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CHARACTERISTIC TIMES IN ONE DIMENSIONAL COLLISIONS

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Recent progress on the temporal characterization of one dimensional collisions by our group in La Laguna and Vancouver is reviewed. Dwell times and their decompositions, arrival times, exponential decay, characteristic asymptotic behaviour at large and short times, transient effects in tunnelling and anomalously short barrier traversal times are discussed.

1 Scattering theory and time dependence

Collisions are intrinsically time dependent but the monographs on scattering theory pay a lot of attention to the solutions of the time independent Schrödinger equation. This is in part because the traditional scattering experiment, aimed at the obtention of *cross sections*, is performed in quasi-stationary conditions and also because the stationary scattering states form a basis to analyze the actual time dependent collision. However it is becoming more and more important to consider explicitly the time dependence. Modern scattering experiments that incorporate femtosecond laser pulses make possible the observation of wave packet motion and the design of particular initial states to achieve specific dynamical behaviour. Also in semiconductor heterostructures the transient regimes are of interest to determine the ultimate speed of the devices. Scattering theory has to adapt to these new trends by developing a formal language in the time domain where the full collision process, and not just the asymptotic regimes and their connection, is taken into account.[a] Since the whole information contained in the wave function $\psi(x,t)$ is difficult to assimilate and hardly required this implies a synthesis effort to express the important dynamical features with a few time parameters. Quantities to measure the *duration of the collision*, the *arrival time* at a detector, the *life time* of an unstable state, the *delay* with respect to free motion, the characteristic *asymptotic behaviour* (at short and large time) or the time required to fill a region of space (e.g. to "charge" a well) or to achieve stationary conditions have to be defined and their properties examined. When the collision involves tunnelling the time dependence is particularly challenging. In addition to the

[a]It is not true anymore that the interaction region is not interesting because it is not observed. Precisely the goal of recent experiments in molecular dynamics is to observe the transition state and understand the intimate mechanisms of chemical reactivity.

time parameters mentioned above a *traversal time* for transmitted or reflected wave packet components is of interest.

An important part of our recent work, reviewed here, has been devoted to all these characteristic times of quantum collisions.[b]

2 Dwell time and its separation into transmission and reflection components

The standard measure of the duration of the collision is the *sojourn*, *dwell* or *mean* collision time,

$$\tau(a,b;t_1,t_2;\psi) = \int_{t_1}^{t_2} dt \int_a^b dx\, |\psi(x,t)|^2 \,. \tag{1}$$

Often a and b are chosen to cover the interaction region, t_1 is set to zero (an initial preparation time) and $t_2 = \infty$. The interpretation of this quantity as a mean time spent in the region $[a,b]$ by the *particle* (with the average performed over the members of the ensemble associated with ψ) is not straightforward. In the standard interpretation of the quantum mechanical formalism there are no trajectories and there is no obvious way to assign a time of presence to a given member of the ensemble of particles associated with the quantum state. There are however several formal arguments that provide (1) by extending to the quantum case the classical dwell time (e.g. via Feynmann path integrals,[1] causal or Bohm trajectories,[2] as an expectation value of a hermitian sojourn time operator,[3] or simply by using directly the classical expression for the dwell time[4]). Irrespectively of a hypothetical detailed statistical interpretation of the dwell time, our philosophy is to accept this quantity as a central characteristic quantity of the state ψ that provides a reasonable definition of the duration of the collision. An experimental determination of the dwell time by means of a time-resolved photoluminescence technique with a picosecond laser has been performed by Tsuchiya et al.[5] The dwell time is an important parameter in high speed applications of semiconductor structures.[6]

There is abundant literature on the **separation of the dwell time** into transmission and reflection components, possibly with interference terms. In the stationary case it would read

$$\tau = |T|^2\tau_T + |R|^2\tau_R + \text{interference terms.} \tag{2}$$

[b]Because of space limitations this is not a comprehensive review on the subject and the reference list of related papers is far from complete. The interested reader may find however a more detailed bibliography in the articles quoted.

