Transition from discrete to continuous time-of-arrival distribution for a quantum particle

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We show that the Kijowski distribution for time of arrivals in the entire real line is the limiting distribution of the time-of-arrival distribution in a confining box as its length increases to infinity. The dynamics of the confined time-of-arrival eigenfunctions is also numerically investigated and demonstrated that the eigenfunctions evolve to have point supports at the arrival point at their respective eigenvalues in the limit of arbitrarily large confining lengths, giving insight into the ideal physical content of the Kijowsky distribution.

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I. INTRODUCTION

The problem of accommodating time as a quantum dynamical observable has a long history and remains controversial to this day [1–10]. The time of arrival (TOA) of a quantum structureless particle at a point or a surface is one aspect of this problematic treatment of time in quantum mechanics in need of clarification [4,5]. Recently significant progress has been made, both at the operational and foundational fronts for the quantum time-of-arrival problem. Most notable at the operational level is the convergence of several analyses of the problem to the axiomatic distribution of arrival for freely moving particles due to Kijowski [6]. Kijowski's distribution was first obtained operationally (under some limiting conditions) by Allcock [7] and later shown to be arising from the quantization of the classical time of arrival [8,11], inspiring extension of the theory to the interacting case [12–14] or multiparticle systems [15]. Most important of these developments in understanding the physical content of Kijowski distribution is the realization that, while axiomatic in nature, it can be obtained from an operational procedure [16,17], whose essence is to modify (filter) the initial state to counterbalance the disturbance introduced by the apparatus, in particular at low energies.

At the foundational level, it has been shown that the non-self-adjointness of the free time-of-arrival operator, widely regarded as due to the semiboundedness of the Hamiltonian in accordance with Pauli's theorem [1,9], can in fact be lifted by spatial confinement [9]. Thus the concept of confined quantum time of arrival (CTOA) was introduced [10]. The CTOA operators form a class of compact and self-adjoint operators canonically conjugate with their respective Hamiltonians in a closed subspace of the system Hilbert space. Being compact, the CTOA operators possess a discrete spectrum and a complete set of mutually orthogonal square integrable eigenfunctions [21]. The eigenfunctions of the CTOA operators are found to be states that evolve to unitarily (i.e., according to Schrodinger's equation) arrive at the origin at their respective eigenvalues—that is, the events of the centroid of the position distribution being at the origin and its width being minimum occur at the same instant of time.

Now we are confronted with the problem of relating the already established results for the unconfined quantum particle to the confined one, in particular the question whether the established Kijowski time-of-arrival distribution is extractable or not from the confined time-of-arrival operators. Therefore in this paper we give meaning to the limit of the discrete time-of-arrival distribution of the CTOA operators defined on succesively larger segments, proving that this limit is Kijowski's distribution. We begin by a short review of the properties of the confined and unconfined time-of-arrival operators; this is followed by numerical indications of the relation between these two cases, numerical indications that are strengthened by the analytical proof of the following statement: The time-of-arrival operator on the full real line is the limit for l tending to infinity of the time-of-arrival operators defined for free motion in a segment of length $2l$. The dynamics of the CTOA eigenfunctions are then numerically investigated in the limit of arbitrarilly large confining lengths. We end by summarizing and providing conclusions.

II. THE QUANTUM FREE TIME-OF-ARRIVAL OPERATOR

From a heuristic perspective, it is quite natural to assume that the quantum TOA may be associated with the quantization of the corresponding classical expression. That is, if a classical free particle, of mass μ in one dimension at initial location q with momentum p, will arrive, say, at the origin at the time $T(q,p)=-\mu q p^{-1}$, then the quantum TOA distribution must be derivable from a quantization of $T(q,p)$, such as the symmetrized

$$\mathsf{T}=-\frac{1}{2}\mu(\mathsf{q}\mathsf{p}^{-1}+\mathsf{p}^{-1}\mathsf{q}), \tag{1}$$

where p and q are the momentum and position operators. Formally the time-of-arrival operator T is canonically conjugate to the free Hamiltonian, $\mathsf{H}=(2\mu)^{-1}\mathsf{p}^2$, i.e., $[\mathsf{H},\mathsf{T}]=i\hbar$. Equation (1) has been separately studied when the motion of the free particle takes place in the entire real line and when it

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is restricted to a segment of the real line. These studies led to some seemingly contradictory descriptions, in that the time-of-arrival operator is not self-adjoint for the full real line, while there is an infinite family of self-adjoint operators playing the corresponding role for the segment. Furthermore, for the full line case there is a well-defined property of time covariance which is lacking in the confined case.

