- \phi_{out}(t) .
\]

Another important operator is

\[
S = \Omega_+^\dagger \Omega_+ ,
\]

which links the two asymptotes,

\[
\phi_{out}(t) = S \phi_{in}(t) .
\]

It is also convenient to introduce the auxiliary “transition” operators \( T_\pm \) as

\[
T_\pm = V \Omega_\pm .
\]

The explicit definition of the Möller operators is given by infinite-time (strong) limits,

\[
\Omega_\pm = \lim_{t \to \pm \infty} e^{iHt/\hbar} e^{-iH_0 t/\hbar} .
\]

The domain of these operators is the Hilbert space of square integrable states, although it is very useful to consider an extension that can be applied on plane waves and allows to work in a momentum representation. To this end let us first define the parameterized operators

\[
\Omega(z) = 1 + G_0(z) T(z) , \\
T(z) = V + V G(z) V ,
\]

where \( z \) is a complex variable with dimensions of energy, and \( G(z) = (z - H)^{-1} \) and \( G_0(z) = (z - H_0)^{-1} \) are the resolvents of \( H \) and \( H_0 \). \( T(z), V, G(z) \) and \( G_0(z) \) are also related by

\[
G(z) = G_0(z) + G_0(z) T(z) G_0(z) \\
T(z) G_0(z) = V G(z) .
\]

We shall see that the matrix elements of the resolvents in coordinate representation are singular on the real positive axis, where there is a branch cut, and at poles on the negative real axis (bound states). Further singularities may occur by analytical continuation on the second energy sheet.

Note that the operators of scattering theory have abstract or parameterized versions \[8\]. Confusion may arise if they are not properly distinguished. The relation between abstract and parameterized operators is found by acting with \( (13) \) on a square integrable state. The resulting infinite-time limits can be substituted by the following limits, see e.g. \[8\],

\[
\Omega_\pm = \lim_{\varepsilon \to 0^+} \varepsilon \int_{-\infty}^0 dt e^{\varepsilon t} e^{iHt/\hbar} e^{-iH_0 t/\hbar} ,
\]

\[
\Omega_- = \lim_{\varepsilon \to 0^+} \varepsilon \int_0^\infty dt e^{-\varepsilon t} e^{iHt/\hbar} e^{-iH_0 t/\hbar} .
\]

Integrating, and introducing a closure relation in momentum,

\[
\Omega_\pm = \int_{-\infty}^\infty dp \Omega(E_p \pm i0) |p\rangle \langle p| ,
\]

\[
T_\pm = \int_{-\infty}^\infty dp T(E_p \pm i0) |p\rangle \langle p| .
\]

The action of these operators on plane waves is now well defined. In particular, the improper eigenvectors of \( H \) are obtained by acting with the parameterized Möller operators on the plane waves,

\[
|p^\pm\rangle = \Omega(E_p \pm i0) |p\rangle = |p\rangle + \frac{1}{E_p \pm i0 - H_0} T(E_p \pm i0) |p\rangle .
\]
where \( E_p = p^2/(2m) \) is the energy of the plane wave and of the corresponding eigenstate of \( H \). This is the Lippmann-Schwinger integral equation for the states \(|p^\pm\rangle\), which are composed by a “free” plane wave and a “scattering” wave. To evaluate the coordinate representation and the asymptotic behaviour of the states at large distances, the matrix elements of the free-motion resolvent are required,

\[
\langle x'|p^\pm\rangle = \pm \frac{i m}{\hbar |p|} e^{\pm i |p|x'-x'|/\hbar}.
\]  

(23) is obtained by introducing a resolution of unity in momentum representation and using contour integration in the complex momentum plane. Note that the two ways of approaching the real axis in (23), from below or from above, imply different boundary conditions at large \(|x|\) for the two states in (23): the scattering wave of \(|p^+\rangle\) is formed by outgoing plane waves moving off the potential region, whereas the scattering wave of \(|p^-\rangle\) involves incoming plane waves towards the potential region.

Since the plane waves \(|p\rangle\) form a complete set, the following resolutions of the operators \( \Omega \), \( T \) and \( S \) can be introduced,

\[
\Omega_\pm = \int_{-\infty}^{\infty} dp \langle p^\pm|p\rangle, \quad \Omega^\dagger_\pm = 1_{\text{op}}. \tag{24}
\]

\[
T_\pm = V \int_{-\infty}^{\infty} dp \langle p^\pm|p\rangle, \quad T^\dagger_\pm = 1_{\text{op}}. \tag{25}
\]

\[
S = \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dp' \langle p'|p\rangle \langle p^\pm\rangle, \quad S^\dagger = 1_{\text{op}}. \tag{26}
\]

Strictly speaking, the operators in (24-26) are not identical to the ones in (10,12,13) since the domain of the former includes plane waves. However, when acting on Hilbert space states they are equivalent so that, to avoid a clumsy notation, the same symbols will be used. A momentum representation is therefore allowed for these operators, which in general involves distributions (generalized functions such as Dirac’s delta or Cauchy’s principal part).

For real potential functions \( V(x) \) the norm is conserved throughout the collision, \( \langle \phi_{\text{in}}|\phi_{\text{in}}\rangle = \langle \psi|\psi\rangle = \langle \phi_{\text{out}}|\phi_{\text{out}}\rangle \). This means that the Möller operators are isometric, i.e.,

\[
\Omega^\dagger_\pm \Omega_\pm = 1_{\text{op}}. \tag{27}
\]

As a consequence,

\[
\langle p^\pm|p'^\pm\rangle = \delta(p - p'). \tag{28}
\]

In general the Möller operators are not unitary because the bound states are not in their range. Contrast this to the the operator \( S \): it conserves the norm too, but it is unitary because it maps the whole Hilbert space onto the whole Hilbert space,

\[
SS^\dagger = S^\dagger S = 1_{\text{op}}. \tag{29}
\]

The scattering states \( \psi \) with incoming and outgoing asymptotes move far away from the potential so they are orthogonal to the bound states \( \{|\Phi_j\rangle\} \) at large (positive or negative) times. Since the overlap amplitude \( \langle \psi|\Phi_j\rangle = 0 \) is independent of time, the space of bound states \( \mathcal{B} \) is orthogonal to the scattering states, namely to the range of the Möller operators. We shall always assume that the ranges of the two Möller operators are equal to the subspace of scattering states \( \mathcal{R} \), and that the whole Hilbert space is the direct sum of the subspaces spanned by scattering and bound states, \( \mathcal{H} = \mathcal{R} \oplus \mathcal{B} \). This assumption is known as asymptotic completeness,

\[
\Omega^\dagger_\pm \Omega_\pm = 1_{\text{op}} - \Lambda = \int_{-\infty}^{\infty} dp \langle p^\pm|p\rangle. \tag{30}
\]

In this expression the “unitary deficiency” \( \Lambda \) is the projector onto the subspace of bound states,

\[
\Lambda = \sum_j |\Phi_j\rangle\langle \Phi_j|. \tag{31}
\]

Taking matrix elements in (26), the momentum representation of \( S \) is given by

\[
\langle p|S|p'\rangle = \delta(p - p') - 2i \pi \delta(E_p - E_p') \langle p|T(E_p + i0)|p'\rangle. \tag{32}
\]
The collision conserves the energy, which is, asymptotically, kinetic energy. That is why $S$ commutes with $H_0$ and its matrix elements are proportional to an energy delta function. It is quite useful to factor out this delta function to define an on-the-energy-shell $S(E)$ matrix. Using

$$
\delta(p - p') = \frac{|p|}{m} \delta(E_p - E'_p) \delta_{pp'},
$$

where $\delta_{pp'}$ is the Kronecker delta,

$$
\delta_{pp'} = \begin{cases} 
1 & \text{if } p = p' \\
0 & \text{if } p \neq p',
\end{cases}
$$

and defining the matrix elements of $S$, $S_{\alpha\beta}$, by

$$
(p|S|p') = |p|m^{-1} \delta(E_p - E'_p) S_{\text{sign}(p)\text{sign}(p')} (E_p),
$$

one finds

$$
S_{\text{sign}(p)\text{sign}(p')} (E_p) = \delta_{pp'} - \frac{2i\pi m}{|p|} (p|T(E_p + i0)|p') , \quad |p| = |p'|.
$$

The subscripts $\alpha, \beta = \pm$ in the matrix elements $S_{\alpha\beta}$, denote the two possible “channels”, which correspond to positive (+) or negative (−) momentum. A difference between the one dimensional scattering on the full line ($-\infty < x < \infty$) and radial scattering on the half line, ($0 < r < \infty$) is that in the former, the $S$ matrix is a unitary $2 \times 2$ matrix while in the later is a complex number of unit modulus.

C. Symmetries

1. Time reversal invariance.

This symmetry holds for real potentials. It implies

$$
S_{\alpha\beta} = S_{-\beta - \alpha}.
$$

2. Parity.

Frequently the potentials are symmetrical with respect to its central position. In that case,

$$
S_{\alpha\beta} = S_{-\alpha - \beta}.
$$

D. Eigenstates of $H$

The eigenstates of $H$ given by the Lippmann-Schwinger integral equations (22) behave asymptotically as a combination of two plane waves with positive and negative momenta. The factors multiplying these plane waves are the reflection and transmission amplitudes according to the following table for asymptotic, long-distance behavior (assume for the time being that $p > 0$)

$$
\frac{1}{\hbar^{1/2}} \begin{cases} 
\exp(ipx/\hbar) + R^t(p) \exp(-ipx/\hbar), & \text{if } x -\infty \\
T^t(p) \exp(ipx/\hbar), & \text{if } x -\infty,
\end{cases}
$$

$$
\frac{1}{\hbar^{1/2}} \begin{cases} 
T^r(p) \exp(-ipx/\hbar), & \text{if } x -\infty \\
\exp(-ipx/\hbar) + R^r(p) \exp(ipx/\hbar), & \text{if } x -\infty.
\end{cases}
$$

For potentials of finite range that vanish outside $[a, b]$ these are in fact exact expressions for $x < a$ and $x > b$. 

5
If \( p > 0 \), the boundary conditions in (39) define the states \( \langle x | p^+ \rangle \) corresponding to an \textit{incoming} plane wave from the left, \( \langle x | p \rangle \), while the boundary conditions in (40) define the states \( \langle x | (-p)^+ \rangle \) corresponding to an \textit{incoming} plane wave from the right, \( \langle x | -p \rangle \). \( T(p) \) and \( R(p) \), with superscripts \( l \) or \( r \) for right or left incidence, are the transmission and reflection amplitudes. A wave packet peaked around a given \( |p^+\rangle \) would be dominated by the plane wave \( |p\rangle \) before the collision, whereas, after the collision, there would be two packets, one reflected and one transmitted with probabilities \( |R(p)|^2 \) and \( |T(p)|^2 \), dominated by \( | -p \rangle \) and \( |p\rangle \) respectively, see e.g. 3.

For \( p < 0 \), however, the states determined by (39) and (40) correspond, respectively, to \( \langle x | p^- \rangle \), with \textit{outgoing} plane wave \( \langle x | p \rangle \), and \( \langle x | (-p)^- \rangle \), with \textit{outgoing} plane wave \( \langle x | -p \rangle \). A wave packet formed around \( |p^-\rangle \) would be close to a plane wave \( |p\rangle \) only \textit{after} the collision occurs. To form this peculiar outgoing state, the incoming asymptote must combine waves incident from both sides of the potential barrier. This may of course be difficult to implement in practice, but it does not preclude the usefulness of these states as basis functions, and in general for applications where some control or selection of the products of the collision is required.

