Quantum arrival time measurement and backflow effect.

J. G. MUGA$^{1,2}$, J. P. PALAO$^1$ and C. R. LEAVENS$^2$

$^1$ Departamento de Física Fundamental y Experimental, Universidad de La Laguna, La Laguna, Tenerife, Spain
$^2$ Institute for Microstructural Sciences, National Research Council of Canada, Ottawa, Canada K1A 0R6

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Abstract.– The current density for a freely evolving state without negative momentum components can temporarily be negative. The “operational arrival time distribution”, defined by the absorption rate of an ideal detector, is calculated for a model detector and compared with recently proposed distributions. Counterintuitive features of the backflow regime are discussed.
The arrival time of a particle at a spatial point is one of the classical concepts whose quantum counterpart is problematic, even for the free particle case considered in this paper. Despite this there are experiments, most notably “time of flight experiments”, that seemingly circumvent the theoretical objections and difficulties exemplified by Alcock’s work.[1] Several researchers have tried in recent years to fill this gap between theory and practice by reexamining the subject using a variety of approaches[2-14]; a recent review provides a brief summary of the methods applied and a discussion of open questions[14].

If all of the particles in an ensemble of freely moving classical particles have positive momenta $p$ then the distribution $\Pi[t(X)]$ of arrival times $t(X)$ at the position $x = X$ is just the particle flux $J[x = X, t]$. (One spatial dimension is always assumed in this paper, the arrival point $X$ is taken as the origin $x = 0$ unless indicated otherwise, and $t(0)$ is written simply as $t$.) Not surprisingly, in many investigations the proposed distribution $\Pi(t)$ of arrival times for quantum particles is closely related to the probability current $J(0, t)$. In both the quantum and classical cases $J(0, t)$ is equal to $dN^+(t)/dt$, where $N^+(t)$ is the probability of finding the particle to the right of $x = 0$ at time $t$ ($N^+(t) = \int_{X=0}^{\infty} \langle |x \psi(t) |^2 \rangle dx$ in the quantum case). Hence, it is tempting to extend the classical result for the arrival time distribution to the quantum regime. But this is not entirely satisfactory because $J(0, t)$ can be negative for a freely evolving quantum state even if its momentum distribution is zero for all negative momentum components, thus invalidating $J(0, t)$ as a probability distribution of arrival times even in the free particle case. Bracken and Melloy showed that the time interval over which $J(0, t) < 0$ can be arbitrarily long but finite[13]. They also derived a least-upper-bound, estimated to be 0.04, for the time integral of $|J(0, t)|$ over an interval of negative $J(0, t)$. But the backflow effect is negligible quantitatively at asymptotic distances from the source or interaction region[4]. This in part explains why the arrival time is not particularly worrisome for the practitioner of time of flight or other arrival time measurement techniques. However, the fundamental difficulty remains and is worth exploring. It is also expected that recent developments in atomic and optical physics will make the backflow regime amenable to experimental study.

In this letter we will model an idealized particle detection setting and investigate the operational arrival time distribution focusing on the backflow regime. We have in mind a scintillation screen or any other device where the detection depends on the passage from the initial channel to one or more final channels (associated with changes in chemical arrangements or internal states of the particle or the apparatus). It is assumed that the experiment is repeated with single particles many times, with the same initial conditions, and that the final number of detection counts for a given $dt$ is proportional to the amount of norm of the initial channel that disappears in that time, $-dt(dN(t)/dt)$, where $N(t) \equiv \int_{-\infty}^{0} dx \langle|x \psi(t)|^2 \rangle$, and $\langle|x \psi(t)| \rangle$ represents the amplitude of the initial channel. In general, in the absence of backflow at $x = 0$, the flux $J(0, t)$ at the front edge of the detector (conventionally located between 0 and $L$) and $-dN(t)/dt$ are close to each other, but the latter is slightly delayed with respect to the former because of the time it takes to absorb (i.e., to pass from the incident to the final channels) the part of the wave inside the detector. More precisely, the time averages evaluated with $J(0, t)$ and $-dN(t)/dt$ differ by the mean dwell time in the detector $\tau_D[4]$. The arrival time distribution is in this context defined operationally, it depends on the apparatus, and it is given by the absorption rate $-dN(t)/dt$ (suitably normalized to account for any incident particles that do not reach the detector). In real detectors additional delays and signal broadening have to be considered because of the amplification of the microscopic signal, for example in a photomultiplier, but we shall ignore that stage of the process, which is highly dependent on the particular detection method or apparatus, to concentrate on the generic first microscopic step.