A. The TOA operator in $\mathcal{H}_p = L^2(-\infty, \infty)$

In momentum representation, Eq. (1) formally assumes the form

$$\mathsf{T} = \frac{i\hbar\mu}{2}\left(\frac{1}{p^2} - \frac{2}{p}\frac{\partial}{\partial p}\right).$$

Under a sensible choice of domain [18], T is a densely defined operator, and unbounded in $\mathcal{H}_p := L^2(\mathbf{R}, dp)$. It is, however, not self-adjoint, and admits no self-adjoint extension. It is in fact a maximally symmetric operator [18]. According to the well-established theory for this kind of operator, there exists a decomposition of unity given by the following degenerate weak (or nonsquare integrable) eigenfunctions:

$$\tilde{\psi}_\alpha^{(t)}(p) = \Theta(\alpha p)\left(\frac{\alpha p}{2\pi\mu\hbar}\right)^{1/2} e^{ip^2 t/2m\hbar}.$$

This is a family of functions parametrized by the eigenvalue t and a discrete parameter α, which can be either $+1$ or -1, and gives the sign of the half-line on which the function presents its support in momentum space. It is straightforward to prove completeness, i.e., $\Sigma_\alpha \int_{-\infty}^{\infty} dt \tilde{\psi}_\alpha^{(t)}(p') \tilde{\psi}_\alpha^{(t)}(p) = \delta(p-p')$, and nonorthogonality,

$$\int_{-\infty}^{\infty} dp \tilde{\psi}_{\alpha'}^{(t')}(p) \tilde{\psi}_\alpha^{(t)}(p) = \frac{1}{2}\delta_{\alpha\alpha'}\left(\delta(t-t') + \frac{i}{\pi}\mathrm{P}\frac{1}{t-t'}\right).$$

The physical content of the eigenfunctions is better examined in coordinate representation [11]. Normalized wave packets with the form of quasieigenstates of T peaked at a given eigenvalue, but with a time width ΔT, have sharp space-time behavior. Their average position travels with constant velocity to arrive at the origin at the nominal arrival time of the packet, in which the packet also attains its minimum spatial width. The passage of probability density from one side of the origin to the other is in summary as sharp as desired by taking $\Delta T \to 0$ [11]. As we shall see later, the unitary evolution of a (generalized) state $|\tilde{\psi}_\alpha^{(t)}\rangle$ leads to a distribution with point support at the origin at the instant corresponding to the eigenvalue t, thus lending support to its interpretation as a time-of-arrival eigenstate.

Using completeness, we can now write the probability density for measured values of the T operator,

$$\Pi_{\psi_0}(t) = \left|\int_0^{\infty} dp \left(\frac{p}{2\pi m\hbar}\right)^{1/2} e^{-ip^2 t/2m\hbar}\psi_0(p)\right|^2 + \left|\int_{-\infty}^{0} dp \left(\frac{-p}{2\pi m\hbar}\right)^{1/2} e^{-ip^2 t/2m\hbar}\psi_0(p)\right|^2,$$

which is, in fact, Kijowski's probability density [6].

An essential property of the distribution of arrivals in Kijowski's axiomatic approach is covariance under transformations generated by the Hamiltonian. It is evident that this property of covariance is indeed held by the distribution above. Physically, it means that the probability of arriving at t for a given state is equal to the probability of arriving at $t-\tau$ for the same state, once evolved a time τ. This is the reflection on the probability density of the canonical commutation relation between H and T.

B. The TOA operator in $\mathcal{H}_l = L^2[-l, l]$

In [10] the naive definition in Eq. (1) T for a free particle in a segment of length $2l$ is supplemented by adequate boundary conditions, leading to properly self-adjoint operators. Physically, the choice of time-of-arrival operator with spatial confinement of the particle in the interval $[-l, l]$ is dictated by the condition that the evolution of the system is generated by a purely kinetic self-adjoint Hamiltonian, i.e., $\mathsf{H} = (2\mu)^{-1}\mathsf{p}^2$, where p is a self-adjoint momentum operator. This requirement demands that the momentum operator p be one of the set $\{\mathsf{p}_\gamma = -i\hbar\partial_q, \gamma \leq \pi/2\}$, with p_γ having the domain consisting of absolutely continuous functions $\phi(q)$ in $\mathcal{H}_l = [-l, l]$ with square integrable first derivatives, which further satisfy the boundary condition $\phi(-l) = e^{-2i\gamma}\phi(l)$. Since T depends on the momentum operator, T is also required to be the corresponding element of the set of operators $\{\mathsf{T}_\gamma\}$.

In coordinate representation, T_γ becomes the Fredholm integral operator $(\mathsf{T}_\gamma\varphi)(q) = \int_{-l}^{l} T_\gamma(q, q')\varphi(q')dq'$, for all $\varphi(q)$ in $\mathcal{H}$, where the kernel is given by

$$T_{\gamma\neq 0}(q, q') = -\mu\frac{(q+q')}{4\hbar \sin\gamma}[e^{i\gamma}H(q-q') + e^{-i\gamma}H(q'-q)], \tag{2}$$

$$T_{\gamma=0}(q, q') = \frac{\mu}{4i\hbar}(q+q')\mathrm{sgn}(q-q') - \frac{\mu}{4i\hbar l}(q^2 - q'^2), \tag{3}$$

in which H is Heaviside's step function and sgn is the sign function.

With this representation, one can show that H_γ and T_γ form a canonical pair in a closed subspace of $\mathcal{H}_l$—a nondense subspace—for every γ. Moreover, the kernel $T_\gamma(q, q')$ of T_γ is square integrable, i.e., $\int_{-l}^{l}\int_{-l}^{l}|T_\gamma(q, q')|^2 dq dq' < \infty$. This means that T_γ is compact, and, as a consequence, that it has a complete set of (square integrable) eigenfunctions and its spectrum is discrete. This, it should be stressed, is a radically different situation from that in the full line, where the operator has a continuous spectrum and is not self-adjoint.