(where T and R are respectively transmission and reflection amplitudes) with a similar relation for wave packets. This separation was initially one of our major objectives.[4,7,8,9] Separations, in principle measureable, based on the flux have been proposed,[4,9] and also based on projection operators. In quantum mechanics this separation is not unique and in general the partial times $\tau_{T,R}$ do not fulfill *classical conditions* (such as additivity, reality or positivity). In our opinion this is not necessarily a drawback if these quantities are shown to contain useful information.

Two sets of complementary projectors are associated with the questions: Is the particle in the region $[a,b]$? [D (yes), $1-D$ (no)] and; Will the particle be transmited? [P (yes), $Q=1-P$ (no)]. The dwell time is simple written as

$$\int_0^\infty dt\,\langle\psi|D|\psi\rangle\,, \tag{3}$$

and can be decompose by means of several resolutions of the projector D,[7,8,9]

$$\begin{aligned} D &= (P+Q)D = PD+QD = PDP+QDQ+PDQ+QDP \\ &= DPD+DQD = \frac{1}{2}[P,D]_+ + \frac{1}{2i}i[P,D]_- + \frac{1}{2}[Q,D]_+ + \frac{1}{2i}i[Q,D]_-\,, \end{aligned} \tag{4}$$

that lead to different decompositions of the dwell time. These projectors provide a compact classification scheme for many of the proposed times and simplify their connection and study.[10] The formalism also allows a probability theory analysis in terms of conditional and marginal probabilities.[7,8,9]

3 Arrival times

An important characteristic quantity is the arrival time at a detector. Allcock many years ago denied the possibility of defining an arrival time in quantum mechanics.[11] But the situation has changed drastically in the last few years and there is now renewed interest in the subject. Allcock's main objection was based on the fact that his model of a detector (a step imaginary potential) could not absorb the wave in a short spatial interval. But we have found conterexamples to Allcock's claim, i.e., complex potentials that absorb in a broad range of energies and occupy a small spatial interval.[c] A systematic procedure to construct potentials with the desired properties has been described.[12,13,14] To justify the expression proposed for the time of arrival [Eq.(6) below] an

[c]There is experimentl evidence of the existence of good enough absorbers: The agreement between measured and calculated collisional cross sections.

operational time of arrival is first defined based on the rate of absorption of the complex potential that models the detector,

$$\langle t\rangle_N = \frac{\int_0^\infty dt\, t\,(dN/dt)}{\int_0^\infty dt\,(dN/dt)}\,. \tag{5}$$

($N \leq 1$ is the norm.) A simple theoretical treatment then shows that for sufficiently good detectors and asymptotic positions this quantitity is essentially equal to the *ideal time* obtained from the flux J *without* complex potential,[17,13]

$$\langle t\rangle_J(x_1) = \frac{\int_0^\infty dt\; J(x_1,t)t}{\int_0^\infty\; dtJ(x_1,t)}. \tag{6}$$

When the contribution of negative momenta in the initial state is negligible the arrival time at $x_1 > d$ can be expressed as an average of stationary phase times (see Eq. (32) below),[9]

$$\langle t\rangle_J(x_1) = \frac{1}{\langle T\rangle}\int_0^\infty dp\,|\langle p\,|\psi(0)\rangle|^2|T(p)|^2\tau_p(x_0,x_1), \tag{7}$$

where $\langle T\rangle$ is the transmission probability of the wave packet.[15,16]

4 Exponential decay. Short and long time behaviour

Resonant tunneling has become a major research field. Many theoretical approaches on the time dependence in resonant scattering are devoted to justify the exponential decay. An ideal description of the decay of states influenced by resonances would allow an understanding of both the dominant exponential decay and the deviations from it. Progress in this direction has been achieved by representing the *survival amplitude* $A(t,\psi) \equiv \langle\psi(0)|\psi(t)\rangle$ as a discrete sum over resonant terms.[18] The possibility of tayloring the effective interaction potential for electronic motion in semiconductor structures [19] makes feasible the investigation of deviations from the exponential decay.