The previous discussion should make clear that \( T(p) \), for \( p < 0 \), is \textit{not} a standard transmission amplitude, because it \textit{is} the amplitude of the transmitted plane wave of the state \( |p^+\rangle \), \( p < 0 \). However, it analytically continues the standard transmission amplitude \( (T(p) \text{ for } p > 0) \) onto the \( p < 0 \) domain, so the term “transmission amplitude” will be used irrespective of the sign of \( p \), even though the physical meaning is different for the two possible signs. According to our notational convention, positive arguments of the amplitudes correspond always to states \( |p^+\rangle \), while negative momentum arguments correspond to \( |p^-\rangle \) states.

E. Relation between scattering amplitudes and basic operators

Comparing the asymptotic (large \( |x| \)) behaviour of the states in (39) and (40) with the asymptotic behaviour in (23), the amplitudes \( R(p) \) and \( T(p) \) can be related to on-the-energy-shell elements of the transition matrix. We shall work out one case in detail: the scattering part of \( \langle x | p^+ \rangle \) for \( p > 0 \) and \( x \rightarrow \infty \) is

\[
\int_{-\infty}^{\infty} dx' \langle x | G_0(E_p + i0) | x' \rangle \langle x' | T(E_p + i0) | p \rangle \\
= -\frac{2\pi m_i e^{i\pi x/h}}{h} \int_{-\infty}^{\infty} e^{-i\pi x'/h} | x' \rangle \langle T(E_p + i0) | p \rangle \\
= -\frac{2\pi m_i}{p} \langle x | p \rangle \langle p | T_+ | p \rangle.
\]

Adding the free wave, \( h^{-1/2} e^{i\pi x/h} \), and comparing with (39), there results \( T^l(p) = 1 - 2i\pi m \langle p | T_+ | p \rangle / p \) for \( p > 0 \). The rest of the cases can be worked out similarly (Because of time reversal invariance, \( \langle p | T_\pm | p \rangle = \langle -p | T_\pm | -p \rangle \), and \( T^r(p) = T^l(p) \). Therefore the superscript for the transmission amplitude will be dropped hereafter):

\[
T(p) = 1 - \frac{2i\pi m}{p} \langle p | T_{\rm sign(p)} | p \rangle, \\
R^l(p) = -\frac{2m\pi}{p} \langle -p | T_{\rm sign(p)} | p \rangle, \\
R^r(p) = -\frac{2m\pi}{p} \langle -p | T_{\rm sign(p)} | -p \rangle.
\]

Some useful relations follow from (12),

\[
[T(-p)]^* = T(p), \quad p \text{ real.} \\
R^{\pm,l}(-p)^* = R^{\pm,l}(p), \quad p \text{ real.}
\]

From (39) and (40), the \( S \) matrix is given by

\[
S(p) \equiv S(E) = \begin{pmatrix} T(p) & R^r(p) \\ R^l(p) & T(p) \end{pmatrix}, \quad p > 0.
\]
It is quite useful to consider $S$ as a (matrix) function of $p$. In simple applications we only use $S(p)$ with $p > 0$, but in fact we may also define $S(p)$ for $p < 0$ or even for complex $p$ in terms of the analytical continuations of the amplitudes $T(p)$, $R^r(p)$, and $R^l(p)$. This extension will be discussed in sec. I.G.

F. The diagonal $S_d$ matrix

The $S$ matrix (52) has been obtained from the momentum representation of $S$ using plane waves incident form one side, $|±p\rangle$, but other on-shell matrices may be defined in terms of a different basis formed by combinations of $|±p\rangle$. Of particular interest is the set $|u_j\rangle$, $j = 0, 1$, that provides a diagonal matrix

$$S_d(p) = \begin{pmatrix} S_0(p) & 0 \\ 0 & S_1(p) \end{pmatrix}.$$  \hspace{1cm} (46)

Unitarity implies that $|S_j| = 1$, so the matrix elements may be written in terms of real eigenphase shifts $\delta_j$, $S_j = e^{2i\delta_j}$. The $|u_j\rangle$ are not mixed by the collision; these incident states produce an outgoing combination equal to the incident one, except for a phase factor. The diagonal $S_d$ matrix is most advantageous for parity invariant potentials, since the linear combinations become simply even and odd wavefunctions,

$$|u_0\rangle = 2^{-1/2}(|p\rangle + |−p\rangle), \hspace{1cm} (47)$$

$$|u_1\rangle = 2^{-1/2}(|p\rangle − |−p\rangle). \hspace{1cm} (48)$$

From the asymptotic behaviour of $|u_j^\pm\rangle = \Omega_+|u_j\rangle$ and $|±p^+\rangle$ we may relate reflection and transmission amplitudes for even potentials to the eigenphase shifts,

$$R(p) = 2^{-1} \left(e^{2i\delta_0} − e^{2i\delta_1}\right), \hspace{1cm} (49)$$

$$T(p) = 2^{-1} \left(e^{2i\delta_0} + e^{2i\delta_1}\right). \hspace{1cm} (50)$$

(Eq. (54) is in fact valid for arbitrary potentials.) The boundary conditions for the states $|u_j^+\rangle$ are

$$\lim_{x \to -\infty} \langle x|u_0^+\rangle = e^{i\delta_0} \left(\frac{2}{\hbar}\right)^{1/2} \cos(px/\hbar + \delta_0),$$

$$\lim_{x \to -\infty} \langle x|u_1^+\rangle = e^{i\delta_0} \left(\frac{2}{\hbar}\right)^{1/2} \cos(px/\hbar + \delta_0),$$

$$\lim_{x \to \infty} \langle x|u_0^+\rangle = ie^{i\delta_1} \left(\frac{2}{\hbar}\right)^{1/2} \sin(px/\hbar − \delta_1),$$

$$\lim_{x \to \infty} \langle x|u_1^+\rangle = ie^{i\delta_1} \left(\frac{2}{\hbar}\right)^{1/2} \sin(px/\hbar + \delta_1). \hspace{1cm} (51)$$

It will be convenient for later manipulations to drop the constant complex phase factors and define real eigenfunctions of $H$ as

$$\langle x|\psi_0\rangle = e^{-i\delta_0} \langle x|u_0^+\rangle,$$

$$\langle x|\psi_1\rangle = ie^{-i\delta_1} \langle x|u_1^+\rangle. \hspace{1cm} (52)$$

3Keep in mind that $p > 0$ in the arguments of $S$ or of the scattering amplitudes does not mean “incidence from the right”. According to the sign convention described in I.F, it means that the amplitudes correspond to states with outgoing scattering parts: $|p^+\rangle$ for right incidence, and $|−p^+\rangle$ for left incidence.
G. Complex momentum

The properties of $T(p)$ as a function of the complex momentum $p$ are of importance for many applications. Let the potential function $V(x)$ be such that

$$\int_{-\infty}^{\infty} dx \, |V(x)|(1 + x^2) < \infty.$$  

(53)

Then $T(p)$ is meromorphic in $\text{Im} \, p > 0$ with a finite number $n_b$ of simple poles $i\beta_1, i\beta_2, \ldots, i\beta_n$, $\beta_j > 0$, on the imaginary axis. The numbers $-\beta_j^2/(2m)$ are the eigenvalues of $H$. Moreover,

$$T(p) = 1 + O(1/p) \quad \text{as} \quad |p| \to \infty, \quad \text{Im} \, p \geq 0,$$  

(54)

and there can only be a zero at the real axis, at $p = 0$,

$$|T(p)| > 0 \quad \text{Im} \, p \geq 0, \quad p \neq 0.$$  

(55)

In the generic case $T(0) = 0$, and

$$T(p) = \gamma p + o(p), \quad \gamma \neq 0, \quad \text{as} \quad p \to 0, \quad \text{Im} \, p \geq 0.$$  

(56)

Since $T(p)$ is meromorphic and it does not have zeros in the upper plane, the integral

$$\frac{1}{2\pi i} \int_{\mathcal{A}} dp \, \frac{d\ln T(p)}{dp} = -n_b$$  

(57)

along the contour $\mathcal{A}$ consisting of $[-R, -\epsilon]$, $[\epsilon, R]$, a semicircle of radius $\epsilon$ around the origin, and a large semicircle of radius $R$ in the upper half-plane, provides, according to a theorem of complex plane integration, the number of zeros (none in this case) minus the number of poles of $T(p)$ enclosed (the bound states). The integral may also be evaluated using (43), (54), and (56); this gives $2i\Phi_T(R) - 2i\Phi_T(\epsilon) - i\pi$, where $\Phi_T(p)$ is the phase of $T$,

$$T(p) = |T(p)| \exp(i\Phi_T).$$  

(58)

Combining the two results,

$$\Phi_T(0) - \Phi_T(\infty) = \pi(n_b - 1/2),$$  

(59)

which is Levinson’s theorem for the case $T(p = 0) = 0$. Otherwise, there is no $-i\pi$ contribution from the small semicircle and the phase difference becomes just $\pi n_b$. The convention followed is that $\Phi_T(\infty) = 0$, so the theorem establishes the value of $\Phi_T(0)$.

The possibility to continue analytically $T(p)$ to the lower half plane will depend on the potential considered [10]. Here we shall assume that the continuation can be performed (this is the case for example for potentials of finite range) and discuss the properties that these continuations must obey. From $T^l(z) = T(z^*)$ and the relations (52) we find

$$(R^{r,l}(p))^* = R^{r,l}(-p^*),$$  

(60)

$$(T(p))^* = T(-p^*),$$  

(61)

so that if there is a pole of $T(p)$ in the fourth quadrant at $p_R - ip_I$ ($p_R, p_I > 0$), there must be also a pole in the third quadrant at $-p_R - ip_I$. For an isolated pole, and if $p_I$ is small, the phase of $T(p)$ along the positive real line will increase rapidly by $\pi$. From (50) we see that poles of $T(p)$ are generally poles of $S_0$ or of $S_1$. Since $|T(p)| = |\cos(\delta_0 - \delta_1)|$, if the resonance eigenphase shift also jumps by $\pi$, while the other one remains approximately constant, the transmission probability along the real axis will pass across a maximum (1), or a minimum (0), or both, depending on the initial phase difference of the two eigenphase shifts. The above simplified picture will be blurred if the resonances are very close to each other, or the pole is far from the real line.
H. Unitarity and its consequences

The unitarity of the collision $S$ matrix, $SS^\dagger = S^\dagger S = 1$, reflects the conservation of norm in the collision. It provides two relations: from the diagonal elements,

$$|T(p)|^2 + |R^{r,l}(p)|^2 = 1,$$

(62)

and from non-diagonal ones,

$$T(p)[R^l(p)]^* + [T(p)]^* R^r(p) = 0, \quad p \text{ real}.$$

(63)

Eq. (63) leads to a relation for the phases,

$$2\Phi_T - \Phi_{R^r} - \Phi_{R^l} = (2n + 1)\pi, \quad n = 0, \pm 1, \pm 2, \ldots,$$

(64)

where, as in (58),

$$R^r,l(p) = |R^r,l(p)| e^{i\Phi_{r,l}(p)}.$$

(65)

III. A MEASURE OF THE COLLISION DURATION: THE DWELL TIME

In classical mechanics the quantity

$$\tau_D(a, b; t_1, t_2)_{\text{classical}} = \int_{t_1}^{t_2} dt \int_a^b dx \varrho(x, t),$$

(66)

where $\varrho(x, t)$ is the probability density of an ensemble of independent particles, is the average over the ensemble of the time that each particle trajectory spends between $a$ and $b$ within the time window $[t_1, t_2]$. In other words, this is an average "dwell" or "sojourn" time in the selected space-time region. Its formal quantum mechanical counterpart is

$$\tau_D(a, b; t_1, t_2; \psi) = \int_{t_1}^{t_2} dt \int_a^b dx |\psi(x, t)|^2.$$

(67)

In principle the coordinates $a, b > a$ and the instants $t_1$ and $t_2 > t_1$ are arbitrary but most often $a$ and $b$ are chosen so that $V(x)$ is zero or negligible for $x < a$ and $b > a$. Hereafter $t_1$ will be, by default, $-\infty$, or occasionally 0, an initial preparation time; and $t_2 = \infty$.

