Title: Times of arrival and gauge invariance

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Abstract: "We revisit the arguments underlying two well-known arrival-time distributions in quantum mechanics, viz., the Aharonov-Bohm and Kijowski (ABK) distribution, applicable for freely moving particles, and the quantum flux (QF) distribution. An inconsistency in the original axiomatic derivation of Kijowskiâ€™s result is pointed out, along with an inescapable consequence of the â€œnegative arrival timesâ€• inherent to this proposal (and generalizations thereof). The ABK free-particle restriction is lifted in a discussion of an explicit arrival-time setup featuring a charged particle moving in a constant magnetic field. A natural generalization of the ABK distribution is in this case shown to be critically gauge-dependent. A direct comparison to the QF distribution, which does not exhibit this flaw, is drawn (its acknowledged drawback concerning the quantum backflow effect notwithstanding).

Based on a recent paper (https://arxiv.org/abs/2102.02661), to be published in Proceedings of the Royal Society A."

Times of arrival and gauge invariance

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Times of arrival and gauge invariance

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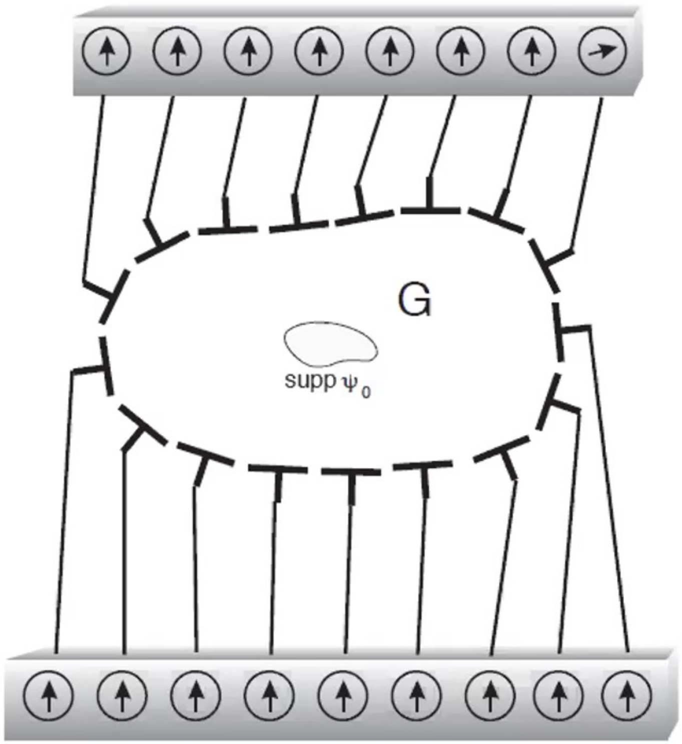
We revisit the arguments underlying two well-known arrival-time distributions in quantum mechanics, viz., the Aharonov–Bohm–Kijowski (ABK) distribution, applicable for freely moving particles, and the quantum flux (QF) distribution. An inconsistency in the original axiomatic derivation of Kijowski's result

Essentials of a TOF experiment

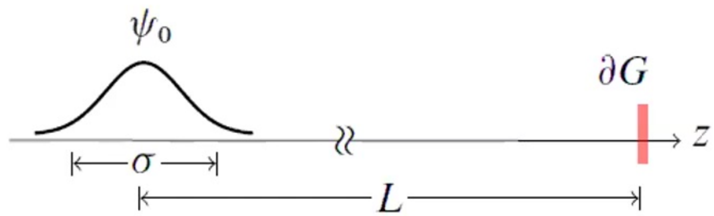


An idealized TOF experiment. Figure courtesy of Dürr.

- Given ψ_0 and ∂G,
- What is the probability density of arrival or detection times $\Pi(\tau)$ as a functional depending on ψ_0 and on ∂G?
- Note that $\Pi(\tau)\,d\tau$ is the probability that the particle is detected on ∂G between times τ and $\tau + d\tau$.
- It follows that,

$$\int_0^\infty d\tau \; \Pi(\tau) + P(\infty) = 1.$$

Aharonov-Bohm (1961), Paul (1962)



quantize classical arrival-time expressions ($\hbar = m = \sigma = 1$)[1]

$$\tau = \frac{L - z}{p}$$

---

[1] The correct classical TOF formula valid for an arbitrary initial point (z, p) in phase space is

$$\tau = \begin{cases} (L - z)/p, & \operatorname{sgn} p = \operatorname{sgn}(L - z), \\ \infty, & \text{otherwise}, \end{cases}$$

quantizing which seems nothing short of impossible.