In what follows, we will need only the spectral properties for the periodic confined quantum time-of-arrival operators (that is to say, $\gamma = 0$). The operator T_0 commutes with the parity operator. Furthermore, it changes sign under time inversion, which entails that its spectrum is symmetric about 0. This suggests classifying its eigenfunctions in even and odd subspaces (which will be denoted by the subscripts e and o, respectively), and, within each of those subspaces, by a discrete index n and the sign of the eigenvalue (indicated as a superscript). In this manner, and as computed elsewhere [10], the odd eigenfunctions are

$$\varphi^{\pm}_{n,o}(q) = A_n q f^{\pm}\left(\frac{s_n q^2}{l^2}\right) \tag{4}$$

with

$$f^{\pm}(\xi) = e^{\mp i\xi}\xi^{1/4}[J_{-1/4}(\xi) \mp iJ_{3/4}(\xi)], \tag{5}$$

while the even ones are given by

$$\varphi^{\pm}_{n,e}(q) = B_n g^{\pm}\left(\frac{r_n q^2}{l^2}\right) \tag{6}$$

with

$$g^{\pm}(\xi) = e^{\mp i\xi}\xi^{3/4}[J_{-3/4}(\xi) \mp iJ_{1/4}(\xi)] + \frac{e^{\mp i r_n}J_{1/4}(r_n)}{r_n^{1/4}}. \tag{7}$$

A_n and B_n are the normalization constants, while s_n and r_n are the solutions of the secular equations for the operator, namely the positive roots of $J_{-3/4}(r)+\frac{2}{3}J_{5/4}(r)+1/rJ_{1/4}(r)=0$ for the even case and of $J_{-1/4}(s)=0$ for the odd case. The eigenvalues are determined by

$$\tau^{\pm}_n = \pm\frac{\mu l^2}{4\rho_n \hbar}, \tag{8}$$

where ρ_n stands for either r_n or s_n.

It has been demonstrated in [10] that a CTOA eigenfunction is a state that evolves unitarily—that is according to Schrodinger's equation—to being concentrated around the origin at its eigenvalue along a classical trajectory, i.e., a state in which the events of the centroid of the position distribution being at the origin and its width being minimum occur at the same instant of time equal to the eigenvalue.

III. RECOVERING KIJOWSKI'S DISTRIBUTION FROM THE CTOA OPERATORS

A. Numerical examples

We have thus seen that the time-of-arrival operators for confined and unconfined free motion have radically different properties, and it is not immediate how Kijowski's distribution follows from the spectral properties of the CTOA operators. In this section we show that indeed Kijowski's distribution is extractable from the discrete time-of-arrival distribution defined by the CTOA operator. But before doing so we first provide further justification from numerical results.

One basic difference between the two cases being examined is that the spectrum is continuous for the full line, whereas it is discrete for the segment. As a consequence, the same can be predicated of the probability distributions for times of arrivals. Therefore in order to compare like with like, it is convenient to use the accumulated probability of having arrived at the origin before a given instant for both cases.

Also in order to perform sensible comparisons we shall consider initial states with compact support on the real line, which can also be defined for all segments which would include that compact support. In this manner the probability of having arrived at the origin before instant t can be computed for the same function both for the segment and the line.

In the case of the segment, the probability of having arrived at the origin before instant t for the initial state ψ_0 is calculated according to the standard quantum mechanical prescription,

$$F_{\psi_0}(t) = \sum_{\tau_{\gamma,s}\leq t} |\langle\varphi_{\gamma,s}|\psi_0\rangle|^2, \tag{9}$$

where $\varphi_{\gamma,s}$ and $\tau_{\gamma,s}$ are the eigenfunctions and eigenvalues of T_{γ}. This distribution is in turn investigated for increasing l and compared with the accumulated probability for Kijowski's distribution,

$$F^K_{\psi_0}(t) = \int_{-\infty}^{t} \Pi_K[\tau,\psi_0]d\tau, \tag{10}$$

where $\Pi_K[\tau,\psi_0]$ is the Kijowsky time-of-arrival density.

As the length of the segment l increases, the discrete eigenvalues of the corresponding time-of-arrival operators become denser, and we take advantage of this property to have another representation for comparison with Kijowski's distribution; namely plotting Kijowski's time-of-arrival density together with a discrete derivative of the probability of having arrived at the origin before a given instant, in the case of the segment, discrete derivative that can be understood as a time-of-arrival density. This allows us an easier recognition of some features that would otherwise be obscured in the accumulated probability.

Figures 1–3 show the accumulated probability for the discrete case and for the Kijowski distribution, together with their corresponding time-of-arrival densities. In Fig. 1 we depict a simple situation for an initial Gaussian state, with a good match between the distributions for both the full line and the segment. Figure 2 corresponds to an initial state that presents the backflow effect [19], that is, that at some instants the quantum probability flux can become negative even if all the components of the state are of positive momentum. In the situation depicted in Fig. 2, therefore, we can discriminate whether the discrete distribution associated with the segment approaches Kijowski's distribution or, rather, the flux, which is also related to the density of arrivals. The result, as can be ascertained from the inset in Fig. 2, is that Kijowksi's distribution is the one selected in the limit of large l. Figure 3 is a depiction of accumulated probabilities for different values of l, clearly showing convergence to Kijowski's accumulated probabilities; similarly with the discrete derivatives.