The effect of such a measuring device on the incident channel can be characterized by complex reflection and transmission amplitudes, $R(p)$ and $T(p)$, that depend on
the momentum. Within the spirit of “optical models” a complex potential may be constructed subject to the constraint of generating functions $R(p)$ and $T(p)$ with specified properties. This phenomenological approach retains the basic features of the apparatus-particle system avoiding the explicit treatment of all the degrees of freedom involved. A good detector will absorb completely over a broad range $\Delta_p$ of incident momenta,

$$R(p) = T(p) = 0, \quad (p \text{ in } \Delta_p). \tag{1}$$

With perfect amplification, all particles with incident energies in the working range will then be detected. Another desirable feature of a “time of arrival detector” is that its spatial width $L$ be small. Clearly, these ideal conditions are difficult to meet in actual detectors, and known complex potentials do not satisfy them exactly either. It is however rewarding to study theoretical models as close as possible to the ideal limit to ascertain what to expect of “ideal measurements”.

Consider an initial ($t = 0$) wavefunction with no negative momentum components and negligible overlap with the complex potential region $[0, L]$. In the absence of this potential the freely evolving wavefunction can be written as

$$\langle x | \phi_{in}(t) \rangle = \int_0^\infty dp \langle x | p \rangle e^{-ip^2t/(2m\hbar)} \langle p | \phi_{in}(0) \rangle,$$  \tag{2}

whereas, if the potential is present the wavefunction is given by

$$\langle x | \psi(t) \rangle = \int_0^\infty dp \langle x | p^+ \rangle e^{-ip^2t/(2m\hbar)} \langle p | \phi_{in}(0) \rangle,$$  \tag{3}

where the $|p^+\rangle$ are scattering eigenstates of $H$ associated with the incident plane waves $|p\rangle$, and $|\phi_{in}\rangle$ is the freely evolving incoming asymptote to which the state $|\psi\rangle$ tends before the collision. The validity and meaning of this equation are not trivial. The elements of scattering theory with complex potentials required to obtain (2) are described in the Appendix B. For a “perfect absorber” the reflection amplitudes $R(p)$ are zero for those momenta for which $\langle p | \phi_{in}(0) \rangle$ is nonnegligible, so for $x \leq 0$ the plane wave and the eigenstate of $H$ coincide, $\langle x | p \rangle = \langle x | p^+ \rangle$. Therefore, $\langle x | \psi(t) \rangle = \langle x | \phi_{in}(t) \rangle$ for $x \leq 0$, namely, the wave function to the left of the model detector is unaltered by the presence of the perfectly absorbing complex potential. The corresponding fluxes for $\phi$ and $\psi$ are also equal up to the potential edge,

$$J_\psi(x,t) = J_\phi(x,t), \quad x \leq 0. \tag{4}$$

This means that it is possible for a perfect absorber to emit probability! This counterintuitive phenomenon happens whenever probability backflow occurs at $x = 0$ in the absence of the complex potential, i.e. $J_\phi(x = 0, t) < 0$ for some finite time range $\delta_t$. Since the perfectly absorbing detector reproduces this negative flux region exactly it must “give back” part of the probability that had entered $[0, L]$ before $\delta_t$: $dN^-(t)/dt = -J_\psi(x = 0, t) = -J_\phi(x = 0, t) > 0$ for $t$ in $\delta_t$, where $N^-(t) = \int_0^t |\langle x | \psi(t) \rangle|^2 dx$. There is, however, no paradox because the leftward probability flow out of the detector volume is only temporary and does not imply a permanent reflection for a fraction of the particles since eventually all particles are absorbed. Thus a perfect absorber defined according to (4) does not require that $J(0, t)$ always be nonnegative at its front edge. Moreover, the fact that $dN(t)/dt \leq 0$ at all times for a complex potential with a negative imaginary part is not necessarily inconsistent with $dN^-(t)/dt$ being positive for a finite range $\delta_t$ of $t$. These surprising, non-classical results will be demonstrated for an explicit choice of state and complex potential. The complex potential model is constructed by means of a series of complex square barriers with negative imaginary parts, see Appendix B. This enables us to know the scattering eigenfunctions exactly, and to calculate easily the absorption rate for a given wavepacket by quadrature (also quantities such as the total absorption, or the dwell time). The method allows for efficient absorption at moderate to
large momenta (where Eq. (1) can be essentially satisfied with absorptions higher than 99.9\%) but not for very low momenta. The wave packet is selected accordingly without too low momenta, and as a consequence the amount of backflow that we shall study is far from the upper bound found by Bracken and Melloy [12], but this is not essential for demonstrating the effect and for illustrating the general theoretical prediction of Eq. (4).