First the **short time behaviour** of the decay of the survival probability $S = |A|^2$ is discussed. Several authors have described a short time t^2 dependence of the *decay probability* $P_{\rm decay} \equiv 1 - S$, see e.g. papers related to the "quantum Zeno paradox". On the other hand a formal treatment and examples by Moshinsky and coworkers suggest a $t^{1/2}$ dependence of the decay probability at short times.[20,21] These two seemingly different claims are in fact compatible if one considers the possibility of initial states with infinite first or second energy moments.[22,23]

The survival amplitude $A(t,\psi)$ can be written in terms of the evolution operator $e^{-iHt/\hbar}$ as

$$A(t,\psi) = \langle\psi|e^{-iHt/\hbar}|\psi\rangle = \frac{i}{2\pi}\int_C dq e^{-izt/\hbar} M(q), \tag{8}$$

$$M(q) \equiv \frac{q}{m}\langle\psi|\frac{1}{z-H}|\psi\rangle \tag{9}$$

where $z = q^2/(2m)$ is a complex energy and q a complex momentum. The contour C goes from $-\infty$ to $+\infty$ passing above all of the singularities of the resolvent due to the spectrum of H. Let us assume that the function $M(q)$ can be analytically continued into the lower half q−plane. $M(q)$ has in general a set of *core* singularities, depending only on the potential, plus possibly other *structural* singularities depending on the particular state ψ. Let us also assume that a pole expansion of the form

$$M(q) = \sum_k \frac{a_k}{(q-q_k)}, \quad \Im\mathrm{m}\, q_k < 0 \tag{10}$$

is possible.[d] Here $k = 1, 2, 3\cdots$ indexes the poles. It is useful to deform the original integration contour to being along the diagonal D of the second and fourth quadrants of the q-plane (steepest descent path). The poles q_k crossed on carrying out this deformation contribute to $A(t)$ exponentially,

$$E_k(t) = a_k e^{-iq_k^2 t/(2m\hbar)} = a_k e^{-u_k^2}, \tag{11}$$

where $u = q/f$ is a convenient new variable which takes real values along D,

$$u_k \equiv q_k/f, \quad f \equiv (1-i)\sqrt{(m\hbar/t)}. \tag{12}$$

Independently of being crossed or not crossed by the contour deformation, all poles contribute because of the integral along the diagonal. Each pole contribution is expressed in terms of a known function, the w-function,[24] as

$$D_k(t) = -\frac{a_k}{2}\mathrm{sign}(\Im u_k)\, w[\mathrm{sign}(\Im u_k) u_k]. \tag{13}$$

Combining the contributions,

$$A(t) = \sum_k [E_k(t) + D_k(t)] = \sum_k \frac{1}{2} a_k w(-u_k). \tag{14}$$

[d] Higher order poles can be treated in a similar fashion and an example of a more complex case is described in section V.

($E_k(t) = 0$ for poles that have not been crossed when deforming the contour). In the first form of (14), the exponential decay in E_k is separated from the "correction" D_k. However the second compact expression is very useful for studying the short time behaviour.

The Taylor series of the w–function[24] gives a series for $A(t)$ in powers of $t^{1/2}$. This suggests a short time $t^{1/2}$ dependence of the decay probability, as claimed by Moshinsky and coworkers.[20,21] On the other hand, if we formally expand the evolution operator, $e^{-iHt/\hbar} = 1 - iHt/\hbar + ...$, there results a t^2 dependence,

$$P_{\text{decay}} = \frac{t^2}{\hbar^2}\left(\langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2\right) + \cdots. \tag{15}$$

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. Let us consider the first two derivatives of A at time $t = 0$ first from the formal series of the evolution operator and then by assuming a general short time dependence of the form $A \sim 1 + b\,t^c$, where b and c are finite constants,

$$\left.\frac{dA}{dt}\right|_{t=0} = \frac{-i}{\hbar}\langle\psi|H|\psi\rangle = b\,c\,t^{c-1}\Big|_{t=0} \tag{16}$$

$$\left.\frac{dA^2}{dt^2}\right|_{t=0} = -\frac{1}{\hbar^2}\langle\psi|H^2|\psi\rangle = b\,c\,(c-1)t^{c-2}\Big|_{t=0}. \tag{17}$$

