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DOES POSITIVE FLUX PROVIDE A VALID DEFINITION OF TUNNELLING TIMES?

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One of the possible definitions ($\langle\tau_{OR}\rangle$) of the quantum transmission tunnelling time is based on the (normalized) positive flux at the barrier edges. Two recent articles in this journal hold conflicting views on the validity of this definition and on the existence of negative values of $\langle\tau_{OR}\rangle$ in some cases [**85,** 115 (1993) and **89,** 31 (1994)]. We have performed independent calculations that show unambiguously that $\langle\tau_{OR}\rangle$ can be negative. Arguments are given against the interpretation of $\langle\tau_{OR}\rangle$ as a tunnelling time for transmitted particles.

IN QUANTUM mechanics, there is no obvious or generally accepted way to define a quantity for the time that a particle which is finally transmitted through a barrier has spent in it [1]. This is the *tunnelling time problem.* The difficulties can be traced back to the non commutativity of the operators associated with "being in the barrier" and "being finally transmitted" [2].

Olkhovsky and Recami [3] proposed a definition of the average tunnelling time as the difference between an average exit instant, $\langle t\rangle_{out}$, at the right edge of the barrier ($x = d$) and an average entrance instant, $\langle t\rangle_{in}$, at the left edge ($x = 0$):

$$\langle\tau_{OR}(0,d)\rangle = \langle t\rangle_{out} - \langle t\rangle_{in}$$

$$\equiv \frac{\int_{-\infty}^{\infty} \mathrm{d}t\, tJ_+(d,t)}{\int_{-\infty}^{\infty} \mathrm{d}t\, J_+(d,t)} - \frac{\int_{-\infty}^{\infty} \mathrm{d}t\, tJ_+(0,t)}{\int_{-\infty}^{\infty} \mathrm{d}t\, J_+(0,t)}. \quad (1)$$

(We shall limit the present discussion to square barriers for simplicity, assuming that the initial wave packet is incident from the left.) Here the "positive flux" $J_+(x,t) \equiv \Theta(J)J(x,t)$, where Θ is the Heaviside or "unit step" function and $J(x,t)$ is the quantum current density at position x and time t, plays (when normalized) the role of a distribution of passage times. Olkhovsky and Recami interpreted $\langle\tau_{OR}(0,d)\rangle$ as the "average transmission time". Since this time remains for nearly monochromatic packets essentially constant with respect to d in the "Hartman regime", effective superluminal speeds were described. Olkhovsky and Recami suggested that the infinitely large speeds could perhaps disappear in a "self-consistent relativistic quantum theoretical treatment". If, on the contrary, the effect were not to disappear, they related it to other superluminal phenomena described within relativistic theories [3]. Later on, Leavens criticized this approach [4] because of its "inability to isolate the contribution of *to be transmitted* electrons to the probability current density at the leading edge of the barrier" and showed by numerical evaluation of equation (1) with d replaced by $x < d$ and the lower limit $-\infty$ replaced by 0, that $\langle\tau_{OR}(0,x)\rangle$ can be negative. In their response Olkhovsky, Recami and Zaichenko [5] claimed that the integration limits should be maintained as in equation (1) and that "by using parameters very near to the ones adopted by Leavens..." no negative values were obtained [6].

First of all it should be emphasized, as pointed out in [7], that the initial conditions imposed on the wave packets in papers [4] and [5] are different and therefore different numerical values can be expected. Leavens uses the standard convention in numerical wave packet computations: A "minimum" Gaussian packet (with a minimum position-momentum uncertainty product) at a large distance from the barrier ($\langle x\rangle < 0$) is the initial state at time $t = 0$. In his calculation the lower time limit of equation (1) becomes the "preparation time" $t = 0$. Instead, the lower time limit in the calculations by Olkhovsky, Recami and Zaichenko is $t_i < 0$ because they use a convention in which the centroid of the incident wave packet would reach the origin $x = 0$ at $t = 0$ in the absence of the barrier. Moreover they choose the wave packet so that at $t = 0$ and in the absence of the barrier it is a minimum Gaussian [8]. Since the initial wave packet used by Leavens is a minimum packet with $\langle x \rangle < 0$, there is not an exact correspondence between the two calculations. Because different conventions are used for the origin of time $t = 0$, the lower time limit used by Leavens is, in fact, consistent with the way in which the authors of [5] interpret equation (1) in their own calculations. Of course, in any numerical computation, and in real experiments, the integration limits are finite, say $t = t_i$ and $t = t_f$. These values are in practice chosen so that at t_i and t_f the packet is far from the barrier.