In spite of the formal similarity of the classical and quantum expressions, the interpretation of (67) as a “mean time” spent in the region $[a, b], [t_1, t_2]$ by quantum particles is not straightforward, since in the standard interpretation of the quantum mechanical formalism there are no trajectories and therefore there is no obvious way to assign a time (duration) of presence to a given member of the ensemble of particles associated with the quantum state. There are however several arguments that provide (67) by extending to the quantum case the classical dwell time, e.g. via Feynmann path integrals, causal or Bohm trajectories, or as an expectation value of a hermitian sojourn time operator, see also Chapter ... for an interpretation in terms of weak measurements. Irrespective of a hypothetical statistical interpretation of the dwell time in terms of individual members of the ensemble, the dwell time is at the very least a characteristic quantity of the ensemble represented by the state $\psi$, that quantifies the duration of the wave packet collision. For example, the dwell time is considered an important parameter in high speed applications of mesoscopic semiconductor structures.

$\tau_D$ can be written in several ways, in particular as

$$\tau_D = \tau_D(a, b; -\infty, \infty) = \int_{-\infty}^{\infty} dt P_{ab}(t) = \langle \psi(t = 0)|T_D|\psi(t = 0)\rangle.$$

(68)

---

4 The concept of a “dwell time” for a finite space region in the stationary regime is due to Buttiker. Previously, integrals of the form had been used to define time delays by comparing the free motion to that with a scattering center and taking the limit of infinite volume, see e.g.
where \( P_{ab}(t) = \int_a^b dx \, g(x, t) \), \( T_D \) is the *sojourn time operator*,
\[
T_D = \int_{-\infty}^{\infty} dt \, e^{iHt/\hbar} D(a, b)e^{-iHt/\hbar}, \tag{69}
\]
and \( D(a, b) \) is the projector onto the selected space region,
\[
D(a, b) = \int_a^b dx \, |x\rangle \langle x|. \tag{70}
\]

An experimental determination of the dwell time may be carried out by monitoring the time evolution of the probability inside the selected spatial region, \([18]\). This is admittedly an indirect route, where the first moment of \( T_D \), \( \tau_D \), is obtained without having measured individual dwell times for the members of the ensemble. It remains to be seen if second and higher moments of \( T_D \) may be associated with some simple operational procedure.

Let us now find other useful expressions for the dwell time. Integrating the continuity equation over \( x \) between \( a \) and \( b \), and over time between \( -\infty \) and \( t \), \( P_{ab} \) takes the form
\[
P_{ab}(t) = \int_{-\infty}^t dt' \left[ J(a, t') - J(b, t') \right] = \int_{-\infty}^t dt' \Delta J(a, b, t'), \tag{71}
\]
where \( J(x, t') \) is the current density, \( \Delta J(a, b) = J(a) - J(b) \), and the boundary condition \( P_{ab}(-\infty) = 0 \) has been assumed. Substituting (71) into (68), one finds
\[
\tau_D = \lim_{t \to \infty} \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' \Delta J(t''), \tag{72}
\]
Unless \( P_{ab}(t) \) decays faster than \( t^{-1} \), the dwell time will diverge. The existence of a potential function leads generically to an asymptotic decay \( \sim t^{-3} \), as discussed in section \([19]\). However, for free motion the dwell time will diverge unless the momentum wave function vanishes at \( b = 0 \), because of the dependence \( \sim t^{1/2} \) of the free motion propagator, see \([21]\) below and the related discussion. In terms of the sojourn time operator (69) for \( H_0 \), the possible divergence is due to a \(|p|^{-1} \) factor,
\[
T_{D,H_0} = \sum_{\alpha = \pm} \int_{-\infty}^{\infty} \frac{dp}{|p|} \frac{m\hbar}{|p|} |\langle p|D|\alpha p\rangle\rangle |\langle \alpha p|\rangle\rangle. \tag{73}
\]
In this and the following sections we shall limit ourselves in general to incoming asymptotes in the positive momentum channel (+) that vanish at \( p = 0 \), so that the dwell time for free motion does exist. This will allow to compare dwell times with and without potential and to define delay times. These states, with a bounded support in momentum space, have necessarily a Fourier transform in coordinate space that can only vanish at some set of points of measure zero. But this is not a problem since the total probability for positive positions tends to zero as \( t \to -\infty \),
\[
\lim_{t \to -\infty} \int_{-\infty}^{\infty} dx \, |\langle x|\phi_{in}(t)\rangle\rangle|^2 = \int_{-\infty}^{0} dp \, |\langle p|\phi_{in}(0)\rangle\rangle|^2 \tag{74}
\]
for any \( a \) and any \( \phi_{in} \) [4].

Assuming that \( tP_{ab}(t) \to 0 \) as \( t \to \infty \), the dwell time (58) takes the local form
\[
\tau_D(a, b) = \int_{-\infty}^{\infty} dt' \left[ J(b, t') - J(a, t') \right] t'. \tag{75}
\]

Other expression for states incident in the positive momentum channel may be obtained by using resolutions of the identity in terms of the states \(|p^+\rangle\rangle,
\[
\tau_D(a, b; \psi) = \int_{0}^{\infty} dp \, |\langle p|\phi_{in}(0)\rangle\rangle|^2 \tau_D(p), \tag{76}
\]

10
where
\[ \tau_D(a, b; p) \equiv \frac{\int_a^b dx \langle x \rvert p^+ \rangle^2}{p/mh}, \] (77)
which suggests the interpretation of \( \tau_D(a, b; p) \) as a dwell time for particles of definite momentum \( p \) [12].

Suppose now that \( a < 0 \) and \( b > 0 \) are both far from the barrier region, before and after the barrier respectively, so that the first passage of the wave packet across \( a \) can be described accurately in terms of the free motion asymptote \( \phi_{in} \), while the passage of the transmitted and reflected wave packets can be evaluated with the asymptotic expressions
\[
\psi_T(b, t) = \frac{1}{\sqrt{h}} \int_0^\infty dp \langle p \rvert \phi_{in}(0) \rangle T(p) e^{i(p_b-Et)/h}, \quad (78)
\]
\[
\psi_R(a, t) = \frac{1}{\sqrt{h}} \int_0^\infty dp \langle p \rvert \phi_{in}(0) \rangle R(p) e^{-i(p_a+E_t)/h}. \quad (79)
\]
(For a potential with support between \( 0 \) and \( d \), \( b = d \), but \( a \) cannot be 0, because of the strong interference between the incident and reflected parts. \( |a| \) should be much greater than the incident wave packet width in order to distinguish clearly the entrance passage from the reflected one.) Then,
\[
\int_{-\infty}^{\infty} dt' J_T(b, t') = \int_0^\infty dp \langle J(p) \rvert^2 \rangle \langle p \rvert \phi_{in}(0) \rangle^2 = P_T, \quad (80)
\]
\[
\int_{-\infty}^{\infty} dt' J_I(a, t') = \int_0^\infty dp \langle p \rvert \phi_{in}(0) \rangle^2 = 1, \quad (81)
\]
\[
\int_{-\infty}^{\infty} dt' J_R(a, t') = -\int_0^\infty dp \langle J(p) \rvert^2 \rangle \langle p \rvert \phi_{in}(0) \rangle^2 = -P_R, \quad (82)
\]
where the subscripts \( I, T \) and \( R \) in \( J_I, J_T \) and \( J_R \) mean that \( \phi_{in}, \psi_T \) and \( \psi_R \) have been used to calculate the fluxes. One can then write (73) as
\[
\tau_D = P_T \langle t \rangle_b^{\text{out}} - \langle t \rangle_a^{\text{in}} + P_R \langle t \rangle_a^{\text{out}}, \quad (83)
\]
where
\[
\langle t \rangle_b^{\text{out}} = \frac{\int_{-\infty}^{\infty} dt' J_T(b, t') t'}{\int_{-\infty}^{\infty} dt' J_T(b, t')} \quad (84)
\]
\[
\langle t \rangle_a^{\text{in}} = \frac{\int_{-\infty}^{\infty} dt' J_I(a, t') t'}{\int_{-\infty}^{\infty} dt' J_I(a, t')} \quad (85)
\]
\[
\langle t \rangle_a^{\text{out}} = -\frac{\int_{-\infty}^{\infty} dt' J_R(a, t') t'}{\int_{-\infty}^{\infty} dt' J_R(a, t')} \quad (86)
\]
In each case the “average passage instant” is obtained by properly normalizing the fluxes. One may rightly wonder whether the notation and terminology used (as average passage times) are justified. The “averages” are taken over the current density \( J \), a quantity that is not definite positive even for an incident wave packet without negative momentum components [20] [22]. It turns out, however, that the above “averages” over \( J \) are equal to averages over a positively defined arrival time distribution (Kijowski's arrival time distribution) [23], as will be discussed in Chapter ...

Models of detectors based on complex non-hermitian potentials lead also to these average times, delayed only by the small (dwell) time that the particle spends in the detector before being detected [24]. In the next section we shall relate these times to the “phase times”.

Finally, note that (81) could be, and has been, used to partition the dwell time into transmission and reflection components [4] [25], see also the closely related approach of Olkhovsky and Recami [26]. The main drawback is that the defined entrance average instant is common for both contributions, see [27] [28], which is not a correct in the classical ensemble limit, and may lead to negative transmission times [29] even in the classical case [27]. A two-detector model avoided this problem by assigning different entrance instants for each member of the ensemble [23]. The distinction between the dwell time and its components was first done by Buttiker [12], and raised some controversy. As summarized in chapter 1, Muga, Brouard and Sala have emphasized the multiplicity of possible quantum partitionings versus the uniqueness of the classical case, and developed a systematic theory to generate partitionings with the correct classical limit. Some of these include interference terms that cannot be assigned to transmission or reflection but to both of them [11].
IV. IMPORTANCE OF THE PHASES. TIME DELAYS.

If the S matrix is known or simply one of the amplitudes \( R^l \) or \( R^r \) is given as a function of momentum and there are no bound states, necessary and sufficient conditions are known for a unique potential to exist, and there are well established construction procedures \([30,6]\). However a knowledge of the probabilities is not enough to determine the coefficients. The phases are associated with observable time dependent properties.

Consider a wave-packet impinging from the left on a barrier potential located near \( x = 0 \) (The exact barrier position is not important for our present purposes. Two typical choices for \( x = 0 \) are the center of a symmetrical barrier, or the left edge of a finite range potential). Let us take as before the spatial interval \([a, b]\) well outside the barrier, so that there is a clear separation between incoming and reflected passages.