All together, these numerical results suggest strongly that the $l\to\infty$ limit of the time-of-arrival operators for the segment of length $2l$ tend to the time-of-arrival operator on the real line, in some sense.

B. The limit for large l

A first hint into the relationship between the confined and unconfined TAO operators is provided by the kernel of the

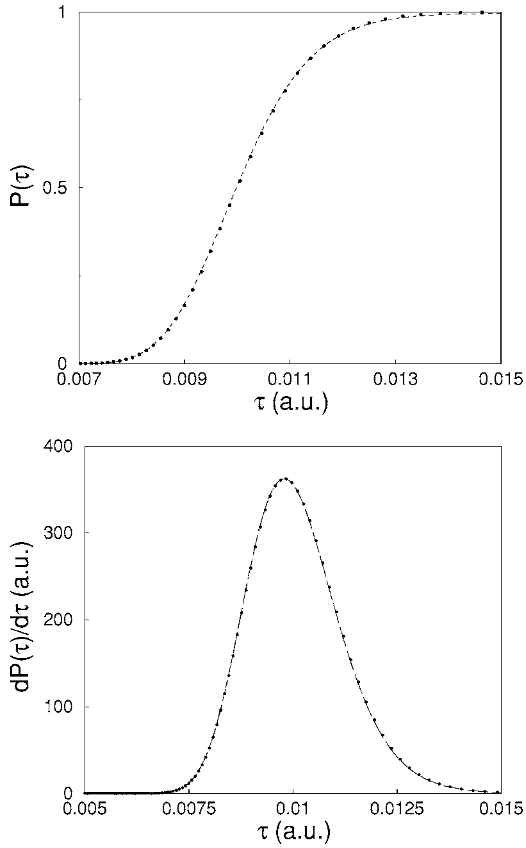

FIG. 1. The top figure shows the accumulated probability of arrival vs time at the origin for a Gaussian wave packet with mean momentum $\langle P\rangle=100$, full width at half maximum $\sigma_x=0.05$, and initial expected value $\langle X\rangle=-1$ (all the quantities in atomic units). The dots correspond to confined motion with $l=10$, and the solid line to the full line. In the lower figure we depict the corresponding probability densities (with the same notation), defined as explained in the text.

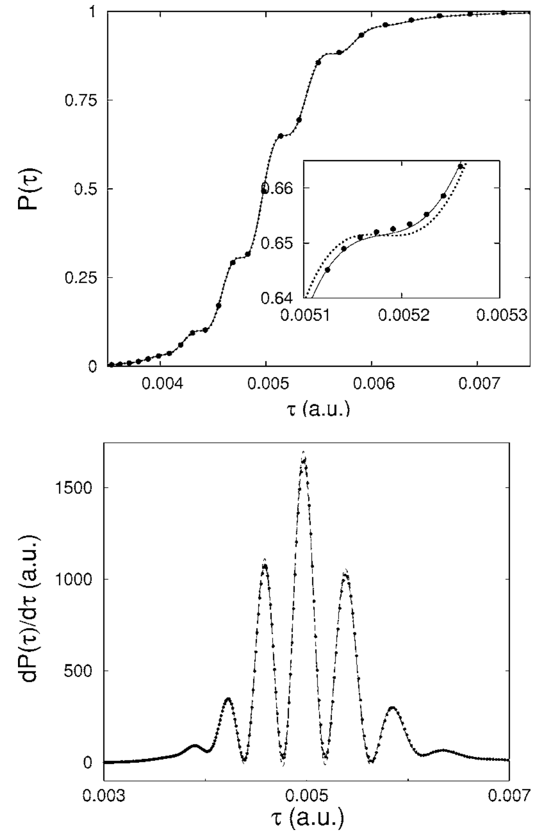

FIG. 2. Accumulated probability of arrival (upper figure) vs time at the origin for two Gaussian wave packets with mean momentum $\langle P_1\rangle=200$ and $\langle P_2\rangle=100$ with maximum interference at the origin, e.g., $\langle X_1\rangle=-1$ and $\langle X_2\rangle=-0.5$. The full width at half maximum is $\sigma_x=0.05$ for both Gaussians. The dots correspond to confined motion with $l=10$, while the solid line corresponds to the full line. For completeness the dotted line depicts the quantum probability flux at the origin, integrated up to the relevant instant. The inset shows the zone of maximal discrepancy between integrated flux and accumulated Kijowski's probability, where the accumulated probability for confined motion matches Kijowski's. In the lower figure we show the corresponding probability densities (with the same notation) defined as explained in the text, as well as the quantum probability flux at the origin: in this situation there is a backflow effect [19].

later in position representation. In q representation, the T operator takes on the form of the integral operator

$$(\mathsf{T}\varphi)(q)=\int_{-\infty}^{\infty}\langle q|\mathsf{T}|q'\rangle\varphi(q')dq', \tag{11}$$

where the kernel is given by

$$\langle q|\mathsf{T}|q'\rangle=\frac{\mu}{4i\hbar}(q+q')\mathrm{sgn}(q-q'). \tag{12}$$

Clearly this is the $l\rightarrow\infty$ formal limit of the kernel $T_0(q,q')$. It is also the limit as $\gamma\rightarrow 0$ of kernels $T_\gamma(q,q')$, and, since the large l limit washes out the effect of the boundary conditions, (i.e., the wave functions must necessarily vanish at infinity) this implies that the kernels match up in the large l limit. For this reason, it will be sufficient for us to consider the periodic confined time of arrivals in the limit of arbitrarily large confinement lengths.