We may first consider an incident state $|\psi\rangle$ that leads to analytical expressions for $\langle x|\psi(t)\rangle$ and $J(x,t)$, and that satisfies the stated restrictions of the arrival time theories of references [17,5,9,10,12],

$$\langle p|\psi(0)\rangle = C(1 - e^{-\alpha p^2/\hbar^2})e^{-\delta^2(p-p_0)^2/\hbar^2 - ipx_0/\hbar}\Theta(p),$$

with $\delta^2 + \alpha > 0$ and $x_0 \ll -\delta$. Note the absence of negative momentum components and the $p^2$ dependence as $p \to 0$. The Fourier transform can be compactly expressed using $w$–functions [18],

$$\langle x|\psi(t)\rangle = C'\left\{ \frac{w(-ig/2A^{1/2})}{A^{1/2}} - \frac{w[-ig/2(A + \alpha)^{1/2}]}{(A + \alpha)^{1/2}} \right\}. \tag{6}$$

Here $w(z) = e^{-z^2}\text{erfc}(-iz)$, and

$$A = \delta^2 + iht/(2m),$$

$$g = i(x - x_0) + 2k_0\delta^2, \tag{7}$$

$$C' = \frac{C\hbar^{1/2}}{4\pi^{1/2}e^{k_0^2\delta^2}} = \frac{1}{\sqrt{2^{3/4}\pi^{1/4}} \left\{ \frac{w(-i2^{1/2}k_0\delta)}{2^{3/2}\delta} \right\}},$$

$$\frac{w[-2ik_0\delta^2/(2\delta^2 + \alpha)^{1/2}]}{(2\delta^2 + \alpha)^{1/2}} + \frac{w\{-2ik_0\delta^2/[2(\delta^2 + \alpha)]^{1/2}\}}{[8(\delta^2 + \alpha)]^{1/2}} \right\}^{-1/2}. \tag{9}$$

where $k_0 = p_0/\hbar$. The derivative with respect to $x$, and therefore the flux, are also analytical since $dw(z)/dz = -2zw(z) + 2i/\pi^{1/2}$. The momentum distribution of this wave packet is too close to zero energy to be efficiently absorbed, so we shall use instead a new state obtained from (3) by a "boost" at time $t = 0$,

$$\langle p|\psi'(0)\rangle = \langle p - b|\psi(0)\rangle. \tag{10}$$

The flux for the new state can be related to the flux and probability density of the original one,

$$J_{\psi'}(0,t) = J_{\psi}(-bm/t, t) + (b/m)\langle x = -bt/m|\psi(t)\rangle^2. \tag{11}$$

The last term may be understood as the flux contribution due to the displacement of an observer with velocity $-b/m$. Since $b > 0$, it is always positive, so if the boost is strong enough the backflow region disappears. We have chosen a value of $b$ small enough that the effect remains and large enough that essentially full absorption can be achieved (99.97\%). The complex potential has been improved in successive optimizations until the prediction of Eq. (4) has been numerically confirmed by the converged flux results. Figures 1 and 2 show the flux at $x = 0$ (with and without complex potential), and $-dN(t)/dt$. The two fluxes, with and without complex potential, are indistinguishable on the scale of the figures. This means in particular that, during the backflow regime detailed in Figure 2, the potential region $[0,L]$ returns probability to the left half space $[-\infty,0]$ at exactly the rate required to maintain the same negative flux as the freely evolving state. Fig. 1 shows global agreement in shape between the flux and the absorption rate $-dN/dt$, the latter being
slightly delayed. It is of interest to compare the operational arrival time distribution \(-dN(t)/dt\) with other theoretical proposals for the time of arrival distribution. Also shown in Figures 1 and 2 are Kijowski’s distribution