If the first and/or second moments are infinite the possible values of c are restricted. In particular, in the following table the behaviour described on the right column is in principle possible when the condition on the left column is satisfied

$$\langle\psi|H|\psi\rangle = \infty \qquad P_{\text{decay}} \sim t^{1/2} \tag{18}$$

$$\langle\psi|H|\psi\rangle < \infty \text{ and } \langle\psi|H^2|\psi\rangle = \infty \qquad P_{\text{decay}} \sim t^{3/2} \tag{19}$$

$$\langle\psi|H|\psi\rangle < \infty \text{ and } \langle\psi|H^2|\psi\rangle < \infty \qquad P_{\text{decay}} \sim t^2 \tag{20}$$

Examples where $t^{1/2}$, $t^{3/2}$ and t^2 dominate the short time behaviour of P_{decay} are provided in ref.[22]. It is shown that when the decay probability behaves as $t^{3/2}$ or t^2 the coefficients for lower powers of t vanish because of cancellations between different pole contributions.[25]

The **long time behaviour** of the probability density in one dimensional collisions is discussed next.[26] It is assumed for simplicity that there are no bound states. The propagator in terms of the contour C in the complex momentum q-plane is given by

$$\langle x|e^{-iHt/\hbar}|x'\rangle = \frac{i}{2\pi}\int_C dq\, I(q)e^{-izt/\hbar}, \tag{21}$$

$$I(q) \equiv \frac{q}{m}\langle x|\frac{1}{z-H}|x'\rangle\,. \tag{22}$$

Due to the exponential $e^{-izt/\hbar}$ in (21) the large t behaviour is dominated by the region around the origin (saddle point). Assuming that the resolvent matrix element $\langle x|(z-H)^{-1}|x'\rangle$ can be analytically continued into the lower half q-plane (This is valid in particular for finite range potentials.[27]) and provided that the analytically continued function is analytical at the origin it has a Taylor series expansion If this is the case then $I(0)=0$. Because of the (odd) q factor in (22), the first term, a_0, does not contribute to the integral (21). The asymptotic formula for the propagator comes therefore from the second term. Introducing again the variable $u=q/f$ and deforming the contour along the steepest descent path,

$$\langle x|e^{-iHt/\hbar}|x'\rangle \sim \frac{i}{2m\pi}a_1 f^3\int du\, u^2 e^{-u^2} = \frac{1-i}{2m\sqrt{\pi}}a_1\left(\frac{m\hbar}{t}\right)^{3/2}. \tag{23}$$

So when $I(0)$ vanishes a t^{-3} asymptotic behaviour of the probability density occurs. This can arise either via a cancellation between free and scattering parts, i.e., $I_s(0)=-I_f(0)\neq 0$ or both terms can vanish separately, $I_s(0)=I_f(0)=0$. Examples of both cases are provided in ref. [26]. An exception is the free motion on the full line. In this case the resolvent matrix element diverges at the origin and $I_f(0)=-i/\hbar\neq 0$. The asymptotic behaviour of the probability density for free motion on the full line is t^{-1}.

5 Transient and asymptotic effects in tunnelling

A possible route to define a fundamental tunnelling time implies regarding quantum mechanics as a statistical theory where the concept of *particle trajectory* is a valid one.[2,28] But we don't know at present if any of the hidden variable theories is a faithful representation of reality. Instead of emphasizing the *particle*, we may concentrate on the *wave* aspect of the quantum state and look for a condensed description in terms of characteristic times. This simplification is frequently achieved by means of asymptotic approximation methods. Localizing the origin of the main contributions to the wave is not only of conceptual interest, it also improves the efficiency of numerical calculations. The simplest result in this direction is the asymptotic "phase time" that results from applying the *stationary phase approximation*. A more complete asymptotic analysis is based on deforming the contour integrals in order to single out dominant contributions from *critical points* (poles, saddle points, branch points).[30] Stevens used this idea to examine a sequence of "tunnelling problems" involving a step potential barrier. His work has been later extended.[31–35]

A clear limitation of asymptotic methods is their inability to deal with non asymptotic situations. A second drawback of too simple an expansion is known as "non uniformity", a single asymptotic expansion may not be valid for all values of the parameters involved. Another pitfall to be avoided is the temptation to assign too much importance to "mathematical events" of a particular critical point (for example, to the crossing of a pole by a steepest descent path). The order of magnitude of the contribution of other critical points can be similar (and its interference effect destructive) or larger.