Since the incoming state is in the positive momentum channel,

\[
\langle x | \phi_{in}(t) \rangle = \int_0^\infty dp \langle x | p \rangle \langle p | \phi_{in}(0) \rangle e^{(ipx - Et)/\hbar},
\]

and, applying the Möller operator \( \Omega_+ \),

\[
\langle x | \psi(t) \rangle = \int_0^\infty dp \langle x | p^+ \rangle \langle p | \phi_{in}(0) \rangle e^{(ipx - Et)/\hbar}.
\]

(If the zero of time is taken well before the wave packet interacts significantly with the barrier, the substitution \( \langle p | \psi(0) \rangle = \langle p | \phi_{in}(0) \rangle \) does not introduce any significant error.)

Substituting \([82], [78] \) and \([79] \) in the time averages \([82-84] \), and using the standard expression for the current density,

\[
J(x, t) = \frac{\hbar}{m} \text{Im} \left( \psi(x, y)^* \frac{\partial \psi(x, t)}{\partial x} \right),
\]

the derivative of an energy Dirac’s delta may be identified and then used to perform one of the momentum integrals. The results are

\[
\langle t \rangle^\text{out}_b = \frac{1}{T} \int_0^\infty dp |\langle p | \phi_{in}(0) \rangle|^2 |T(p)|^2 \frac{m}{p} [b - x_0 + \hbar \Phi'_T(p)] , \tag{88}
\]

\[
\langle t \rangle^\text{out}_a = \frac{1}{T} \int_0^\infty dp |\langle p | \phi_{in}(0) \rangle|^2 |T(p)|^2 \frac{m}{p} [-a - x_0 + \hbar \Phi'_R(p)] , \tag{89}
\]

\[
\langle t \rangle^\text{in}_a = \int_0^\infty dp |\langle p | \phi_{in}(0) \rangle|^2 \frac{m}{p} [a - x_0] , \tag{90}
\]

where the prime means derivative with respect to \( p \), and

\[
x_0 \equiv \hbar \text{Im} \left( \langle \phi_{in}(0) | p^+ \rangle \langle p | \phi_{in}(0) \rangle \right). \tag{91}
\]

These results do not require to assume a narrow packet in momentum representation.

The quantity

\[
\tau_T^{ph}(x_0, b; p) \equiv m [b - x_0 + \hbar \Phi'_T(p)] / p \tag{92}
\]

in the integrand of \([88] \) consists of a time that a classical free particle with mass \( m \) and momentum \( p \) would spend from \( x_0 \) to \( b \), plus the time delay \( m \hbar \Phi'_T(p) / p \). Similarly, the term in brackets in \([84] \),

\[
\tau_R^{ph}(x_0, a; p) \equiv m [-a - x_0 + \hbar \Phi'_R(p)] / p , \tag{93}
\]

is a time spent by a classical particle that travels freely from \( x_0 \) to \( x = 0 \), where its momentum is instantly reversed, and from \( x = 0 \) to \( a \), plus a delay contribution. It is to be noted that unless \( a = -b \) the reference time associated with classical free motion is different in the transmission and reflection cases. We shall see a consequence of this disparity afterwards when calculating average delays in \([1B] \).

Formally we may use \([92] \) and \([93] \) to define “phase times” for arbitrary values of \( a, b, \) and \( x_0 \). In particular, for a finite range barrier between \( x = 0 \) and \( d \) let us define
by substracting from $\tau_T^{ph}(x_0, d; p)$ the classical flight time between $x_0$ and $0$, $-mx_0/p$. These “extrapolated phase times” for traversal should not be overinterpreted as actual traversal times \[13\] \[12\] not only because, as pointed out in Chapter 1, there is not a unique traversal time, but because a wave packet peaked around $p$ is very broad in coordinate representation, so it is severely deformed before the hypothetical “entrance” instant $t_{out} = |x_0|/m/p$, and at $x = 0$ there is an important interference effect between incident and reflected components. The wavefunctions $\phi_{in}$ and $\psi_R$ used to calculate the fluxes $J_I$ and $J_R$ do not faithfully represent the actual wave, so that the average instants \[22\] \[21\] loose their physical meaning as average detection times.

### A. The Hartman effect

Relation (88) is suitable for examining the “Hartman effect” \[33\] \[31\] \[26\] \[25\]. Hartman \[33\] studied the evolution of a wave-packet with momentum distribution centered around $p_c$, colliding with a rectangular barrier of height $V_0 > p_c^2/(2m)$, and width $d$. He found three regions according to the value of $d$. For large barrier widths (opaque barrier conditions), the stationary phase time associated with $p$, under the barrier, goes to a constant, $\tau_T^{ph}(x_0, d; p) = 2m/(p\kappa) - x_0m/p$, independent of $d$, where

$$\kappa = [2m(V_0 - E)]^{1/2}/\hbar.$$

When transmission is dominated by momentum components below the barrier, the transmitted wave-packet seems to traverse the potential region in a time interval independent of $d$. This is the “Hartman effect”. If $d$ is increased further, plane waves with momentum above the barrier height dominate the transmission, and classical behaviour results, i.e., time grows linearly with $d$. Finally, for small barrier widths, Hartman defined a “thin barrier region” where the phase time depends generally on $d$.

To be more specific, let us consider the initial Gaussian wave-packet

$$\langle x|\phi_{in}(0)\rangle = \left[\frac{1}{2\pi\delta^2}\right]^{1/4} \exp\left[ip_c x/\hbar - (x - x_c)^2/(4\delta^2)\right],$$

of average momentum $p_c = \hbar k_c$ and spatial width (square root of the variance) $\delta$. Here $x_0$ becomes equal the wave packet center $x_c$. The initial momentum distribution is a Gaussian distribution with variance $\sigma^2 = [\hbar/(2\delta)]^2$. We assume that $p_c >> \sigma^2$ so that the truncation at $p = 0$ in \[88\] is not significant. For an energy distribution peaked around $E_c < V_0$ the following results can be drawn \[25\]:

If $\kappa d = \sqrt{2m(V_0 - E_c)}d/\hbar >> 1$, $\langle t\rangle^{out}$ does not vary appreciably when $d$ increases, thus showing Hartman effect. When $d$ is sufficiently large, the components of the wave-packet under the barrier are so strongly depressed by $|T(p)|^2$ that higher momenta start to dominate, and $\langle t\rangle^{out}$ grows almost linearly, as one expects classically. As $\delta$ is increased, larger values of $d$ are needed to pass from the first regime to the second one. An estimation of the value of $d$ which gives the transition between Hartman effect and quasiclassical behaviour can be obtained for each value of $\delta$ by equating the factor $|T(p)|^2/|\phi_{in}(p)|^2$ for $p = p_c$ and for $p = p_r$, where $p_r$ is the momentum of the first resonance above the barrier. This leads to the relation

$$\delta = \frac{\hbar}{|p_r - p_c|} \ln |T(p_c)/T(p_r)| \approx \frac{\hbar \sqrt{\kappa d}}{|p_r - p_c|}.$$

between $\delta$ and $d$, that clearly separates quantum and quasiclassical behaviour. Also, for fixed $\delta$, the transition is sharper at larger $\delta$ as a consequence of the narrower momentum distribution.

We have already warned the reader against a naive overinterpretation of the extrapolated phase time $\tau_T^{ph}(0, d; p)$, which becomes $2m/(p\kappa)$ for the barrier traversal in the Hartman effect, mainly because of the strong deformation of the broad incident wavepacket. We could try to avoid the interpretational pitfalls of this quantity and look instead at the time $\langle t\rangle^{out}$ for a wave packet which is initially localized near the edge of the barrier, and with a small spatial width compared to the barrier length $d$, to identify the entrance time and the preparation instant with a tolerable small uncertainty. However, Low and Mende speculated \[23\], and then Delgado and Muga have shown \[26\], that this localization leads to the dominance of over-the-barrier components. Similar conclusions are drawn from a two detector model, one before and one after the barrier, when the detector before the barrier localizes the particle into a small spatial width compared to $d$ \[25\].
B. The lifetime and delay time matrices

The four delay times corresponding to reflection and transmission for right and left incidence form the delay time matrix introduced by Eisenbud in his thesis [37],

$$\Delta t_{\alpha\beta} = \text{Re} \left[ -\frac{i}{\bar{h}} \frac{1}{S_{\alpha\beta}} \frac{dS_{\alpha\beta}}{dE} \right] .$$

(98)

The matrix element $\Delta t_{\alpha\beta}$ is the delay time in the appearance of the peak outgoing signal in channel $\beta$, after the injection of a pulse narrowly peaked in momentum in channel $\alpha$. The “delay” may in fact become negative as discussed already. These delay times have been traditionally obtained by means of the “stationary phase argument”. Let us rewrite the transmitted wave function as

$$\langle x|\psi_T(t)\rangle = \hbar^{-1/2} \int_0^{\infty} dp e^{i\bar{p}t/\hbar + i\Phi_T(p)} |\phi_{\text{in}}(0)\rangle |T(p)| .$$

(99)

If the initial state is narrowly peaked around $p_0$, the integral will be appreciably different from zero only if the phase of the exponential function is stationary near $p = p_0$. This implies a “spatial delay” with respect to the free-motion wave packet,

$$\Delta x = \hbar \frac{d\Phi_T}{dp} \bigg|_{p=p_0} ,$$

(100)

and a corresponding “time delay”

$$\Delta t_++(p_0) = \hbar m \frac{d\Phi_T}{dp} \bigg|_{p=p_0} .$$

(101)

The time delays are also related to the on-the-energy-shell lifetime matrix of Smith [38],

$$Q(E) = i\hbar S(E) \frac{dS(E)^\dagger}{dE} ,$$

(102)

$S$ is unitary, so $Q$ is Hermitian. Thus the diagonal matrix elements of $Q$ are real and take the form

$$Q_{\alpha\alpha} = \sum_\beta |S_{\alpha\beta}|^2 \Delta t_{\alpha\beta} .$$

(103)

Since the particle has a probability $|S_{\alpha\beta}|^2$ to emerge in the channel $\beta$, $Q_{\alpha\alpha}$ is the average delay experienced by the particle injected in channel $\alpha$.