1. Kijowski distribution in position representation

In what follows we will need the position representation of the degenerate eigenfunctions of T. In q representation, the eigenfunctions assume the form

$$\psi_t^{\pm}(q)=\frac{1}{\sqrt{2\pi\hbar}}\int_0^{\infty}e^{\pm iqp/\hbar}\left(\frac{p}{2\mu\hbar}\right)^{1/2}e^{ip^2t/2\mu\hbar}dp, \tag{13}$$

where the integration is understood in the distributional sense. Even and odd combinations of these are likewise eigenfunctions with the same eigenvalue t,

$$\varphi_t^{e/o}(q)=\frac{1}{\sqrt{2}}[\psi_t^{+}(q)\pm\psi_t^{-}(q)]. \tag{14}$$

The full explicit expression for $\varphi_t^{e/o}(q)$ is obtained by direct substitution, leading to

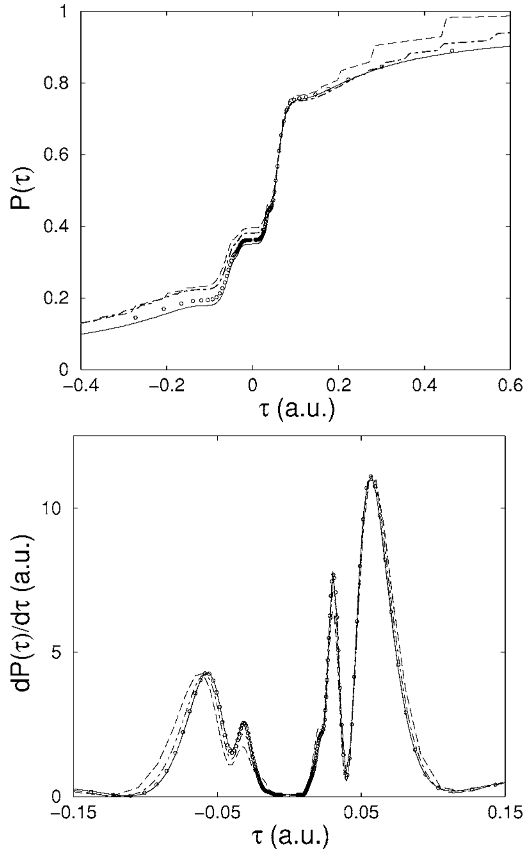

FIG. 3. The upper figure shows the accumulated probability of arrival at the origin vs time for two Gaussian wave packets with mean momentum $\langle P_1\rangle=5$ and $\langle P_2\rangle=1.5$ with $\langle X_1\rangle=-1$ and $\langle X_2\rangle=-0.5$. The full width at half maximum is $\sigma_x=0.05$ for both Gaussians. The distinct lines correspond to different values of l: $l=3$, long dashed line; $l=5$, dotted-dashed line, and $l=15$, circles. The solid line corresponds to Kijowski's distribution. In the lower figure we show the corresponding probability densities (with the same notation), as defined in the text.

$$\varphi_t^{e/o}(q) = e^{i[(1\pm 2)\pi/8]}\frac{1}{4}\sqrt{\frac{2}{\pi t}}\left(\frac{\mu}{\hbar t}\right)^{1/4}\exp\left(-i\frac{\mu q^2}{4\hbar t}\right) \times\left[D_{1/2}\left(-e^{i(\pi/4)}\sqrt{\frac{\mu}{\hbar t}}q\right)\pm D_{1/2}\left(e^{i(\pi/4)}\sqrt{\frac{\mu}{\hbar t}}q\right)\right], \tag{15}$$

where D_ν is the parabolic cylinder function, and the even and odd case correspond to positive and negative sign, respectively.

In momentum representation it is known that these eigenstates form a resolution of the identity. It thus follows, owing from the unitarity of the Fourier transform, that the same happens in the position representation Hilbert space, $L^2(\mathbb{R})$, i.e., $\Sigma_\beta\int_{-\infty}^{\infty}dt\overline{\varphi_t^\beta}(q')\varphi_t^\beta(q)=\delta(q-q')$, with β standing for e and o. They are likewise nonorthogonal.

Because of the invariance of Kijowski's distribution under parity, it can be split in even and odd components of the wave function. In terms of $\varphi_t^{e/o}(q)$, it then assumes the form

$$\Pi_{\psi_0}(t) = \Pi_{\psi_0}^e(t) + \Pi_{\psi_0}^o(t) \tag{16}$$

where

$$\Pi_{\psi_0}^{e/o}(t) = \left|\int_{-\infty}^{\infty}\overline{\varphi_t^{e/o}(q)}\psi_0(q)dq\right|^2. \tag{17}$$

In the following section, we will show that $\Pi_{\psi_0}^{e/o}(t)$, and, hence, Kijowski's distribution itself, can be obtained from the accumulated probability of arrival $F_{\psi_0}^{(l)}(t)$ in the limit $l\to\infty$.