We have recently overcome some of these difficulties by working out an *exact* solution of the dynamics that retains the basic philosophy of expressing the wave function in terms of contributions from critical points.[36] Specifically the collision of a state initially prepared as a "half plane wave",

$$\psi(x,0) = \begin{cases} h^{-1/2}\exp(ip_0x/\hbar), & x<0 \\ 0, & \text{otherwise,} \end{cases} \tag{24}$$

with a square barrier from 0 to d and height V_0 has been studied. This work follows a series in the wake of Stevens [31–35] but emphasizes and determines quantitatively the role of resonances by means of resonance-decomposition techniques.[18] Indeed, the contribution of the resonances is essential for the description of the transient regime.

The basic formalism can be illustrated with the free motion case. This problem was first solved by Moshinsky.[37] By expanding the evolution operator in a plane wave basis the wave function is written as

$$\psi_0(x,t) = \frac{i}{2\pi h^{1/2}}\int_{-\infty}^{\infty}\frac{e^{i[px-p^2t/2m]/\hbar}}{p-p_0+i0}\,dp \qquad (x,t>0). \tag{25}$$

As done before, the integration contour can be deformed to a $-45°$ straight line $\Gamma(t)$. The novelty now is that the saddle point of the exponent is at $p = mx/t$ so that the contour "moves". For a fixed position x the saddle point goes from ∞ to 0 as t grows from 0 to ∞, larger times being associated with low momenta and shorter times with high momenta. At $t_c = mx/p_0$ the structural pole at p_0 is crossed and for $t > t_c$ the integration contour $\Gamma(t)$ includes a circle around the pole p_0. Alternatively, for fixed t, the pole is crossed at $x_c = p_0t/m$. The crossing of the pole by the contour as t (or x) varies selects an instant (or coordinate) which describes approximately the motion of the wave front, and assigns a velocity of propagation to that part of the wave function. A crude approximation to the integral (25) retains only the residue due to the deformation of the contour around the pole. This leads to an approximate "step" wave function that keeps the shape of the original state but displaces the front with velocity p_0/m. A better approximation would consider in addition the contribution of the saddle point. But since saddle and pole do eventually coincide (as t or x vary), a special uniform expansion would be required. Actually the integral can be carried out exactly by completing the square in the exponential and using the variable $u = \frac{p-mx/t}{f}$. Then, Eq. (25) and the contour deformation lead to

$$\psi_0(x,t) = \frac{e^{imx^2/2t\hbar}}{2h^{1/2}}\, w(-u_0) \qquad u_0 = (p_0 - mx/t)/f;\ (x,t > 0)\,. \tag{26}$$

This expression incorporates all the information including the situations before, at and after the crossing and the wave front shape is exactly described. An interesting property of the w–function is $w(-u_0) = 2e^{-u_0^2} - w(u_0)$. After the crossing the exponential is the part that one would get from the residue. The $w(u_0)$ term corrects this crude estimate. u_0^2 is purely imaginary and the exponential does *not* decay with time while $w(u_0)$ does decay At fixed x, $u_0^2 \sim ip_0^2 t/2m\hbar$ as $t \to \infty$ and a stationary regime with constant probability density is reached. However, when the poles have a negative imaginary part, as discussed next, the exponential contribution from the residue decays.