We shall now relate the $Q$ matrix with the “wave packet lifetime”, defined as the difference between dwell times with and without potential [38,39],

$$\langle Q \rangle \equiv \tau_{D,\psi} - \tau_{D,\phi_{\text{in}}} .$$

(104)

As before, the incidence is in the positive momentum channel. $\tau_{D,\psi}$ is given by [31], whereas the dwell time for free motion is

$$\tau_{D,\phi_{\text{in}}} = \langle t \rangle_{b,\phi_{\text{in}}}^{\text{out}} - \langle t \rangle_{a,\phi_{\text{in}}}^{\text{in}} = \int_0^{\infty} dp \langle |\phi_{\text{in}}(0)\rangle |^2 \frac{m}{p} [b-a] ,$$

(105)

where, similarly to (90),

$$\langle t \rangle_{b,\phi_{\text{in}}}^{\text{out}} = \int_0^{\infty} dp \langle |\phi_{\text{in}}(0)\rangle |^2 \frac{m}{p} [b-a] .$$

(106)

Since, by hypothesis, $\langle t \rangle_{a,\psi}^{\text{in}} = \langle t \rangle_{a,\phi_{\text{in}}}^{\text{in}}$, $\langle Q \rangle$ takes the form

$$\langle Q \rangle = \int_0^{\infty} dt \int_a^b dx \left( |\langle x|\psi(t)\rangle|^2 - |\langle x|\phi_{\text{in}}(t)\rangle|^2 \right)$$

$$= P_T[\langle t \rangle_{b,\psi}^{\text{out}} - \langle t \rangle_{b,\phi_{\text{in}}}^{\text{out}}] + P_R[\langle t \rangle_{a,\psi}^{\text{in}} - \langle t \rangle_{b,\phi_{\text{in}}}^{\text{out}}] .$$

(107)
Substituting all the integral expressions obtained for the passage times, and writting \( c = -a - b \),

\[
\langle Q \rangle = \hbar \int_0^\infty dp \frac{m}{p} |\langle p|\phi_n(0)\rangle|^2 \left[ \Phi_T^* |T(p)|^2 + \left( \Phi_R^* + \frac{c}{p} \right) |R(p)|^2 \right]. 
\]  

(108)

Note the term proportional to \( c \) in the reflection part. It arises because of the mismatch between the free motion reference times used to define the reflection and transmission time delays when \( c \neq 0 \). Choosing \( c = 0 \), \( \langle Q \rangle \) represents the weighted momentum average of the mean delay for each momentum\(^5\).

\[
\langle Q \rangle = \int_0^\infty dp |\langle p|\phi_n(0)\rangle|^2 Q(E)_{++}.
\]  

(109)

The eigenvalues of \( Q \) have been used as good indicators of resonances \[1\], see \[IVC\] below, and may be interpreted for symmetrical potentials as the delays associated with symmetrical or antisymmetrical bilateral incidence \[40\]. However their operational interpretation in terms of individual measurements is puzzling. An asymptotic measurement of the arrival time at \( b \) in the transmission side could be done in principle for one of the identically prepared systems represented by the wave packet. Because of the coordinate spread of the wavepacket, however, there is a large uncertainty in the time that the \emph{same} particle enters the region \([a,b]\). If a detector is placed at \( a \) before the collision occurs, the entrance time can be determined, but in general either the particle is destroyed or its behaviour afterwards is modified by the measurement. We are thus faced with an intrinsic difficulty to measure \emph{individual} delays. This means that, at variance with other quantum mechanical averages which are interpreted as averages of the eigenvalues measured for the individual members of the ensemble, the operational meaning of (109) does not require to assign a lifetime to a given particle. It depends on the average times defined in (82-84), which are measurable, at least in principle, by the time-of-flight technique (Other operational procedure making use of particle absorption along the chosen interval has been described by Golub et al. \[12\]). This peculiarity of the delay time was already noted by Goldrich and Wigner \[43\]. A consequence is that the ordinary quantum fluctuations around the average value are not operationally meaningful. Instead, the relevant fluctuations refer to variations of the average values themselves, corresponding to \( S \) matrix (or Hamiltonian) ensembles \[13\].

The trace of (102) in the on-shell space is related to the change in density of states \( \Delta \rho(E) = \text{Tr}[\delta(E-H) - \delta(E-H_0)] \) which is a fundamental quantity to characterize the continuous spectrum \[16\] according to the “spectral theorem” (The three dimensional elastic and multichannel versions of the spectral theorem have been extensively discussed and proven rigorously \[40\].)

\[
\Delta \rho(E) = -\pi^{-1} \text{Im} \text{Tr}[G(E+i0) - G_0(E+i0)] = \frac{1}{\hbar} \sum_\alpha Q(E)_\alpha = \pi^{-1} \frac{d \Phi_T(E)}{dE}.
\]  

(110)

The second equality (spectral theorem) follows from a result of Dashen, Ma and Bernstein \[17\]. To obtain the final expression, use has been made of \[62\] and \[13\] \[48\], see \[13\] for an alternative derivation consisting in evaluating \( \Delta \rho \) for a finite system and then going to infinity. Note that the maxima of the trace of \( Q \) may be used to identify resonance energies and widths \[50\]. For further relations between the density of states and the dwell time see \[51\] \[52\]. Chapter ... discusses the concept of local density of states and its relation to the Larmor clock and transport properties.

C. Breit-Wigner resonances

The simplest model of resonance behaviour is the Breit-Wigner model for an isolated resonance,

\[
S(E) = 1 - \frac{i A}{E - E_0 + i \Gamma/2}.
\]  

(111)

By imposing unitarity to \( S \), and assumming that \( A \) and the resonance parameters \( E_0 \) and \( \Gamma \) are independent of \( E \), it follows that \( A = A^\dagger \) and

---

\(^5\)Additional oscillatory terms, see e.g. \[32\] \[40\], appear when the no-interference condition between the reflected and incident wave packets is not imposed.
\[ A^2 = \Gamma A. \]  

(112)

This means that the matrix \( A \) factorizes as \( A_{\alpha \beta} = \gamma_{\alpha} \gamma_{\beta}^* \), and that it is proportional to a projector matrix \( P = A/\Gamma \) with eigenvalues 1 and 0. Thus, the equation (112) takes the form

\[ \Gamma = \sum_{\alpha} |\gamma_{\alpha}|^2. \]  

(113)

The corresponding \( Q \) matrix may now be written as

\[ Q = P q_m, \]  

(114)

with eigenvalues \( q_m \) and zero, where

\[ q_m = \frac{\hbar \Gamma}{(E - E_0)^2 + \Gamma^2/4}. \]  

(115)

is the maximum value allowed for a diagonal element of \( Q \). The Breit-Wigner model for \( S \) and \( Q \) can be generalized in various ways, in particular to account for multiple overlapping resonances [44].

D. Negative delays

In partial wave analysis of three dimensional collisions with spherical potentials, the time delay has been used mainly as a way to characterize resonance scattering. One of the standard definitions of a resonance is a jump by \( \pi \) in the eigenphases of the \( S \) matrix. In one dimensional collisions the time delay has been also used frequently to characterize (non-resonant) tunnelling, where it may become negative. In fact the different delay signs associated with the two types of effects, resonances and tunnelling, are not independent. In 3D it was soon understood by Wigner [54] that the increases and decreases of the phase should balance each other. Since Levinson’s theorem imposes a fixed phase difference from \( p = 0 \) to \( \infty \), there must be intervals of negative delay to compensate for the phase increases associated with the resonances. A similar analysis applies in 1D to the transmission amplitude. In Figure 1, the phase of the transmission amplitude for a square barrier is shown versus \( p \) for different values of the barrier width \( d \).

![Figure 1](image)

**FIG. 1.** Phase of the transmission amplitude versus momentum for a square barrier of “height” \( V_0 = 5 \) and for three different widths, \( d = 1 \) (solid line), 2 (short dashed line), and 3 (long dashed line). \( m = 1 \). (all quantities in atomic units)
As $d$ increases, the scattering resonances “above the barrier” $p > p_0 = (2mV_0)^{1/2}$ become more dense and are defined better because of the approach of the resonance poles in the fourth quadrant to the real axis. The corresponding increases of the phase are compensated by a more and more negative delay in the tunneling region.

Negative delays also arise if a pole of $T(p)$ crosses the real axis upwards, when varying the interaction strength, to become a loosely bound state in the positive imaginary axis. Levinson’s theorem, see [53], imposes then a sudden jump in the phase $\Phi_T(0)$ that must be compensated by a strong negative slope. This effect is more important near threshold, i.e., when the pole is very close to the real axis [53]. Similar effects have been described for non-bound state poles in complex potential scattering [54].

Wigner also found a bound for the negative (partial wave) delay time of a potential of finite radius. Whereas positive delays can be arbitrarily large, negative delays are restricted by “causality conditions” [57]. Some back-of-the-envelope causality arguments may however be misleading. For example, assume a barrier of length $d$, and let $a$ coincide with the left edge and $b$ with the right edge. If the total time $\tau_T^{th}(0,d)$ is to be positive, the delay cannot be more negative than the reference free time,

$$\Delta t_{++} > - \frac{md}{p},$$

see e.g. [58]. In fact this bound may be violated, in particular at low energy in the proximity of a loosely bound state. This should not surprise the reader after our repeated warnings against an overinterpretation of the extrapolated time $\tau_T^{th}(0,d)$. The flaw in the argument is the assumption of positivity of $\tau_T^{th}$. Nevertheless, rigorous bounds have been established by Wigner himself and various authors in 3D collisions, see [54,57] for review. In 1D collisions the following bound holds for even potentials with finite support between $-b$ and $b$ [55,60]:

$$\Delta t_{++} \geq \frac{m}{p} \left\{-2b + \frac{1}{4p} \sin(2pb/h + 2\delta_0) - \sin(2pb/h + 2\delta_1)\right\} \geq \frac{m}{p} \left(-d - \frac{1}{2p}\right).$$

This may be proven by using the even and odd eigenfunctions $\langle x|\psi_j \rangle$ introduced in (52), in particular the fact that $\int_{-b}^{b} dx \psi_j^2 > 0$. We start by calculating the logarithmic derivative of $\langle x|\psi_0 \rangle$ at $x = b$ from the known expression for the outer region, see [54],

$$L_b = \frac{d\langle x|\psi_0 \rangle/dx}{\langle x|\psi_0 \rangle} \bigg|_{x=b} = -\frac{p}{h} \tan(pb/h + \delta_0).$$

Taking the derivative of $L_b$ with respect to $p$,

$$\frac{d\delta_0}{dp} = -\left\{\frac{\hbar}{p} \frac{dL_b}{dp} \cos^2(pb/h + \delta_0) + \frac{1}{2p} \sin[2(pb/h + \delta_0) + \frac{x}{h}]\right\}. \tag{119}$$

The first term on the right hand side may also be written as

$$\frac{\hbar}{m} \left\{\langle x|\psi_0 \rangle E \langle x|\psi_0 \rangle x - \langle x|\psi_0 \rangle \langle x|\psi_0 \rangle E, x \rangle \right\}(x = b), \tag{120}$$

where the subscripts $E$ and $x$ are shorthand notation for the derivatives with respect to $E$ and $x$. Repeating the same operations for $x = -b$ one finds that

$$\langle x|\psi_0 \rangle E \langle x|\psi_0 \rangle x - \langle x|\psi_0 \rangle \langle x|\psi_0 \rangle E, x \rangle \big|_{x=b} = -\left\{\langle x|\psi_0 \rangle E \langle x|\psi_0 \rangle x - \langle x|\psi_0 \rangle \langle x|\psi_0 \rangle E, x \rangle \right\}(x = -b). \tag{121}$$

We shall now prove that this is a positive quantity. Taking the derivative of the stationary Schrödinger equation with respect to energy one obtains for real eigenfunctions of $H$ the identity [58]

$$\langle x|\psi|^2 = -\frac{\hbar^2}{2m} \frac{\partial}{\partial x} \left(\langle x|\psi \rangle \langle x|\psi \rangle E, x - \langle x|\psi \rangle E \langle x|\psi \rangle x \right), \tag{122}$$

so that, using (121),
\[ \int_{-b}^{b} dx \langle x|\psi_0|^2 = \frac{\hbar^2}{m} (\langle x|\psi_0\rangle_E\langle x|\psi_0\rangle_x - \langle x|\psi_0\rangle \langle x|\psi_0\rangle_E.x) (x = b). \]  

(123)

Carrying out similar manipulations for the odd wavefunction \( \langle x|\psi_1\rangle \), (117) is found as a consequence of the positivity of the probability to find the particle in the barrier region.

According to this bound the negative delay may be arbitrarily large for small enough momenta and may diverge at \( p = 0 \), as it occurs when a bound state appears when making the potential more attractive [53]. For the square barrier, which does not have bound states, the time advancement of the Hartman effect is less important and it is actually bound by (118). Thus, whereas the experiments looking for anomalously large traversal velocities (“superluminal effects”) have been frequently based on evanescent conditions in square barriers (tunneling), square wells with the proper depth may in fact lead to much larger advancement effects at threshold energies.