Leavens initial packet is far from the barrier and it is physically unjustified to change his lower time limit of $t = 0$ to negative values. In any case the extension of the lower limit to $t_i = -\Delta$ in his calculation does not alter the result, because before $t = 0$ the flow of density at the barrier is negligible. On the contrary, with the convention for the origin of time used by Olkhovsky, Recami and Zaichenko, times $t < 0$ do provide an important contribution and cannot be neglected. At the risk of being repetitive we shall emphasize that in [3, 5] $t = 0$ is a time in the midst of the collision, but in [4] $t = 0$ is a preparation time when the collision has not yet started.

Leavens [4] uses a fourth order in time step symmetrized product formula grid method to evaluate the evolved state $\psi(t)$, while Olkhovsky, Recami and Zaichenko [5] use an integration over momentum with the cutoff $\Theta(p_b - p)$, where p_b is the barrier "height" in momentum units. Although the results calculated by Leavens were consistent with a number of numerical checks, he recognized the possibility that the unphysical negative values obtained for $\langle \tau_{OR}(0,x) \rangle$ "could arise from mistakes in the numerical calculations" [7]. In order to check the accuracy of these results we have done the calculation independently with a numerical method based on the quadrature

$$< x|\psi(t)\rangle = \int_{-\infty}^{\infty} \mathrm{d}p \langle x|p^+ < p^+|\psi(0)\rangle \mathrm{e}^{-iE_p t/\hbar}, \qquad (2)$$

where $|p^+\rangle$ is the solution of the Lippmann–Schwinger equation [therefore an eigenstate of the Hamiltonian H with eigenvalue $E_p = p^2/(2m)$] with outgoing scattered part and ingoing plane wave $|p\rangle$.

Standard scattering theory allows one to simplify this equation by using the relation $\langle p^+|\psi(0)\rangle = \langle p|\phi(0)\rangle$, where ϕ is the ingoing ("free") asymtote of the state ψ. Provided that the momentum representation of $\psi(0)$ has negligible negative momentum component and that $\psi(0)$ is sufficiently far from barrier $\phi(0)$ and $\psi(0)$ can actually be equated in this integral [9], and the lower limit can be changed to 0 in equation (2). We have numerically checked the validity of this procedure in all cases [10].

We have recalculated the curve showing negative values of $\langle \tau_{OR}(0,x) \rangle$ for $x \lesssim 7$ Å in Fig. 3 of [4] with the same initial conditions. Our converged results, see Table 1, are in excellent agreement with the calculation by Leavens.

The negative values of $\langle \tau_{OR}(0,x) \rangle$ obtained in this particular calculation are very small in absolute value and refer to points x in the interior of the barrier considerably less than the barrier width d of 10 Å. In order to dissipate any doubt on the existence of negative values of $\langle \tau_{OR} \rangle$ we have looked for initial conditions that enhance this effect several orders of magnitude and allow for negative times $\langle \tau_{OR}(0,d) \rangle$ for the entire barrier. Figure 1 shows $\langle \tau_{OR}(0,d) \rangle$ for a minimum Gaussian packet, which is very far from the barrier at time $t = 0$, as a function of the barrier width d (the detailed numerical data are provided in the figure caption). The negative values arise as the combination of an initial negative slope of $\langle t \rangle_{out}$ and a saturation of $\langle t \rangle_{in}$ for large enough d, see Fig. 2. Recalling the exponential decay of the transmission with d for opaque barriers, the saturation of $\langle t \rangle_{in}$ can be associated with the fact that the amount of density finally transmitted has negligible effect in this quantity, which for sufficiently large d has already the value it would take in the limit $d \to \infty$, where $\langle t \rangle_{in}$ is