Putting hats on τ

- Two proposals

$$\hat{\tau}_{\mathrm{AB}} = L\,\hat{p}^{-1} - \frac{1}{2}\left(\hat{p}^{-1}\,\hat{z} + \hat{z}\,\hat{p}^{-1}\right)$$

$$\hat{\tau}_{\mathrm{GRT}} = L\,\hat{p}^{-1} - \hat{p}^{-1/2}\,\hat{z}\,\hat{p}^{-1/2}$$

- It turns out, formally,

$$[\hat{\tau}, \hat{p}^2] = 2i\mathbb{1} \quad \left(\overset{?}{\Rightarrow}\ \Delta E\,\Delta\tau \geq 1/2\right)$$

- Echoes of "Pauli's Theorem" (1933).

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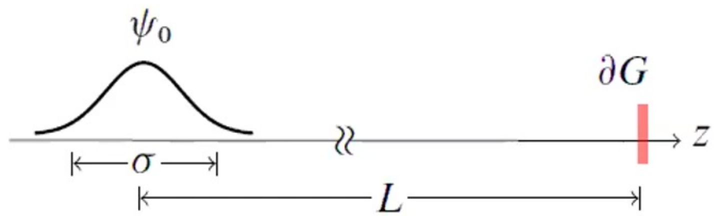

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Arrival-time distribution

- Operators are not self-adjoint, have negative eigenvalues, never mind, ...
- Provide well-defined Positive Operator Valued Measure (POVM).
- In particular,

$$\Pi_{\mathsf{AB}}(\tau) = \frac{1}{2\pi} \sum_{\alpha=\pm} \Bigg| \int_{-\infty}^{\infty} dp\; \theta(\alpha p)\, \sqrt{|p|}\, \langle p|\psi_0\rangle \times \exp\Big(-\frac{i\tau}{2} p^2 + i p L \Big) \Bigg|^2 .$$

The problem of negative eigenvalues

- Normalization $\int_{-\infty}^{\infty} d\tau \; \Pi_{\mathsf{AB}}(\tau) = 1$
- Discard $\tau \leq 0$, i.e., $P_{\mathsf{AB}}(\infty) = \int_0^{\infty} d\tau \; \Pi_{\mathsf{AB}}(-\tau)$.
- Cannot use usual quantum formulas like $\langle \tau \rangle = \langle \psi | \hat{\tau} | \psi \rangle$.
- And, if we do, $\langle \tau \rangle = 0$ vanishes for any real $\psi_0(z)$:

$$\langle \psi | \hat{\tau} | \psi \rangle = \frac{i}{4} \int_{\mathbb{R}^2} dz \, dz' \; (2L - z - z') \, \mathrm{sgn}(z - z') \times \psi_0^*(z) \, \psi_0(z'),$$

Status of the time-energy uncertainty relation

- $\Pi_{\mathsf{AB}}(\tau)$ decays too slowly to have a finite $\Delta\tau$, unless

$$\lim_{p\to 0} p^{-3/2} \langle p|\psi_0\rangle = 0.$$

- This then precludes states $\propto \exp\big(-\alpha z^2 + i\beta z\big)$ that are experimentally accessible.
- Even if we restrict attention to finite $\Delta\tau$ wave functions, the Robertson-Schrödinger uncertainty relation does not obtain.

Kijowski's axiomatic derivation (1979)

- Freely moving particles, for which

$$\langle \mathbf{p}|\psi_t\rangle = \langle \mathbf{p}|\psi_0\rangle \exp\left(-\frac{it}{2}\,p^2\right).$$

- Applicable for $\partial G = \{\mathbf{x} \in \mathbb{R}^3 \,|\, z = L\}$.
- Initially, focused on $\langle \mathbf{p}|\psi_0\rangle = 0,\ p_z \leq 0$.
- Arrival-time distribution of the form:

$$\Pi_{\text{Kij}}(\tau) = F\left(e^{ip_z L}\,\langle \mathbf{p}|\psi_0\rangle\right)$$

Kijowski's derivation cont.