V. TIME DEPENDENCE OF SURVIVAL PROBABILITY: EXPONENTIAL DECAY AND DEVIATIONS

The quantum mechanical decay of unstable states can be described in many different ways [61,62]. In many theoretical works the emphasis has been on justifying the approximately valid exponential decay law. A possible treatment for the survival amplitude \( A(t, \psi) \equiv \langle \psi(0)|\psi(t) \rangle \) decomposes the state \( \psi \) by the usual resolution into proper and improper eigenstates of the Hamiltonian \( H \), corresponding to bound and continuum states. Even though it contains all the information, this is not convenient in general either for calculational purposes or for rationalizing the decay behaviour in a simple manner, except in favourable circumstances where the integral is easily approximated and parameterized, e.g. for isolated resonances and particular initial states. An ideal description would handle arbitrarily complex initial states and potentials in simple terms, and allow for an understanding of both the dominant exponential decay and the deviations from it.

Much progress in this direction has been achieved by representing \( A(t, \psi) \) as a discrete sum over resonant terms [63,64]. The discretization allows a clear identification and separation of the physically dominant contributions, different terms being important for different time regimes. Here we follow the treatment presented in [63-65].

The survival amplitude \( A(t, \psi) = \langle \psi(0)|\psi(t) \rangle \) requires the diagonal matrix elements of the unitary evolution operator \( e^{-iHt}/\hbar \). When this operator is expressed in terms of the resolvent, \( A(t, \psi) \) takes the form

\[ A(t, \psi) = \langle \psi|e^{-iHt}/\hbar|\psi \rangle = \frac{i}{2\pi m} \int_{\mathcal{C}} dq \ q \langle \psi| e^{-izt/\hbar} |\psi \rangle = \frac{i}{2\pi} \int_{\mathcal{C}} dq \ e^{-izt/\hbar} M(q), \]

(124)

where \( z = q^2/2m \) is a complex energy and the contour \( \mathcal{C} \) goes from \(-\infty \) to \(+\infty \) passing above all the singularities of the resolvent due to the spectrum of \( H \) (discrete poles for bound states and the natural boundary of the real axis for the continuum), and

\[ M(q) = \frac{q}{m} \langle \psi| \frac{1}{z-H} |\psi \rangle. \]

(125)

The survival probability is to be calculated as \( S(t, \psi) = |A(t, \psi)|^2 \).

A. Predicted time behaviour

The function \( M(q) \) is evaluated in the upper half \( q \)-plane and then analytically continued into the lower half plane. Provided that the continuation exists, \( M(q) \) has in general a set of core singularities, depending only on the potential, plus possibly other structural state-dependent singularities. It is then useful to deform the original integration contour to the diagonal \( \mathcal{D} \) of the second and fourth quadrants of the \( q \)-plane. This provides both physical insight by identifying the most relevant time dependence (exponential decay) of the survival, and a calculational advantage for the remainder, since for \( t > 0 \) the exponential \( e^{-izt/\hbar} = e^{-iq^2t/(2m\hbar)} \) is a real Gaussian on this diagonal.

Let us assume that a pole expansion of the form

\[ M(q) = \sum_{k} \frac{a_k}{(q - q_k)} \]

(126)

is possible (higher order poles can be treated in a similar fashion). Here \( k = 1, 2, 3 \cdots \) indexes the poles. On deforming the \( q \) integration from contour \( \mathcal{C} \) to \( \mathcal{D} \), the residues of the poles \( q_k \) crossed in the fourth quadrant on carrying out
this deformation provide contributions to $A(t)$ that decay exponentially with time, whereas the residues are purely oscillatory for poles in the upper half plane (bound states),

$$E_k(t) = a_k e^{-i\omega_k^2 t/(2\hbar)} = a_k e^{-u_k^2},$$

where

$$u \equiv q/f, \quad f \equiv (1-i)\sqrt{(m\hbar/t)}.$$  \hspace{2cm} (127)

becomes real along the diagonal $D$. Independently of providing or not providing a residue, all poles contribute because of the integral along the diagonal. Each pole contribution is expressed in terms of the $w$-function, see [66], as

$$D_k(t) = -\frac{a_k}{2} \text{sign}(Imu_k)w[\text{sign}(Imu_k)u_k].$$

The exponential term may be added to this contribution to give the compact result [66],

$$A(t) = \sum_k [E_k(t) + D_k(t)] = \sum_k \frac{1}{2} a_k w(-u_k).$$

(It is understood that $E_k(t) = 0$ for poles in the lower half plane that have not been crossed when deforming the contour.) The second expression is very useful for studying the short time behaviour, but the first one has the advantage of separating explicitly the exponential decay, $E_k$, from the “correction” $D_k$, which is given in terms of the known entire function $w$ parameterized by the pole position and time. Numerical values and asymptotic properties of this function for small or large times are easy to calculate.

The above treatment is easily extended for an $M(q)$ that includes an entire function in addition to the pole expansion. This would add to the $w$-functions the integral along $D$ of the entire function times a real Gaussian.

**B. Short time behaviour**

The short time behaviour of the quantum survival probability is easily analyzed in terms of the above formalism, which allows to classify several possible non exponential dependences.

Many authors have described a short time $t^2$ dependence of the decay probability $P_{\text{decay}} \equiv 1 - S$ provided the mean energy and second energy moment of these states exist, see in particular the work related to the “quantum Zeno paradox” [67]. Less attention has been paid to the short time behaviour if these conditions are not fulfilled. A formal treatment and examples by Moshinsky and coworkers suggest a $t^{1/2}$ dependence of the decay probability at short times [68,69]. We shall clarify how these two seemingly different claims can be compatible, and describe other possible dependences.

The Taylor series (17) of the $w$ functions in (130) gives a series in powers of $t^{1/2}$,

$$A(t) = \sum_k \frac{a_k}{2} \sum_{n=0}^{\infty} \frac{[2^{-1}g_k(1-i)(t/m\hbar)^{1/2}]^n}{\Gamma(\frac{3}{2} + 1)}.$$  \hspace{2cm} (131)

This suggests a short time $t^{1/2}$ dependence of the decay probability, as claimed by Moshinsky and coworkers [68,69]. On the other hand, the formal series based on expanding the evolution operator,

$$A(t, \psi) = \langle \psi | e^{-iHt/\hbar} | \psi \rangle = 1 - \frac{it}{\hbar} \langle \psi | H | \psi \rangle - \frac{t^2}{2\hbar^2} \langle \psi | H^2 | \psi \rangle + \cdots,$$

provides a $t^2$ dependence,

$$P_{\text{decay}} = \frac{t^2}{\hbar^2} \left( \langle \psi | H^2 | \psi \rangle - \langle \psi | H | \psi \rangle^2 \right) + \cdots.$$  \hspace{2cm} (132)

However, the expectation values of $H$ and/or higher powers of $H$ may not exist. Several behaviours are possible depending on the existence of these moments. The question of the physical realizability of Hilbert space states with infinite first or second energy moments is subject to debate [70]. We shall leave this debate aside, and determine the possible implications on the short time behavior.
Consider the first two derivatives of $A$ at time $t = 0$ first from (132) and then by assuming a general short time dependence of the form $A \sim 1 + bt^c$, where $b$ and $c$ are finite constants,

\[ \frac{dA}{dt}\bigg|_{t=0} = -\frac{i}{\hbar} \langle \psi | H | \psi \rangle = bc t^{c-1}\bigg|_{t=0} \]  
\[ \frac{dA^2}{dt^2}\bigg|_{t=0} = -\frac{1}{\hbar^2} \langle \psi | H^2 | \psi \rangle = bc (c-1) t^{c-2}\bigg|_{t=0}. \]  

(134)  
(135)

If the mean energy of the initial state does not exist, a $t^{1/2}$ dependence of the decay probability is possible, see examples in [53] and [59].

If the mean energy is finite so that $dS/dt|_{t=0} = 2\text{Re}(dA/dt|_{t=0}) = 0$, then $c \geq 1$. This rules out a $t^{1/2}$ dependence of $A$ since a $t^{1/2}$ dependence implies an infinite time derivative of $A$ at $t = 0$. The corresponding coefficient for $t^{1/2}$ in [131] must vanish by compensation between the different pole contributions.

The second derivative is only finite at time zero if $c \geq 2$. This means that if the first energy moment exists but not the second, a dependence $t^c$ where $1 \leq c < 2$ is possible for $A$ (and for the decay probability), in particular $t^{3/2}$. (The coefficient for $t^{3/2}$ must also vanish in this case.) Otherwise, one can expect that the series (132) will be effective at short times for states with finite moments $\langle \psi | H^n | \psi \rangle$ leading to a $t^2$ behaviour. Examples where $t^{3/2}$ and $t^2$ dominate the short time behaviour of $P_{\text{decay}}$ are provided in [67].

C. Large time behaviour

At first sight the asymptotic expansion of the $w$-function for $t \sim \infty$ in the correction term to the exponential decay suggests a long time dependence of the survival probability as $t^{-1}$, but in fact the general behaviour is $t^{-3}$ because of the cancellation of all the $t^{-1}$ contributions. Due to the exponential $e^{-izt/\hbar}$ in (138) the large $t$ behaviour is dominated by the region around the origin. The origin is actually a saddle point for the steepest descent path for this exponential factor that crosses the origin along the diagonal $D$ of the second and fourth quadrants. By introducing $u$ and $f$ variables as in (128) the exponential becomes $e^{-u^2}$ and $u$ remains real along the steepest descent path.

The resolvent matrix element $\langle \psi | (z - H)^{-1} | \psi \rangle$ which is defined for Im$q > 0$ (first energy sheet) has to be analytically continued into the lower half $q$-plane (or second sheet of the complex $z$ plane) to allow for this type of analysis, which will be valid in particular for finite range potentials. Provided that the analytically continued function is analytical at the origin it has a Taylor series expansion

\[ \langle \psi | (z - H)^{-1} | \psi \rangle = a_0 + a_1 q + a_2 q^2 + ... \]  

(136)

with coefficients $a_i$ depending on $\psi$. But because of the (odd) $q$ factor in (125), the first term, $a_0$, does not contribute to the integral (138). The asymptotic formula for the survival amplitude comes therefore from the second term and takes the form

\[ \langle \psi | e^{-iHt/\hbar} | \psi \rangle \sim \frac{i}{2m\pi} a_1 f^3 \int_{-\infty}^{\infty} du u^2 e^{-u^2} = \frac{1 - i}{2m\sqrt{\pi}} a_1 \left( \frac{m\hbar}{t} \right)^{3/2}. \]  

(137)

This formal result depends on the validity of (136), and on the assumption that no additional contributions due to the deformation of the contour are to be considered asymptotically. In general the analytically continued matrix elements of the resolvent will have poles in the lower half $q$-plane that may be crossed when deforming the contour, but these can only yield contributions that decay exponentially with time, so they are negligible at long times.