We will do so by a proper identification of the limit of the eigenfunctions of the confined quantum time of arrivals for l approaching infinity as the eigenfunctions given by Eqs. (15). To this end we will need the position representation of the eigenvalue problem for T, which is explicitly given in momentum representation in the form

$$\frac{i\mu\hbar}{2}\frac{1}{p^2}\psi_t(p) - i\mu\hbar\frac{1}{p}\frac{d\psi_t(p)}{dp} = t\psi_t(p). \tag{18}$$

Multiplying both sides of the equation by p^2 and then Fourier transforming the resulting expression leads to the position representation of the above eigenvalue equation

$$\frac{d^2\varphi_t(q)}{dq^2} + \frac{\mu i q}{t\hbar}\frac{d\varphi_t(q)}{dq} + \frac{3\mu i}{2t\hbar}\varphi_t(q) = 0, \tag{19}$$

where $\varphi_t(q)=1/\sqrt{2\pi\hbar}\int_{-\infty}^{\infty}\exp(i/\hbar qp)\psi_t(p)dp$. Straightforward substitution of $\varphi_t^{e/0}(q)$ in the differential equation shows that they are linearly independent solutions of Eq. (19).

2. $F_{\psi_0}^{(l)}(t)$ for large l

As we have pointed out above, both in the case of the full real line and in that of the segment the Hamiltonian and the operators T and T_0 are invariant under parity. It follows that, if we rewrite an initial function in terms of an even and an odd component, their separate distributions for times of arrival sum to the distribution for the total function, with no interference term being required. It is thus useful to separate the analysis in the even and odd sectors. That is, we need to examine whether the distributions $F_{\psi_0}^{(l)e/o}(t)$ (which are the separate contributions to the probability of having arrived at the origin prior to instant t of the even and odd components of the initial state ψ_0) do indeed tend to $\int_{-\infty}^{t}dt'\,\Pi_{\psi_0}^{e/o}(t')$, respectively, as l approaches infinity.

First let us consider the contributions from the odd eigenfunctions for the accumulated probability. This is given by

$$F_{\psi_0}^{(l)o}(t) = \sum_{\tau_n^\pm\leq t}\frac{1}{l^3J_{3/4}^2(s_n)s_n^{1/2}}\left|\int_{-l}^{l}qe^{\pm is_nq^2/l^2}\left(s_n\frac{q^2}{l^2}\right)^{1/4} \times\left[J_{-1/4}\left(s_n\frac{q^2}{l^2}\right)\pm iJ_{3/4}\left(s_n\frac{q^2}{l^2}\right)\right]\psi_0(q)dq\right|^2, \tag{20}$$

where the sum includes only contributions from eigenfunctions with eigenvalues smaller than t, l is large enough such that the interval $[-l,l]$ contains the support of $\psi_0(q)$, and we have used the explicit value of the normalization factor A_n.

As our numerical computations demonstrate, for increasing l the dominant eigenfunctions contributing in the calculation of the accumulated probability come from large values of n. But as n increases the eigenvalues of the dominant contributors become denser. Therefore for every time t and large l there exists a corresponding $n(l,t)$ such that $|t| - \tau_{n(l,t)}$ (that is, the difference between the eigenvalue closest to $|t|$—for that value of l—and $|t|$) tends to 0 as l tends to infinity. For any given τ then we can write the corresponding s_n as $\mu l^2/4\tau\hbar$, with the adequate sign, in the inner integrand.

As for the normalization factor, it is clearly the case that s_n tends to infinity, in which limit we can use the asymptotic properties of Bessel functions and their zeroes to write $l^3 J_{3/4}(s_n)^2 s_n^{1/2}$ in the form $2l^3/\pi s_n^{1/2}$ or, alternatively, $(4l^2/\pi)\sqrt{\hbar|\tau|/\mu}$. Finally, since the spacing between the roots of $J_{-1/4}$ tends to π as n tends to infinity, we have the result that the spacing between successive values of τ_n (with either sign) is $4\pi\hbar\tau^2/(\mu l^2)$, whence it follows that the sum $\Sigma_{\tau_n^\pm \leq t}$ can be substituted by the integral $\mu l^2 \int_{-\infty}^{t} d\tau/4\hbar\pi\tau^2$.

Putting together all these asymptotic expressions, we see that Eq. (20) becomes

$$F_{\psi_0}^{(l)o}(t) \to \frac{2\hbar}{\mu}\int_{-\infty}^{t} d\tau \left(\frac{\mu}{4\tau\hbar}\right)^{5/2} \left| \int_{-\infty}^{\infty} q e^{i\mu q^2/4\tau\hbar}\left(\frac{\mu}{4\tau\hbar}q^2\right)^{1/4} \times \left[J_{-1/4}\left(\frac{\mu}{4\tau\hbar}q^2\right) + iJ_{3/4}\left(\frac{\mu}{4\tau\hbar}q^2\right)\right]\psi_0(q)dq\right|^2. \tag{21}$$