- Postied axioms:
  - $F(\psi) \geq 0,$
  - $F(\psi^*) = F(\psi),$
  - $F(\hat{U}\psi) = F(\psi),$
  - $\int_{-\infty}^{\infty} dt\ F(\psi_t) = \langle \psi_0 | \psi_0 \rangle = 1,$
  - $\int_{-\infty}^{\infty} dt\ t^2\, F(\psi_t) < \infty,$
- Many $F(\cdot)$ satisfy this, but

$$F_0(\psi) = \frac{1}{2\pi} \int_{\mathbb{R}^2} dp_x\, dp_y \left| \int_0^{\infty} dp_z\ \sqrt{p_z}\ \tilde{\psi}(\mathbf{p}) \right|^2$$

is special.

Kijowski's derivation cont.

- $F_0(\cdot)$ was *unique*, in that

$$\int_{-\infty}^{\infty} dt\; t\, F(\psi_t) = \int_{-\infty}^{\infty} dt\; t\, F_0(\psi_t),$$

  and

$$\int_{-\infty}^{\infty} dt\; t^2\, F(\psi_t) \geq \int_{-\infty}^{\infty} dt\; t^2\, F_0(\psi_t),$$

  given any admissible F.

- Form generic wave functions, he suggested,

$$\Pi_{\mathrm{Kij}}(\tau) = \frac{1}{2\pi} \sum_{\alpha=\pm} \int_{\mathbb{R}^2} dp_x\, dp_y \left| \int_{-\infty}^{\infty} dp_z\, \theta(\alpha p_z) \times \sqrt{|p_z|}\; \langle \mathbf{p}|\psi_\tau\rangle \right|^2 \quad \left(\stackrel{1D}{\equiv} \Pi_{\mathrm{AB}}(\tau) \right)$$

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$$\left. \times \sqrt{|p_z|}\ \langle \mathbf{p}|\psi_\tau\rangle \right|^2 \quad \left(\overset{1D}{\equiv} \Pi_{\mathsf{AB}}(\tau) \right)$$

Quantum Flux distribution

- Defined by

$$\boxed{\Pi_{\mathrm{QF}}(\tau) = \int_{\partial G} \mathbf{J}(\mathbf{x}, \tau) \cdot d\mathbf{s},}$$

- where

$$\mathbf{J}(\mathbf{x}, t) = \frac{\hbar}{m} \mathrm{Im}\big[\psi^*(\mathbf{x}, t) \boldsymbol{\nabla} \psi(\mathbf{x}, t)\big] - q\mathbf{A}(\mathbf{x}, t)$$

- Naturally motivated from Scattering considerations, correct physical dimensions, automatically normalized.
- Defined for generic ∂G and electromagnetic potentials.
- But doesn't define a (POVM) [Vona,Hinrichs, and Dürr, Phys. Rev. Lett. **111**, 2013]

spreading is observed, thanks to an effective harmonic confinement $\propto r^2$ induced by the magnetic field (3.1).

The 'standard arrival-time distribution' for the primed wave function can be evaluated as follows: First, in view of (2.20), we note

$$\tilde{\psi}_t'(\mathrm{p}) = \frac{\mathrm{e}^{-\mathrm{i}t}}{\pi^{3/4}}\sqrt{\frac{\sigma(t)}{1+\mathrm{i}t}}\exp\left[-\frac{1}{2}(p_x^2+p_y^2+\sigma(t)p_z^2)\right], \tag{3.8}$$

where

$$\frac{1}{\sigma(t)} = \frac{1}{1+\mathrm{i}t} + \mathrm{i}\eta. \tag{3.9}$$

Incorporating the same into (2.19), and performing the Gaussian integrals over p_x and p_y, we are left with

$$\Pi_{\mathrm{STD}}(\tau) = \frac{|\sigma(\tau)|}{2\sqrt{\pi^3(1+\tau^2)}}\sum_{\alpha=\pm}\left|\int_{-\infty}^{\infty}\mathrm{d}p_z\,\theta(\alpha p_z)\sqrt{|p_z|}\exp\left(-\frac{\sigma(\tau)}{2}p_z^2+\mathrm{i}p_z L\right)\right|^2. \tag{3.10}$$