A similar analysis may be performed for the propagator (no bound states) [71]

\[ \langle x | e^{-iHt/\hbar} | x' \rangle = \frac{i}{2\pi} \int_C dq I(q)e^{-izt/\hbar}, \]  

(138)

\[ I(q) = \frac{q}{m} \frac{1}{|z - H|} \langle x | x' \rangle, \]  

(139)

substituting $M(q)$ by $I(q)$. Quite generally, $I(q)$ vanishes at $q = 0$, and a $t^{3/2}$ dependence results. An exception is free motion on the full line, where

\[ \langle x | \frac{1}{z - H_0} | x' \rangle = -\frac{im}{\bar{q}\hbar} e^{i|x - x'|/q\hbar}, \]  

(140)
so that $I(0) = -i/\hbar \neq 0$. As a consequence, the asymptotic behaviour of the probability density for free motion on the full line is generically $t^{-1}$. This is an important case in which (136) is not satisfied. Explicitly, by carrying out the integral in (138), the well known propagator

$$\langle x | e^{-iH_0 t/\hbar} | x' \rangle = \left( \frac{m i \hbar t}{\Theta} \right)^{1/2} e^{i m (x-x')^2/(2 \hbar t)}$$

is obtained. A $t^{-1}$ behaviour will also occur exceptionally when the potential allows for a zero energy pole of the resolvent.

The free-motion probability density may decay faster than $t^{-1}$ when the momentum amplitude $\langle p | \psi(0) \rangle$ vanishes at $p = 0$, so that the $q^{-1}$ singularity is cancelled, see Figure 2. The exceptional cases of decay slower than $t^{-1}$ has been studied by Unnikrishnan [72].

In the previous section we have seen how contour deformation techniques in the complex plane allow to single out contributions to the survival amplitude from resonance poles. In general the integral that provides the time dependent wave function may involve other critical points, “structural” poles, saddle points, or branch points, that determine the transient and asymptotic behaviour of the wave propagation. It is frequently possible to write explicit expressions or asymptotic expansions for the contributions of these critical points. In simple cases the effect of (the dominant term of) one of the critical points provides already a good approximation and a simple picture emerges, where characteristic times or velocities for the arrival of the main signal may be identified. Also typical is the transition from the dominance of one critical point to another, which may lead to a change in qualitative behaviour and to a characteristic time for the transition. The pioneering work in this direction is due to Stevens [73,74], who followed the techniques that Sommerfeld and Brillouin introduced in their study of the propagation of light in dispersive media [75]. Examples of application to quantum scattering off a square barrier and a separable potential may be found in [76] and [77]. Here we shall examine, following [78], the somewhat simplified case corresponding to a point source producing evanescent waves.

**VI. OTHER CHARACTERISTIC TIMES OF WAVE PROPAGATION**

In the previous section we have seen how contour deformation techniques in the complex plane allow to single out contributions to the survival amplitude from resonance poles. In general the integral that provides the time dependent wave function may involve other critical points, “structural” poles, saddle points, or branch points, that determine the transient and asymptotic behaviour of the wave propagation. It is frequently possible to write explicit expressions or asymptotic expansions for the contributions of these critical points. In simple cases the effect of (the dominant term of) one of the critical points provides already a good approximation and a simple picture emerges, where characteristic times or velocities for the arrival of the main signal may be identified. Also typical is the transition from the dominance of one critical point to another, which may lead to a change in qualitative behaviour and to a characteristic time for the transition. The pioneering work in this direction is due to Stevens [73,74], who followed the techniques that Sommerfeld and Brillouin introduced in their study of the propagation of light in dispersive media [75]. Examples of application to quantum scattering off a square barrier and a separable potential may be found in [76] and [77]. Here we shall examine, following [78], the somewhat simplified case corresponding to a point source producing evanescent waves.

**FIG. 2.** $d \ln |\psi(t)|^2 / d \ln t$ versus $d \ln t$ for two different wave packets: one of them vanishes at $p = 0$, $\langle p | \psi(0) \rangle = C(1 - e^{-\alpha p^2/\hbar}) e^{-\delta^2 (p-p_0)^2/\hbar^2 - i p x_0/\hbar} \Theta(p)$ (solid line), and the other one is a a Gaussian wave packet, $\langle p | \psi(0) \rangle = C' e^{-\delta^2 (p-p_0)^2/\hbar^2 - i p x_0/\hbar}$ (dashed line). $C$ and $C'$ are normalization constants; the parameters are $p_0 = 1$, $x_0 = -10$, $\alpha = 0.5$, $\delta = 1$, $x = 0$, $m = 1$ (all quantities in atomic units). Note the asymptotic dependences of the probability densities: $t^{-3}$ and $t^{-1}$ respectively.
waves following [78]. This is not a “scattering problem” in the standard sense, but it illustrates quite clearly the techniques and concepts involved in more conventional scattering problems, and in other time dependent phenomena where a stationary state is achieved after a transient behaviour.

In order to summarize essential aspects of the time dependence of wave phenomena other characteristic velocities or times have been traditionally defined. (We’ll see that some of them coincide with times associated with critical points.) The phase velocity, \( \omega/k \), is the velocity of constant phase points in the stationary wave (assume \( k > 0 \) for the time being)

\[
e^{i(kx-\omega t)}.
\]  

(142)

The boundary conditions, the superposition principle and the dispersion relation \( \omega = \omega(k) \) between the frequency \( \omega \) and the wavenumber \( k \) determine the time evolution of the waves in a given medium. If a “group” is formed by superposition of stationary waves around a particular \( \omega \), it propagates with the group velocity \( d\omega/dk \). In dispersive media (where \( \omega \) depends on \( k \)), the group velocity can be smaller (normal dispersion) or greater (anomalous dispersion) than the phase velocity. It was soon understood that these velocities could be both greater than \( c \) for the propagation of light; Sommerfeld and Brillouin [73], studying the fields that result from an input step function modulated signal in a single Lorentz resonance medium, introduced other useful velocities, such as the velocity of the very first wavefront (equal to \( c \)), or the signal velocity for the propagation of the main front of the wave.

The above description is however problematic for evanescent waves, characterized by imaginary wavenumbers instead of the real wavenumbers of propagating waves. The role played by the imaginary part of the group velocity \( d\omega/dk \) and the possible definition of a signal velocity in the evanescent case have been much discussed. Assume that a source is placed at \( x = 0 \) and emits with frequency \( \omega_0 \) from \( t = 0 \) on. If \( \omega_0 \) is above the cutoff frequency of the medium (the one that makes \( k = 0 \) a somewhat distorted but recognizable front propagates with the velocity corresponding to \( \omega_0 \). For the dimensionless Schrödinger equation

\[
\frac{\partial \psi}{\partial t} = -\frac{\partial^2 \psi}{\partial x^2} + \psi.
\]

(143)

the dispersion relation takes the form

\[
\omega = 1 + k^2,
\]

(144)

and the signal propagation velocity for the main front is equal to the group velocity, \( v_p = (d\omega/dk)\omega_0 = 2(\omega_0 - 1)^{1/2} \).

In other words, at some distance \( x \) form the source, the amplitude behaves, in first approximation, as

\[
\psi(x,t) \approx e^{-i\omega_0 t}e^{ik_0 x} \Theta(t-x/v_m)
\]

(145)

where \( k_0 = (\omega_0 - 1)^{1/2} \) is the wavenumber related to \( \omega_0 \) by the dispersion relation, and \( \Theta \) is the Heaviside (step) function. In the evanescent case, \( \omega_0 < 1 \), a preliminary analysis by Stevens [73,74,78], following the contour deformation techniques used by Brillouin and Sommerfeld suggested that a main front, moving now with velocity \( v_m = 2(1-\omega_0)^{1/2} = \text{Im}(d\omega/dk)\omega_0 \), and attenuated exponentially by \( \exp(\kappa_0 x) \) (where \( \kappa_0 = (1-\omega_0)^{1/2} \), could be also identified,

\[
\psi(x,t) \approx e^{-i\omega_0 t}e^{-\kappa_0 x} \Theta(t-x/v_m).
\]

(146)

The contour for the integral defining the field evolution was deformed along the steepest descent path from the saddle point; and the main front [140] was associated with a residue due to the crossing of a pole at \( i\kappa_0 \) by the steepest descent path.

The result seemed to be supported by a different approximate analysis of Moretti based on the exact solution [79], and by the fact that the time of arrival of the evanescent front, \( \tau = x/v_m \), had been found independently by Büttiker and Landauer [84,87] as a characteristic traversal time for tunnelling using rather different criteria (semiclassical arguments, the rotation of the electron spin in a weak magnetic field, and the transition from adiabatic to sudden regimes in an oscillating potential barrier).

However, more accurate studies of the point source problem and other boundary conditions have shown that the contribution from the saddle point (due to frequency components above or at the frequency cutoff created by the sharp onset of the source emission), and possibly from other critical points (e.g. resonance poles when a square barrier is located in front of the source [78]) are generally dominant at \( \tau \), so that no sign of the \( \omega_0 \)-front is seen in the total wave density at that instant, see [80,83,76,78], and the subsection VI A below.

Büttiker and Thomas reconsidered the signal sent out by a source which has a sharp onset in time [83]. They proposed two approaches to enhance the monochromatic fronts compared to the forerunners due to the saddle. First,
the dominance of the high frequencies forerunners could be avoided if the source is frequency limited such that all frequencies of the source are within the evanescent case. Of course this makes the onset of the signal unsharp. A second option is not to limit the source but to frequency limit the detection. We can choose a detector that is tuned to the frequency of the source and that responds when the monochromatic front arrives.

These two proposals and the sharp onset case were later implemented and examined in detail by Muga and Buttiker [78]. For a source with a sharp onset, they found that the traversal time $\tau$ plays a basic and unexpected role in the transient regime. For strongly attenuating conditions (in the WKB-limit) the traversal time governs the appearance of the first main peak of the forerunner. In contrast, the transition from the forerunner to an asymptotic regime which is dominated by the monochromatic signal of the source is given by an exponentially long time, see more details in VI A below. If the source is frequency band limited such that it switches on gradually but still fast compared to the traversal time, the situation remains much the same as for the sharp source, except that now the transition from the transient regime to the stationary regime occurs much faster, but still on an exponentially long time-scale. The situation changes if we permit the source to be switched on a time scale comparable to or larger than the traversal time for tunneling. Clearly, in this case a precise definition of the traversal time is not possible. But for such a source the transition from the transient regime to the asymptotic regime is now determined by the traversal time. Much the same picture emerges if we limit instead of the source the detector. Muga and Buttiker model the detector response by means of a “spectrogram”, a time-frequency representation of the wave function at a fixed point. As long as the frequency window of the detector is made sharp enough to determine the traversal time with accuracy, the detector response is dominated by the uppermost frequencies. In contrast, if the frequency window of the detector is made so narrow that the possible uncertainty in the determination of the traversal time is of the order of the traversal time itself, the detector sees a crossover from the transient regime to the monochromatic asymptotic regime at a time determined by the traversal time.

Possibly, the fact that we cannot determine the traversal time with an accuracy better than the traversal time itself tells us something fundamental about the tunneling time problem and is not a property of the two particular methods investigated.