Differentiating this with respect to time yields the corresponding probability density

$$\Pi_{\psi_0}^{odd}(t) = \frac{2\hbar}{\mu}\left(\frac{\mu}{4\hbar t}\right)^{5/2}\left|\int_{-\infty}^{\infty} q e^{i\mu q^2/4t\hbar}\left(\frac{\mu}{4t\hbar}q^2\right)^{1/4} \times \left[J_{-1/4}\left(\frac{\mu}{4t\hbar}q^2\right) + iJ_{3/4}\left(\frac{\mu}{4t\hbar}q^2\right)\right]\psi_0(q)dq\right|^2, \tag{22}$$

from which we extract the limit of the odd eigenfunctions as l approaches infinity. The limit is

$$\varphi_t^{odd}(q) = \sqrt{\frac{2\hbar}{\mu}}\left(\frac{\mu}{4\hbar t}\right)^{5/4} q\left(\frac{\mu}{4t\hbar}q^2\right)^{1/4}\exp\left(-i\frac{\mu q^2}{4t\hbar}\right) \times \left[J_{-1/4}\left(\frac{\mu}{4t\hbar}q^2\right) - iJ_{3/4}\left(\frac{\mu}{4t\hbar}q^2\right)\right]. \tag{23}$$

The relationship between Eqs. (15) and (23) is not immediate; but their relationship can be established by substituting $\varphi_t^{odd}(q)$ back in Eq. (15), and finding that it is a solution to the differential equation, meaning it is an eigenfunction of the time-of-arrival operator in the entire real line with the eigenvalue t. Since $\varphi_t^{odd}(q)$ is odd, then it must differ at most with $\varphi_t^{-}(q)$ by a constant factor. Expanding $\varphi_t^{odd}(q)$ and $\varphi_t^{-}(q)$ about $q=0$, we find that they differ only up to the irrelevant phase factor $e^{-i\pi/4}$. Then we must have $\Pi_{\psi_0}^{odd}(t) = \Pi_{\psi_0}^{-}(t)$ in the limit of infinite l.

The same procedure can be carried out for the contribution of the even eigenfunctions, albeit with more cumbersome algebra, and the corresponding conclusion is derived. As a consequence, we have proved that the $l\to\infty$ limit of the discrete probability distribution for times of arrival for a spatially confined particle is indeed Kijowski's probability distribution.

It might be thought that our proof is lacking in that above we assumed that the initial state has compact support, while Kijowski's distribution must also be defined for other normalizable functions. However, our analysis can be extended to initial states with tails extending to infinity. Let $\psi(q)$ be such a state. There always exists a sequence of states with compact supports, $\psi_n(q)$, $n=1,2,\ldots$, such that $\psi_n(q)\to\psi(q)$. We can, say, pick $\psi_1(q)$ and apply our above analysis to this initial state. Once we get the limit of infinite l, we follow it with the limit in n. The resulting limit is going to be Kijowski's distribution because of the continuity of the inner product.

IV. THE DYNAMICS OF THE CTOA EIGENFUNCTIONS IN THE LIMIT OF INFINITE l

We have shown above that the Kijowski distribution is the limit of the discrete distribution for arbitrarily large l; but what physical insight can we get from this realization? Recall that one of the surrounding issues against an ideal quantum time-of-arrival distribution is the fact that a quantum particle loses the localized property of its corresponding classical particle entity. Classically the concept of time-of-arrival is well-defined because a classical particle has a well defined trajectory. This is contrary to the fact that no such trajectory can be ascribed to the quantum particle—it has no definite position and momentum.

Now the theory of confined quantum time of arrivals demonstrates that the quantum time-of-arrival problem, at the ideal level, i.e., at the level where measuring instruments play no explicit role, can be rephrased to finding states that unitarily arrive at a given point at a definite time—states in which the events of the centroid being at the origin and the position distribution width being minimum occur at the same instant of time. The QTOA problem phrased in this way is well-defined because quantum states have well-defined trajectories according to the Schrodinger equation. All these give us insight to the ideal physical content of the Kijowski distribution. Let us see how.

Let us consider some fixed time τ, and for any given length l of spatial confinement, we can find an n such that the eigenvalue τ_n is closest to τ. Now consider a sequence of monotonically increasing l's, $l_1, l_2, l_3, \ldots$, with $l_1 < l_2 < l_3 < \cdots$. Then there will be an n_1 corresponding to l_1 such that τ_{n_1} is closest to τ; and an n_2 corresponding to l_2 such that τ_{n_2} is closest to τ; and so on. For arbitrarily large lengths, we should have $\tau_{n_1}\approx\tau_{n_2}\approx\cdots\approx\tau$, so that in the limit of infinite lengths they converge to τ.

We know that the eigenfunctions $\varphi_{n_1}, \varphi_{n_2}, \ldots$ will obtain their minimum variances at their respective eigenvalues

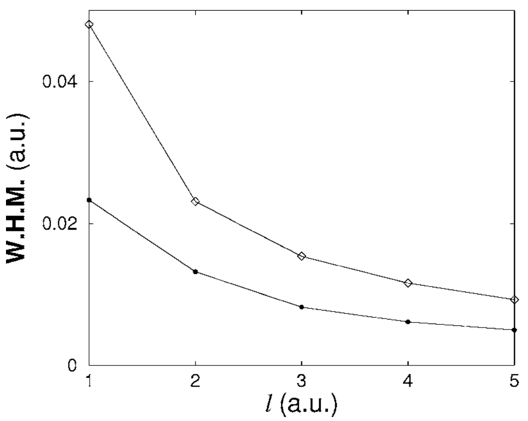

FIG. 4. Width at half maximum (WHM) of the evolved odd and even eigenfunctions (upper and lower lines) at the corresponding eigenvalues closest to $t=0.01$ vs length l.