Table 1. Transmission time $\langle \tau_{OR}(0,x) \rangle$ for various distances x *within the barrier calculated with the same conditions used in Fig.* 3 *of* [4]

x (Å)	Transmission time $\langle \tau_{OR}(0,x) \rangle$ (s)	
	This work	[4]
1	-6.51×10^{-18}	-6.50×10^{-18}
2	-1.30×10^{-17}	-1.30×10^{-17}
3	-1.95×10^{-17}	-1.95×10^{-17}
4	-2.59×10^{-17}	-2.59×10^{-17}
5	-3.12×10^{-17}	-3.12×10^{-17}
6	-2.54×10^{-17}	-2.54×10^{-17}
7	8.50×10^{-17}	8.49×10^{-17}
8	1.01×10^{-15}	1.00×10^{-15}
9	2.20×10^{-15}	2.20×10^{-15}
10	2.36×10^{-15}	2.36×10^{-15}

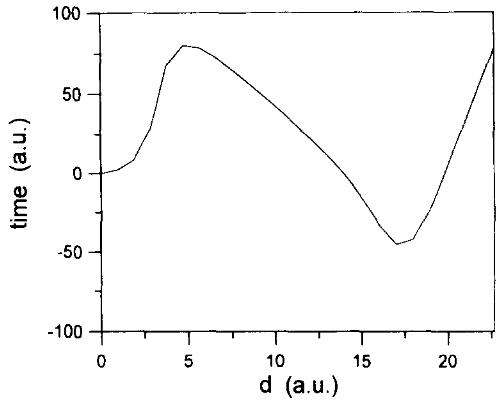

Fig. 1. $\langle\tau_{OR}(0, d)\rangle$ vs d (in atomic units). Mean position and momentum of the packet at time $t = 0$: $\langle x\rangle = -350$ a.u., $\langle p\rangle = 0.494976$ a.u.; square root of position variance $\Delta x = 8$ a.u.; mass $m = 1$ a.u.; barrier energy $V_0 = p_0^2/2$, where $p_0 = 0.8573243$ a.u.

unambiguously due to reflected particles *only*. The interpretation of $\langle\tau_{OR}\rangle$ as a tunnelling time for "transmitted particles" is therfore unjustified. The negative slope of $\langle t\rangle_{out}$ is seemingly in contradiction with the constant value predicted by the "Hartman effect". However, this constant value is only obtained in the strict monochromatic limit. The decrease of $\langle t\rangle_{out}$ with d is due to the filtering effect of the barrier and can be enhanced by increasing the momentum width of the packet and the distance from its initial position to the barrier. At a critical barrier width, the opacity of the barrier is so large that the transmitted packet begins to be dominated by momenta over the barrier. The transition point has been quantitatively estimated in [2]. For larger d values the increase of $\langle t\rangle_{out}$ can be basically understood in terms of classical motion over the barrier. Note that we have *not* imposed a momentum cutoff to exclude such

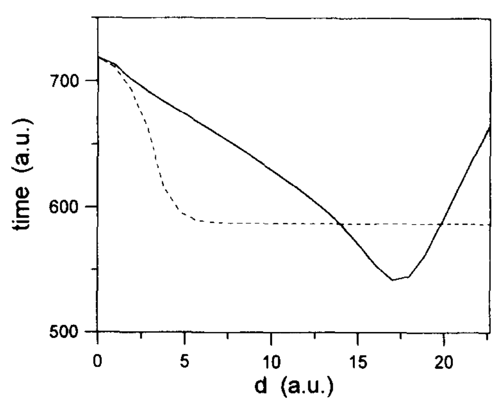

Fig. 2. $\langle t\rangle_{in}$ (dashed line) and $\langle t\rangle_{out}$ (solid line) vs d. Same conditions as for Fig. 1.

motion. But a cutoff could only make the time $\langle\tau_{OR}\rangle$ more negative since the increase of $\langle t\rangle_{out}$ would not be seen. Moreover we find no physical justification for such a cutoff.