**A. Role of the traversal time for a source with a sharp onset**

We shall obtain exact and approximate expressions of the time dependent wave function for $x > 0$ and $t > 0$ corresponding to the Schrödinger equation (143) and the “source boundary condition”

$$\psi(x = 0, t) = e^{-i\omega_0 t} \Theta(t),$$

in the evanescent case $\omega_0 < 1$. (A discussion of the physical meaning of “source boundary conditions” as compared to standard “initial value” conditions has been presented recently [80].) The solution may be constructed from its Fourier transform as

$$\psi(x, t) = -\frac{e^{-it}}{2\pi i} \int_{\Gamma_+} dk \left[ \frac{1}{k + i\kappa_0} + \frac{1}{k - i\kappa_0} \right] e^{ikx - ik^2t},$$

where the contour $\Gamma_+$ goes from $-\infty$ to $\infty$ passing above the pole at $i\kappa_0$, and

$$\kappa_0 = (1 - \omega_0)^{1/2}.$$  

(149)

The contour can be deformed along the steepest descent path from the saddle at $k_s = x/2t$, the straight line

$$k_I = -k_R + x/2t,$$

(150)

($k_R$ and $k_I$ are the real and imaginary parts of $k$) plus a small circle around the pole at $i\kappa_0$ after it has been crossed by the steepest descent path, for fixed $x$, at the critical time

$$\tau = \frac{x}{2\kappa_0}. $$

(151)

This procedure allows to recognize two $w$-functions [66], one for each integral,

$$\psi(x, t) = \frac{1}{2} e^{-it + ik^2t} [w(-u_0') + w(-u_0'')].$$

(152)

Here,
\[ u'_0 = \frac{1 + i}{2^{1/2}} t^{1/2} \kappa_0 \left( -i - \frac{\tau}{t} \right) \]
\[ u''_0 = \frac{1 + i}{2^{1/2}} t^{1/2} \kappa_0 \left( i - \frac{\tau}{t} \right) . \]

It is clear from the exact result (152, 153), that \( \tau \) is an important parameter that appears naturally in the \( w \)-function arguments, and determines with \( \kappa_0 \) the global properties of the solution. Its detailed role will be discussed next.

The simplest approximation for \( \psi(x,t) \) for times before \( \tau \) is to retain the dominant contribution of the saddle by putting \( k = k_s \) in the denominators of (154) and integrating along the steepest descent path,

\[ \psi_s(x,t) = \frac{e^{-it+i\kappa^2 t}}{2 \pi^{1/2}} \left( \frac{1}{u'_0} + \frac{1}{u''_0} \right). \]

The average local instantaneous frequency for this saddle contribution is equal to the frequency of the saddle point \( s \).

\[ \omega_s \equiv 1 + x^2/4t^2 . \]

After the crossing of the pole \( i \kappa_0 \) by the steepest descent path at \( t = \tau \) the residue

\[ \psi_0(x,t) = e^{-i\omega_0 t} e^{-\kappa_0 x} \Theta(t - \tau). \]

has to be added to (154),

\[ \psi(x,t) \approx \psi_s(x,t) + \psi_0(x,t) . \]

The solution given by Eq. (156) describes a monochromatic front which carries the signal into the evanescent medium. The conditions of validity of this approximation can be determined by examining the asymptotic series of the \( w(z) \) functions in (152) for large \( |z| \), see the Appendix. In fact (157) is obtained from the dominant terms of these expansions. Large values of \( \kappa_0 \) are obtained with large values of \( \kappa_0 \), \( \omega_0 \), or \( x \), and also when \( t \to 0 \). Within the conditions that make the saddle approximation valid, the contribution of the pole is negligible. To see this more precisely let us examine the ratio between the modulus of the two contributions,

\[ R(t) \equiv \left| \frac{\psi_0}{\psi_s} \right| = \frac{2\pi^{1/2}}{x} e^{-\kappa_0 x} \left( \frac{1}{2} \kappa_0 t^2 + \kappa_0^2 \right) . \]

Its value at \( \tau \) is an exponentially small quantity,

\[ R(t = \tau) = e^{-\kappa_0 x} (2\pi \kappa_0 x)^{-1/2} . \]

In summary, for the source with a sharp onset described here, the monochromatic front is not visible when the approximation (157) remains valid around \( t = \tau \). A complementary analysis is carried out in Chapter ....

However two very important observable features of the wave can be extracted easily from (157). The first one is the arrival of the \emph{transient front}, characterized by its maximum density at \( t_f \equiv \tau^{3/2} \). This time is of the order of \( \tau \), but the wave front that arrives does not oscillate with the pole frequency \( \omega_0 \), but with the saddle point frequency \( \omega_s \).

The second observable feature that we can extract from (157) is the time scale for the attainment of the stationary regime, or equivalently, the duration \( t_{tr} \) of the transient regime dominated by the saddle before the pole dominates. \( t_{tr} \) can be identified formally as the time where the saddle and pole contributions are equal, \( R = 1 \). Because of (159) we shall assume \( \tau << t_{tr} \) to obtain the explicit result

\[ t_{tr} \approx \left( \frac{x e^{\kappa_0 x}}{2 \kappa_0} \right)^{2/3} . \]

Finally, when \( x \kappa_0 \) is small \( (\lesssim 1) \), the saddle approximation describes correctly the very short time initial growth, but fails around \( \tau \) because the pole is within the width of the Gaussian centered at the saddle point. The pole cancels part of the Gaussian contribution so that the bump predicted by \( \psi_s \) at \( \tau^{3/2} \) is not seen in this regime. \( \tau \) does not correspond to any sharply defined feature, but provides a valid rough estimate of the attainment of the stationary regime.
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APPENDIX: PROPERTIES OF $w$-FUNCTIONS

The $w$-function is an entire function defined in terms of the complementary error function as

$$ w(z) = e^{-z^2} \text{erfc}(-iz). \quad (A1) $$

$w(z)$ is frequently recognized by its integral expression

$$ w(z) = \frac{1}{i\pi} \int_{\Gamma_-} \frac{e^{-u^2}}{u-z} du \quad (A2) $$

where $\Gamma_-$ goes from $-\infty$ to $\infty$ passing below the pole at $z$. For $\text{Im}z > 0$ this corresponds to an integral along the real axis. For $\text{Im}z < 0$ the contribution of the residue has to be added, and for $\text{Im}z = 0$ the integral becomes the principal part contribution along the real axis plus half the residue. From $(A2)$ two important properties are deduced,

$$ w(-z) = 2e^{-z^2} - w(z) \quad (A3) $$

and

$$ w(z^*) = [w(-z)]^*. \quad (A4) $$

To obtain an asymptotic series as $z \to \infty$ for $\text{Im}z > 0$ one may expand $(u-z)^{-1}$ around the origin (the radius of convergence is the distance from the origin to the pole, $|z|$) and integrate term by term. This provides

$$ w(z) \sim \frac{i}{\sqrt{\pi} z} \left[ 1 + \sum_{m=1}^{\infty} \frac{1 \cdot 3 \cdot \ldots \cdot (2m-1)}{(2z^2)^m} \right] \text{Im}z > 0 \quad (A5) $$

which is a uniform expansion in the sector $\text{Im}z > 0$. For the sector $\text{Im}z < 0$ $(A3)$ gives

$$ w(z) \sim \frac{i}{\sqrt{\pi} z} \left[ 1 + \sum_{m=1}^{\infty} \frac{1 \cdot 3 \cdot \ldots \cdot (2m-1)}{(2z^2)^m} \right] + 2e^{-z^2}, \text{Im}z < 0. \quad (A6) $$

If $z$ is in one of the bisectors then $-z^2$ is purely imaginary and the exponential becomes dominant. But right at the crossing of the real axis, $\text{Im}z = 0$, the exponential term is of order $o(z^{-n})$, (all $n$), so that $(A5)$ and $(A6)$ are asymptotically equivalent as $|z| \to \infty$.

$w(z)$ has the series expansion

$$ w(z) = \sum_{0}^{\infty} \frac{(iz)^n}{\Gamma(\frac{n}{2} + 1)}. \quad (A7) $$

The $w$-function is a particular case of the Moshinsky function $[68]$, which can be regarded as “the basic propagator for a Schrödinger transient mode” $[87]$.

[1] A. H. Zewail: Femtochemistry (World Scientific, Singapore 1994)
[2] R. F. Snider: J. Stat. Phys. 61, 443 (1990)
[59] Ph. A. Martin, Acta Phys. Austriae Suppl. 23, 159 (1981)
[60] M. Sassoli de Bianchi: Z. Phys. 35, 2719 (1994)
[61] V. F. Weisskopf and B. P. Wigner: Z. Phys. 63, 54 (1930); 65, 18 (1930)
[62] H. Jakobovits, Y. RothschilD, and J. Lecian: Am. J. Phys. 63, 439 (1995)
[63] G. García Calderón, J. L. Mateos and M. Moshinsky: Phys. Rev. Lett. 74, 337 (1995)
[64] J. G. Muga, G. W. Wei, and R. F. Snider: Ann. Phys. 252, 336 (1996)
[65] J. G. Muga, R. F. Snider and G. W. Wei: Europhysics Letters 35, 247 (1996)
[66] M. Abramowitz and I. A. Stegun: Handbook of Mathematical Functions (Dover, New York 1972); The function \( w \) is a particular case of Moshinsky’s function, see [68] and H. M. Nussenzveig: In Symmetries in Physics, ed. by A. Frank and K. B. Wolf (Springer, Berlin, Heidelberg 1992) pp. 293
[67] B. Misra and E. C. G. Sudarshan: J. Math. Phys. 18, 756 (1977); A. Peres: Am. J. Phys. 48, 931 (1980); W. M. Itano, J. D. Heinzen, J. J. Bollinger and D. J. Winley: Phys. Rev. A 41, 2295 (1990); K. Urbanowski: Phys. Rev. A 50, 2847 (1994)
[68] M. Moshinsky: Phys. Rev. 84, 525 (1951)
[69] G. García Calderón, G. Loyola and M. Moshinsky: In Symmetries in Physics, ed. by A. Frank and K. B. Wolf (Springer, Berlin, Heidelberg 1992) pp. 273.
[70] P. Exner: Open Quantum Systems y Feynman Integrals (Reidel, Dordrecht 1985)
[71] J. G. Muga, V. Delgado and R. F. Snider: Phys. Rev. B 52, 16381 (1995)
[72] K. Unnikrishnan: Am. J. Phys. 66, 632 (1998)
[73] K. W. H. Stevens: Eur. J. Phys. 1, 98 (1989)
[74] K. W. H. Stevens: J. Phys. C: Solid State Phys. 16, 3649 (1983)
[75] L. Brillouin: Wave propagation and Group Velocity (Academic Press, New York 1960)
[76] S. Brouard and J. G. Muga: Phys. Rev. A 54, 3055 (1996)
[77] J. G. Muga and J. P. Palao: J. Phys. A 31, 9519 (1998)
[78] J. G. Muga and M. Buttiker: Phys. Rev. A 62, 023808 (2000)
[79] P. Moretti: Phys. Scr. 45, 18 (1992)
[80] M. Büttiker and R. Landauer: Phys. Rev. Lett. 49, 1739 (1982)
[81] A. Ranfagni, D. Mugnai, P. Fabeni and P. Pazzi: Physica Scripta 42, 508 (1990)
[82] A. Ranfagni, D. Mugnai and A. Agresti: Phys. Lett. A 158, 161 (1991)
[83] N. Teranishi, A. M. Kriman and D. K. Ferry: Superlattices and Microstructures, 3, 509 (1987)
[84] A. P. Jauho nd M. Jonson: Superlattices and Microstructures 6, 303 (1989).
[85] M. Büttiker and H. Thomas: Ann. Phys. (Leipzig) 7, 602 (1998); Superlattices and Microstructures 23 781 (1998)
[86] A. D. Baute, I. L. Egusquiza and J. G. Muga: J. Phys. A, to appear: quant-ph/0007066.
[87] H. M. Nussenzveig: In Symmetries in Physics, ed. by A. Frank and K. B. Wolf (Springer, Berlin, Heidelberg 1992) pp. 293