The solution at time $t > 0$ of the Schrödinger equation for the square barrier can be written in integral form by following similar steps as for the free case,

$$\psi_T(x,t) = \frac{1}{h^{1/2}} \int_{-\infty}^{\infty} dp\, T(p)\, e^{ipx/\hbar}\, e^{-iE_p t/\hbar}\, \langle p|\psi(0)\rangle \quad (x > d), \tag{27}$$

where for negative p, $T(p)$ is the analytical continuation of the (positive p) transmission amplitude. (In spite of its simplicity the derivation and meaning of this equation are are non-trivial.[36])

A similar analysis to the one leading to (27) is possible for the barrier region, $0 \le x \le d$. Because of the rapid oscillations of the integrand these integral expressions are difficult to evaluate numerically, so we look for an alternative integration contour in the complex momentum plane which allows to obtain $\psi(x,t)$ efficiently and to express the result as a sum of contributions from a set of critical points.

For $x > d$, the integrand is considered as a function of the complex variable p and the contour is deformed into a straight -45° line crossing the real axis at the stationary point $p = m[x + \hbar d\alpha/dp|_{p_0}]/t$ (α is the phase of the transmission amplitude, $T(p) = |T(p)|e^{i\alpha}$), plus circles around each of the poles that have been "crossed". Using the variable $u = \frac{p-m[x+\hbar d\alpha/dp|_{p_0}]/t}{f}$ one obtains

$$\psi_T(x,t) = f\, e^{im[x+\hbar d\alpha/dp|_{p_0}]^2/2\hbar t} \int_{\Gamma_u} du\, g_T(u)\, e^{-u^2}, \tag{28}$$

where the function $g_T(u)$ is meromorphic and has resonant poles in the lower p−plane.

At small times and when the saddle at $u = 0$ is far from the nearest pole the saddle is the only important critical point. In this case g_T can be expanded in a power series around $u = 0$ and the resulting series can be integrated term by term.[e] An asymptotic formula for the probability density at the front tail may be obtained by retaining the first term,

$$|\psi(x,t)|^2 \sim \frac{t}{4m\pi^2 x^2} \qquad (x/t \to \infty), \tag{29}$$

which is actually the same expression obtained for free motion.[f] However, when the contour moves closer to the poles the above method is useless. The way out is to extract explicitly the singularities of g_T due to the resonant poles (from $j = 1$ to $j = \infty$) and the structural pole ($j = 0$), leaving the remainder as an entire function $h_T(u)$,

$$g_T(u) = \sum_{j=0}^{\infty} \frac{A_j}{u - u_j} + h_T(u), \tag{30}$$

where $u_j = f^{-1}\,\{p_j - m[x + \hbar d\alpha/dp|_{p_0}]/t\}$ and A_j is the residue of $g_T(u)$ at $u = u_j$. Finally, using the w−functions, $\psi_T(x,t)$ can be written as

$$\begin{aligned} \psi_T(x,t) &= f\, e^{im[x+\hbar d\alpha/dp|_{p_0}]^2/2\hbar t} \\ &\times \left[-i\pi \sum_{j=0}^{\infty} A_j\, w(-u_j) + \int_{-\infty}^{\infty} h_T(u)\, e^{-u^2}\, du \right]. \end{aligned} \tag{31}$$

Since h_T is an entire function it has an infinite power series with infinite convergence radius and the integral can be expressed in terms of its only critical point, the saddle at $u = 0$. An excellent ("uniform") approximation in the full range of times and/or positions is obtained by keeping only the first term in this series. In summary, $\psi_T(x,t)$ **can be written as an explicit sum over critical points: Resonances, the structural pole, and the saddle.** In our calculations two or three summands are enough to accurately follow the propagation even at short (non asymptotic) times.

A velocity of propagation $v_j = [\text{Re}\,(p_j) + \text{Im}\,(p_j)]/m$ can be assigned to each pole contribution by the condition for the crossing of each pole p_j by

[e] The radius of convergence of the series for g_T is the distance from $u = 0$ to the nearest pole.

[f] From another viewpoint this is to be expected since high momentum components behave classically[38] and the free motion of a wave packet can be mimicked classically

the contour [Im $(u_j) = 0$]. The term associated with a pole p_j is observed or not in the shape of the wave function depending on the value of A_j and on the interferences taking place between the different contributions. As a crude estimate, the residue for p_0 has the step shape whereas the residues associated with p_j $(j > 0)$ decay as x decreases, due to the negative imaginary part of p_j.