\[
\Pi_K(t) = \left| \frac{1}{(m\hbar)^{1/2}} \int_0^\infty \sqrt{\theta} e^{-ip^2/2m\hbar} \langle p|\psi(0)\rangle \, dp \right|^2,
\]

and that derived from Bohm’s causal theory \([19,20]\)

\[
\Pi_B(t) = |J(0,t)|/\int_0^\infty |J(0,t')| \, dt',
\]

both evaluated for \(\psi'\). The former distribution was originally derived by imposing a series of conditions consistent with the classical distribution \([17]\), and has been later studied, rederived or generalized by several authors \([2,5-12]\). The transformation (11) does not hold when \(J\) is replaced by \(\Pi_K\) because of the non-linearity introduced by the square root in (12). It arises naturally as the square of the overlap between the initial state (restricted to positive momenta) and the eigenstates of the “time of arrival operator”

\[
\hat{\tau} = -\frac{m}{2} \left( \frac{1}{\hat{p}} - \frac{1}{\hat{q}} \right).
\]

[The different quantization in \([5]\) gives the same result.] As for any other quantity obtained from a formal quantization procedure, its physical meaning and content is not immediately obvious and requires detailed examination and external justification, since in principle other quantizations with the same classical limit may also be constructed \([8,14]\). In the numerical example Kijowski’s distribution \(\Pi_K(t)\) is in overall excellent agreement with the flux (except at the fine scale needed to resolve the backflow region) and, up to the delay, with \(-dN(t)/dt\). With the latter it has in common positivity at all times. The two quantities avoid the negative values of the backflow region smoothly while \(|J(0,t)|\) has downward cusps at the zeroes of \(J(0,t)\).

In Bohm’s theory particle trajectories do not intersect each other so that only a single trajectory contributes to the current density \(J(x,t)\) at each space-time point \((x,t)\). For times \(t\) before \(\delta_t\), when \(J(0,t) > 0\), particles in the ensemble crossing \(x = 0\) do so only from left to right; for times \(t\) during \(\delta_t\), when \(J(0,t) < 0\), some of these particles recross \(x = 0\), moving from right to left to this time - there are no particles crossing \(x = 0\) from left to right during \(\delta_t\); for times \(t\) after \(\delta_t\), when \(J(0,t) > 0\) again, particles cross \(x = 0\) only from left to right. By continuity, at those instants of time \(t\) when \(J(0,t) = 0\) no particle in the ensemble is crossing \(x = 0\) from either direction, leading to the above mentioned cusps. From a classical point of view, the counterintuitive aspect of this picture of backflow, when applied to an ensemble of freely evolving particles, is the necessity for some of these “free” particles to (twice) come to rest and then reverse their direction of motion. However within Bohm’s theory the particles are not truly free but are guided by the wave function \(\psi(x,t)\) \([21]\) which itself undergoes relatively rapid temporal changes in the backflow region considered here. Kijowski’s distribution also contains an obvious counterintuitive feature and is subject to an interpretational puzzle. In different publications \([14,15,11,12]\), which all lead to the arrival time distribution \([12]\) for a freely evolving state containing no negative momentum components, it is claimed that under those circumstances particles arrive at \(x = 0\) only from the left. In the backflow regime this leads to the baffling conclusion that the probability of finding the particle to the left of \(x = 0\) is increasing with time in a time interval during which particles reach \(x = 0\) only from the left. According to Bohm’s theory, the particles that contribute to the backflow region shown in Fig. 2 arrive at \(x = 0\) three times, twice from the left and once from the right, so \(\Pi_B(t)\) is not a “first arrival” time distribution; according to the approaches leading to Kijowski’s distribution \([12]\) they arrive only from the left but...
it is not obvious how this is consistent with $dN^-(t)/dt > 0$ and whether or not one should regard (12) as a distribution of first arrival times. Finally, the operational distribution $-dN/dt > 0$ has the advantage of a clear physical content, and direct relation to an experimental setting, but it should not be overinterpreted, in particular since the present analysis has shown that a perfect absorber can emit probability.