Separating this integral into positive and negative p_z contributions and letting $p_z \to -p_z$ in the latter, yields via [86, eqn 3.462.1]:

$$\Pi_{\mathrm{STD}}(\tau) = \frac{1}{8\sqrt{\pi(1+\tau^2)}|\sigma(\tau)|}\exp\left(-\frac{\mathrm{Re}[\sigma(\tau)]}{2|\sigma(\tau)|^2}L^2\right)\sum_{\alpha=\pm}\left|D_{-3/2}\left(\frac{\mathrm{i}\alpha L}{\sqrt{\sigma(\tau)}}\right)\right|^2. \tag{3.11}$$

Here, $D_\nu(\cdot)$ denotes the parabolic cylinder function of order ν (reducing to the familiar Hermite polynomial for $\nu = 0, 1, 2\ldots$ [86, eqn 9.253]). The 'standard distribution' for the unprimed wave function is obtained by setting $\eta = 0$ in the above.

Since (3.11) depends non-trivially on η (figure 1), and each value of η defines the same physical magnetic field (3.1), the 'standard distribution' is not gauge-invariant. Furthermore, for η non-zero,

$$\Pi_{\mathrm{STD}}(\tau) \sim \sqrt{|\eta|}\,\mathrm{e}^{-L^2/2}\left(\frac{\mathrm{const.}}{\tau} + \mathcal{O}(\tau^{-2})\right), \tag{3.12}$$

as $\tau \to \infty$. Consequently, (3.11) is unnormalizable, hence cannot be a physical probability distribution. At this point, one may be tempted to set $B_0 = 0$, whereby the magnetic field

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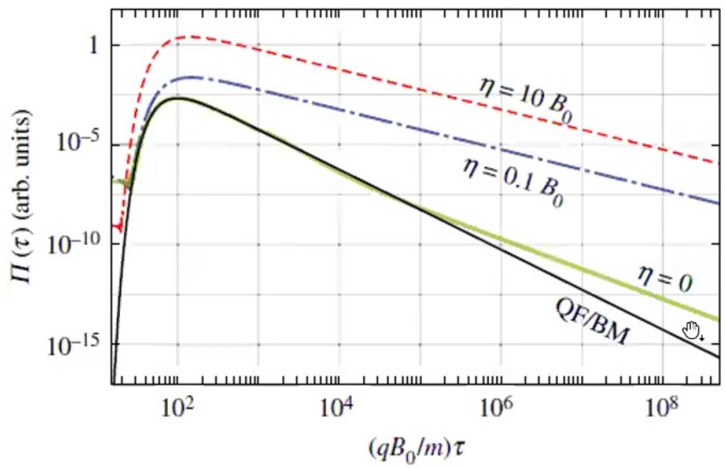

Figure 1. Arrival time distributions $\Pi_{\mathrm{QF/BM}}(\tau)$ and $\Pi_{\mathrm{STD}}(\tau)$ versus (dimensionless) arrival-time $(qB_0/m)\tau$ for $L = 100\sqrt{\hbar/qB_0}$ and select values of η annotated in the figure. The QF/BM distribution is gauge-invariant, hence independent of η. (Online version in colour.)