After crossing each pole the contributions decay with time except for $j = 0$. After having crossed all poles the dominant contribution is $w(-u_0)$. The only remaining term in the strict $t \to \infty$ limit is the residue associated with $w(-u_0)$.

For $0 \leq x \leq d$ the analysis is more complex but it follows similar lines. Because the structural pole $p_0' \equiv (p_0^2 - 2mV_0)^{1/2}$ is now located in the positive imaginary axis, and x is bounded by d it is much easier now than in the transmission region that several critical points contribute simultaneously. Recognizing individual contributions in the total wave becomes impossible because of the interference effects. However, as time increases all contributions except the one from the structural pole decay so the wave function in the barrier can be eventually expressed by a single w–function.

Following similar crude estimates for the main front and resonance forerunners in the transmission region we might try to estimate the wave inside the barrier by the contribution from the residue at the structural pole. This residue gives an attenuated exponential function whose wave front would moves with the "semiclassical velocity" $v_s = (2mV_0 - p_0^2)^{1/2}/m$. However, the front predicted by this contribution[32] is not seen, even approximately, in the real wave. Stevens considered the same initial condition used in this work but an infinitely wide square barrier (a potential step), and claimed that the concept of signal velocity was still valid for the tunnelling regime in the barrier region. It was later shown[34] that this velocity is actually unobservable in the tunnelling case because of the important contribution of the saddle. In our case in addition to the saddle, the branch point and the resonances preclude the identification of a wave front. One of the consequences is that the semiclassical time d/v_s is a poor indication of the "charging or build-up time", a time scale indicating the rate at which the maximum probability is achieved within the barrier.[39] Also, since the crossing of some of the resonant poles occurs (within the barrier) *after* the structural pole in the imaginary axis has been crossed, d/v_s has little to do with the time required to achieve the stationary regime within the barrier.[g] The resonance pole crossings (plus the corresponding exponential decays) determine the relevant time scale for the approach to the stationary regime.

[g]This time is however relevant when a second degree of freedom is coupled to the traslational motion.[44]

6 Anomalously short tunnelling times

One particularly intriguing aspect of the dynamics of collisional tunnelling is that some of the proposed definitions for the tunnelling time imply anomalously short durations for the barrier traversal. This occurs for example in the so called "extrapolated stationary phase times". For packets with a well defined momentum the point of stationary phase of the integrand of the transmitted packet arrives at $x_1 > d$ at time

$$\tau_{p_0}(x_0, x_1) = \frac{m}{p_0}[(x_1 - x_0) + \hbar d\alpha/dp|_{p=p_0}], \tag{32}$$

where x_0 is the center of the initial packet. It is tempting to extrapolate and interpret

$$\tau_{p_0}^{\rm ext} = \frac{m}{p_0}[d + \hbar d\alpha/dp|_{p=p_0}], \tag{33}$$

as a "transversal time" across the barrier. For large enough barriers $\tau_{p_0}^{\rm ext}$ becomes independent of the barrier length. (This is the Hartman effect.[40]) The above interpretation however rests on the assumption that the packet evolves "freely" out of the barrier region $(0, d)$. But wave packets with a well defined momentum are broad in coordinate representation and are severely deformed both before the hypothetical "entrance" instant $t_{\rm ent} = |x_0|m/p_0$ and after the "escape" instant $t_{\rm esc} = t_{\rm ent} + \tau_{p_0}^{\rm ext}$. For arbitrary packets, a common procedure is to define the entrance and escape times by extrapolating the asymptotic free motion of the peaks or centroids of the ingoing and transmitted packets up to their crossing with the barrier edges. But the same type of criticism applies.[h]