Appendix A: Construction of complex absorbing potential

Let us find a potential with support $[0, L]$ that maximizes the absorption in a given momentum interval $[p_1, p_2]$. The method described here is more efficient and numerically robust than previous ones [22]. The proposed functional form is a series of equal length $N$ complex square barriers with complex energies $\{V_j\}$, $j = 1, 2, ..., N$. The real and imaginary values of $V_j$ are found by minimizing (with the restriction $\text{Im}(V_j) < 0$), the sum of the survival probabilities at $s$ values of $p$, $\{p_{\alpha}\}$,

$$f(V_1, ..., V_N; p_1, ..., p_s) = \sum_{\alpha=1}^{s} S(V_1, ..., V_N; p_{\alpha}),$$

where $S(p) \equiv 1 - |T(p)|^2 - |R(p)|^2$, and the $s$ points are evenly spaced in the absorption interval $[p_1, p_2]$. $S$ and its gradient with respect to $\{V_j\}$ are obtained by multiplication of known $2 \times 2$ transfer matrices so that the optimizations are very fast. For the application in the main text we have taken $L = 0.01, N = 4, s = 49, p_1 = 260$, and $p_2 = 740$.

Appendix B: Elements of complex potential scattering theory in one dimension

For the formulation of scattering theory of complex non hermitian potentials it is necessary to consider scattering eigenstates of $H$, $|p^+\rangle$, and their biorthogonal partners $|\hat{p}^+\rangle$, which are eigenstates of $H^\dagger$,

$$|p^+\rangle \equiv |p\rangle + \frac{1}{E_p + i0 - H}V|p\rangle,$$

$$|\hat{p}^+\rangle \equiv |p\rangle + \frac{1}{E_p + i0 - H^\dagger}V^\dagger|p\rangle.$$  \hspace{1cm} (16)

Möller operators that connect the actual state $\psi$ that evolves, respectively, with $H$ or $H^\dagger$, with the freely evolving incoming asymptotic states (to which $\psi$ tends before the collision) can be defined as $\Omega_+ = \int dp |p^+\rangle \langle p|$ and $\hat{\Omega}_+ = \int dp |\hat{p}^+\rangle \langle p|$ respectively. They obey

$$\hat{\Omega}_+^\dagger \Omega_+ = 1_{\text{op}},$$

$$\Omega_+ \hat{\Omega}_+^\dagger = 1_{\text{op}} - \Lambda,$$  \hspace{1cm} (18)

where $\Lambda = \sum_j |\Psi_j\rangle \langle \hat{\Psi}_j|$ is given in terms of the bound states of $H$ ($\Psi_j$, and of $H^\dagger$, ($\hat{\Psi}_j$). Thus the integral form of an arbitrary wave packet evolving with $H$ without bound state component can be written as

$$\langle x|\psi(t)\rangle = \int dp \langle x|p^+\rangle e^{-iE_p t/\hbar} \langle \hat{p}^+|\psi(0)\rangle.$$  \hspace{1cm} (20)
Using the generalized isommetry relation (18) one may substitute \( \langle \hat{p}^+ | \psi(0) \rangle \) by \( \langle p | \phi_{in}(0) \rangle \) in (20). Moreover, if \( \psi(0) \) does not significantly overlap with the potential and there are not negative momenta, \( \phi_{in}(0) \) can also be substituted by \( \psi(0) \) as shown in [23].
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FIGURE CAPTIONS

Figure 1: $J(0, t)$ for free motion (solid line), $J(0, t)$ with the absorber, (short dashed line), $\Pi_K(t)$ (dotted-dashed), and $-dN/dt$ (long dashed line) for the wave packet $\psi'$ in (14), see also (15), with the following parameters (all in atomic units): $\alpha = 1.4$, $p_0 = 1$, $x_0 = -0.22$, $\delta = 0.007$, $b = 300$. The first three curves are indistinguishable in this scale.

Figure 2: $J(0, t)$ for free motion (solid line), $J(0, t)$ with the absorber (short dashed line), $|J(0, t)|$ (dotted line), $\Pi_K(t)$ (dotted-dashed line), $-dN(t)/dt$ (dashed line), and $-dN(t)/dt|_{y+\tau_D}$ (dashed line with squares). Same parameters as in Figure 1. The first two curves are hardly distinguishable. $\tau_D = 1.0515 \times 10^{-5} au$. 