$\tau_{n_1}, \tau_{n_2}, \ldots$. How do the variances compare for the different φ_n's? Equivalently, what is the behavior of the variance with respect to φ_n at the eigenvalue τ_n as l approaches infinity? In this case the variance increases with l. This is not surprising because the φ_n's would be thrown out of the Hilbert space for infinite l, i.e., they acquire infinite variances.

However, if we substitute the width at half maximum (WHM) of the probability density $|\varphi_n(q,\tau_n)|^2$ at the eigenvalue τ_n for the variance, we find that WHM decreases with increasing l. Figure 4 demonstrates this. What is even more important is that the density $|\varphi_n(q,\tau_n)|^2$ at the eigenvalue τ_n tends, as l increases indefinitely, to a function with point support at the origin. Figure 5 demonstrates this. These results imply that the CTOA eigenfunctions in the limit of infinite l (which are already outside of the Hilbert space) evolve to "collapse" at the origin at their respective eigenvalues. This allows us to interpret Kijowski's distribution as the ideal time-of-arrival distribution of collapsing states at the origin.

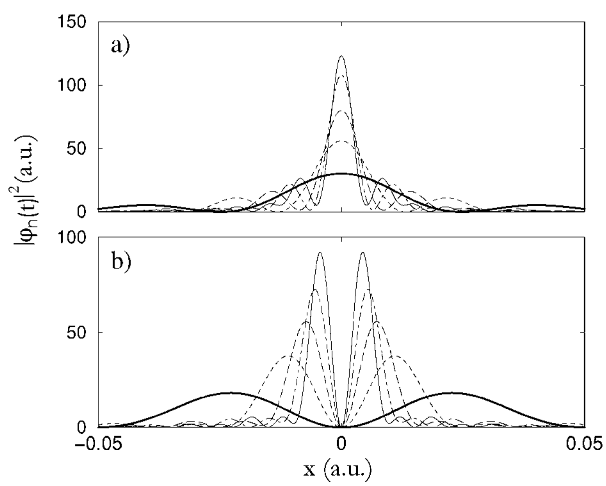

FIG. 5. Probability density $|\varphi_n(\tau)|^2$ vs position at the corresponding closest eigenvalue τ_n to $t=0.01$, for the even (upper figure) and odd (lower figure) eigenfunctions. The different lines are associated with $l=1$ (thick solid line), $l=2$ (dashed line), $l=3$ (long-dashed line), $l=4$ (dotted-dashedline), and $l=5$ (thin solid line).

V. DISCUSSION

From a purely technical point of view, we have shown that Kijowski's (continuum) time-of-arrival distribution for free, unconfined quantum particles can be obtained as the limit of the (discrete) distribution that results from quantizing the time of arrival in a finite box, taking into account the eigenvalue spacing in the transition from sums to integrals. Note that the TOA operator is not self-adjoint in the unconfined case, but it is self-adjoint in the box. There are several possible readings of this fact. We will point out some of them, with the aim of opening a public discussion on the fundamental issues involved, rather than to settle final answers and exhaustive explanations.

For those following a traditional, von Neumann's formulation of quantum mechanics, the connection with a self-adjoint operator may be satisfactory since, within this framework, all observables must be associated with self-adjoint operators. One of the customary roles of self-adjointness is to assure the orthogonality of eigenfunctions so that, according to the projection postulate, repeated measurements would give the same result. It turns out however, that this idealization is not applicable to many observables and/or measurement operations. In particular, improper eigenfunctions for observables with continuum spectrum (such as momentum, energy, or position on the line) are not normalizable, and thus the collapse and repeated measurement idea cannot be applied literally, even in principle, but only approximately. It seems then that, as long as some ideal probability distribution may be computed unambiguously, there is no fundamental need to have a self-adjoint operator in these cases. Indeed, if one adopts the point of view that observables are best formulated in terms of POVMs [3,8], self-adjointness is not essential to describe observables. The eigenfunction orthogonality may, however, be seen anyway as a desirable, simplifying property, whereby a part (component) of the initial state is responsible for a given outcome (eigenvalue) and not for any other. What the present paper shows is that the time-of-arrival eigenfunctions in the unbounded case differ, appart from a normalization factor, only outside the large box or far from the arrival point at the origin. The nonorthogonality in the continuum is thus caused by the distant eigenfunction behavior with negligible overlap with the initial wave packet, and is thus physically irrelevant for computing the distribution.

Another problematic matter is the interpretation of the discrete nature of the time-of-arrival eigenvalues in the box. A discretization of time variables should not be surprising. For any system with discrete energies or eigenmodes the corresponding time periods are also discrete. In the same vein, the TOA operator considered involves the discretized momentum operator in the denominator and therefore discrete eigenvalues. The problem thus is not in accepting the possibility of a discretization but in determining its operational meaning. "Measurements," and "observables" are frequently highly idealized in quantum mechanics, to the point that all explicit reference to an apparatus could disappear. This is useful, but may also leave us without important physical references for its operational interpretation. Whereas an operational interpretation exists for Kijowski distribution in the continuum, a direct operational interpretation of the discrete times of the confined case is still missing and is one of the challenges for future research. In any case, the discrete-continuum smooth transition found here may be a useful tool to generate new theories of, say, first time of arrival with interacting potentials, that can be later translated to the continuum and operationally interpreted or compared with existing operational proposals [20].

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