Contrary to a claim in [3] the expression (1) does not yield even classically the time that a transmitted particle spends in a region $(0, d)$. Assume a classical ensemble of particles with non-zero momentum spread that collides with a linear barrier of maximum height αd, $V(x) = \alpha x\Theta(d - x)\Theta(x)$. The average time that the transmitted particles spend in $(0, d)$ has to be computed by averaging only over the subensamble of transmitted particles, i.e., over those particles with $E > \alpha d$. Thus, while the expression for $\langle t\rangle_{out}$ is correct classically, the expression for the entrance instant is not correct, because "to be reflected" particles contribute also to J_+ at $x = 0$. In fact it is not difficult to find examples where the classical time computed with equation (1) gives negative values. Perhaps the simplest one is an ensemble of two classical particles which start at $x \ll 0$ at $t = 0$, one with energy $E^+ \gg \alpha d$ and the other one with a very small energy $E^- < \alpha d$, close to zero. In this case, $\langle t\rangle_{out} - \langle t\rangle_{in} < 0$ (when computing these averages only the rightwards passage is considered). The negative time is found in this case because the slow particle takes a very long time to cross $x = 0$ while the fast particle crossed $x = d$ much earlier. This does not imply any conflict with relativity!

Finally, the definition of transmission times given in [3] is similar to one proposed by some of us in a previous article [11], where a different definition of J_+ was used. In that article the objective was to find a decomposition of the dwell time into transmitted and reflected parts, but the partial times could not be associated with subensembles of transmitted and reflected particles since the average entrance instant is common for the two partial times.

Our previous analysis does not mean that the flux is not a useful quantity to characterize temporal aspects of collisions. From an operational view, the (normalized) flux is a valid distribution function when it can be associated with the rate of absorption of a detector at a point x_1 (for simplicity we assume here that $x_1 \gg d$). When the detector is essentially a perfect absorber that can be modeled phenomenologically by a complex potential between x_1 and x_2 [12], the continuity equation allows one to find a simple relation between the operational average absorption time, $\langle t_N\rangle$, which describes the average time at which an incident particle is destroyed in the detector, and the average arrival time obtained with the "free" flux, $\langle t_J\rangle = \int_0^\infty J(x_1, t)t\,dt / \int_0^\infty J(x_1, t)\,dt$, i.e., with the flux in absence of detector [13] (for a perfect absorber the integral of the flux is equal to the total norm absorbed, $\int_0^\infty J(x_1, t)\,dt = N_{abs}$),

$$\langle t_N \rangle = \langle t_J \rangle + \Delta_t. \qquad (3)$$

Here Δ_t is the "dwell time" within the absorbing potential divided by the absorbed norm N_{abs}, and it is expected to be negligible in general. This analysis has been used for defining average arrival instants and for relating them to an operational measuring procedure under the asymptotic conditions (far from the barrier) met in a scattering molecular beam time of flight experiment [13]. Asymptotically, at a large positive distance from the potential, the flux is always positive. In practice, even at the barrier d the flux is positive in an overwhelming fraction of time in all our calculations, and the distinction between J_+ and J is, at least numerically, unnecessary. The importance of the arrival time $\langle t_J \rangle$ comes from its measurability and from the fact that it can be regarded as an average over momentum of the "phase times" [14], which involve the phase ϕ of the transmission coefficient $T = |T|e^{i\phi}$ [2]. Because of its relation with the phase times, $\langle t_J \rangle$ contains complementary information with respect to the modulus $|T|$ of the transmission coefficient. In combination with inverse scattering techniques this additional information can be used to obtain the interaction potential.

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6. Later (corrected) calculations by the authors of [3] show a smaller discrepancy than the one stated in [5]. However they still find positive values of $\langle \tau_{OR}(0, x) \rangle$, although they also recognize that for suitable initial conditions negative times may be found (private communication by E. Recami).
7. C.R. Leavens, *Solid State Commun.* **89,** 37 (1993).
8. Note however that with their notation the (wave number) variance of their minimum packet is not $(\Delta k)^2$ but $[(\Delta k)/2]^2$.
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10. In principle, if an "initial" packet (considered as a packet which is far from the barrier at t_i) had a significant negative momentum contribution it would be possible to have two separate time regions where barrier and packet overlap, one at times $t > t_i$, the physical one, and one at times $t < t_i$ associated with the interaction with the barrier due to the negative momentum components. But the overlap at times $t < t_i$ is spurious since, as already stated, it does not make physical sense to consider times before the preparation time. Actual experiments prepare the initial state at a finite time and a finite spatial region.
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14. See, e.g. [1] for the definition and analysis of the "phase times".