Instead of associating the position of the particle with a particular feature of the packet, such as the peak, we prefer to take seriously the statistical interpretation of the wave function and define averages. For the "escape" instant we average the time of arrival using the flux of particles as a distribution of passage times. As discussed before this ideal time, $\langle t \rangle_J$, is essentially coincident with an operational time $\langle t \rangle_N$ defined in terms of an absorbing detector. A proper definition of the entrance time into the barrier is also required. However, this turns out to be more involved since the conditions that allow the approximate equality $\langle t \rangle_N \approx \langle t \rangle_J$ do not generally hold in this case. Moreover there is the serious objection that the flux at this point involves both "to be transmitted" and "to be reflected" amplitudes. Actually the "to be reflected" component becomes dominant for wide enough barriers.[42] Selection of the positive part of the flux alone does not solve this conceptual difficulty. Moreover

[h] There are examples where the transmitted packet emerges *before* the incident peak has arrived at the left edge.[41]

there are many definitions of "positive flux".[43] A reasonable compromise consists in localizing the initial wave packet close enough to the left edge of the barrier with a small spatial width compared to the barrier lenght d, in such a way that one can identify the entrance and the preparation instant within a tollerable small uncertainty.[i] However Low and Mende have shown [45] that due to this localization the "usual wave packet analysis", which makes use of the the passage of the peak of undeformed packets to determine the traversal time, fails due to the incompatibility of a series of conditions: (I) $|x_0| << d$. (II) Negligible contribution to the initial wave packet of negative momentum components; (III) Negligible penetration through the barrier in the initial packet in comparison with the transmission probability; (IV) In order to follow unambiguously the peak position of the wave packet it must propagate without appreciable deformation with respect to the incident packet. This implies low momenta, $p_0 << p_b$, where $p_b = (2mV_0)^{1/2}$ is the barrier height in momentum units; (V) $|T(p)\langle p\,|\psi(0)\rangle|_{p=p_0} >> |T(p)\langle p\,|\psi(0)\rangle|_{p=p_b}$ is also imposed in ref.[45] to assure that expansions around p_0 can be made.

Low and Mende speculated that, under conditions I-IV, the transmitted part of the wave packet would be dominated by momentum components with energies above the barrier height. The eventual dominance of over the barrier components for wide enough barriers was already noted by Hartman.[40] In the recent literature on the Hartman effect this fact has been frequently ignored, perhaps because it is not directly evident from the expression (33) which refers to a single plane wave momentum and not to a real wave packet. The critical barrier length, d_c, where the transition between tunnelling and over the barrier motion takes place is given by [9,46]

$$d_c \approx \left(\frac{(p_b - p_0)^3}{p_b + p_0}\right)^{1/2} \left(\frac{\hbar^{1/2}}{2(\Delta_p)}\right)^2 . \qquad (34)$$

where Δ_p^2 is the momentum variance of the initial wave packet. Using the conditions I-IV and comparing with (34), one finds that $d >> d_c$ as speculated by Low and Mende. However, it has been pointed out [46] that I and III are well motivated on physical grounds but the other conditions are too severe since they are imposed to assure the applicability of the formalism used. Actually the arrival time analysis based on Eq.(6) does not require any predetermined form for the arriving wave packet, i.e., it does not require conditions IV and

[i] A possible solution proposed to the paradox of rapid transmission has been the association of the transmitted peak with the front of the incident wave packet. However in standard quantum mechanics the concept of point to point influence is far from simple.[47] The localization imposed in our approach circunvents the problem of associating the transmitted particles with a particular region of the initial packet.

II. The question then is if the conclusions by Low and Mende are valid for less restrictive conditions and if their speculation is founded. By imposing only the conditions I and III a systematic numerical calculation shows that for initial states localized close enough to the barrier to permit an accurate transmission time measurement, the process is also dominated by over the barrier transmission.[46] Similar conclusions are drawn from a two detector model, one before and one after the barrier, when the first detector has a small spatial width.[48]

7 Concluding remark

Time is always problematic in quantum mechanics and in particular in scattering theory it has been traditionally relegated to a secondary role. There is nowadays a need to develop a new language emphasizing time dependence which incorporates different characteristic quantities that summarize the essential features of the wave dynamics. (The complexity of a quantum mechanical collision, and in particular of collisional tunnelling cannot be trapped with a single quantity unless one is interested in a very specific aspect.) Steps towards this goal have been reviewed.

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