It is also informative to directly compute the Bohmian arrival-time distribution for this case. First, the guiding equation (2.23) implies for either vector potential the component equations

$$\dot{R}_t = 0, \quad \dot{\Phi}_t = 1 \quad \text{and} \quad \dot{Z}_t = \frac{t}{1+t^2} Z_t, \tag{3.16}$$

where $\mathrm{X}_t = R_t(\cos\Phi_t \hat{\mathrm{x}} + \sin\Phi_t \hat{\mathrm{y}}) + Z_t \hat{\mathrm{z}}$ is the position of the particle at time t. For an arbitrary initial condition X_0, the solutions are given by

$$R_t = R_0, \quad \Phi_t = \Phi_0 + t, \quad \text{and} \quad Z_t = Z_0\sqrt{1+t^2}. \tag{3.17}$$

Physically, the Bohmian trajectories are circular helices of radius R_0 that circulate in an

22,35,83], wherein the significance of the backflow effect has been persistently emphasized. For free particles, the differences are indeed negligible, since

$$\Pi_{\mathrm{Kij}}(\tau) \approx \frac{L}{\tau^4} \left| \tilde{\psi}_0 \left(\frac{L}{\tau} \right) \right|^2, \tag{2.28}$$

once $L, \tau \gg 1$ with $L/\tau \sim \mathcal{O}(1)$ (see [4] for details), thereby agreeing with $\Pi_{\mathrm{QF}}(\tau)$ via equation (2.27). In a few examples containing simple interaction potentials, we found good agreement between the QF and the 'standard distribution', although a general argument is far from available.

3. Arrival time statistics in a constant magnetic field

In this section, we consider a direct extension of the 'standard distribution' to vector potentials, letting $\hat{H}$ be the minimally coupled Hamiltonian in equation (2.20). To illustrate its consequences, we describe next a simple arrival-time experiment involving a spin-0 particle of mass m and charge q, moving in a constant magnetic field

$$\mathbf{B}(\mathrm{x}) = 2B_0\hat{\mathbf{z}}, \tag{3.1}$$

directed along the z-axis of a right-handed coordinate system. The particle is prepared in a suitable wave function at time zero, $\psi_0(\mathrm{x})$, and arrival times are monitored at a distant plane $z = L$. As a pretext for the relevance of this problem outside its present context, we mention the TOF measurements of *single* charged particles moving within a Penning trap in mass spectrometry applications, and that of electrons emitted from quantum Hall edge states [84,85, p. 9]. In what follows, we employ cylindrical polar coordinates $\mathrm{x} = (r, \phi, z)$, considering two vector potentials

$$\mathbf{A}(\mathrm{x}) = B_0 r\hat{\boldsymbol{\phi}} \quad \text{and} \quad \mathbf{A}'(\mathrm{x}) = \mathbf{A}(\mathrm{x}) - \eta z\hat{\mathbf{z}}, \tag{3.2}$$

that yield (3.1), i.e. $\nabla \times \mathbf{A} = \nabla \times \mathbf{A}' = \mathbf{B}$. Here, η is a free (real) parameter that can be changed without altering the physical magnetic field under consideration. The vector potential $\mathbf{A}$ corresponds to what is often called the symmetric gauge, and satisfies the Coulomb gauge condition $\nabla \cdot \mathbf{A} = 0$. The vector potentials are related by the gauge transformation time-energy uncertainty relation. Our considerations suggest serious reconsideration of these ambitions, once the unphysical 'negative arrival times' inherent in them are taken seriously. The QF distribution is a natural candidate for the arrival-time distribution in quantum mechanics but does not enjoy unrestricted applicability due to the backflow effect. This defect is remedied by the Bohmian arrival-time distribution from which the QF was derived. On the other hand, there are often serious difficulties met in realizing stable backflow situations experimentally (see, however, [81,87,88]). Thus, Π_{QF} is unproblematic for most practical purposes, even though it does not follow from a generalized quantum observable (or POVM).[12]

Finally, the 'standard distribution', understood as a natural generalization of the ABK free-motion result, cannot be applied to vector potentials in the manner explored in §3, as it fails to be gauge-invariant. Finding a gauge-invariant generalization therefore remains a challenging and important task for its proponents, as electromagnetic fields are essential to any realization of a TOF experiment. As a first step, one might restrict attention to freely moving charged particles alone, where free motion is taken to mean, as usual, vanishing $\mathbf{E}$ and $\mathbf{B}$. The electromagnetic potentials, however, are non-zero, satisfying $\mathbf{A} = \nabla\lambda$ and $V = -\partial\lambda/\partial t$, where $\lambda(\mathbf{x}, t)$ is an arbitrary real function. The most general Hamiltonian describing this motion is thus $\hat{H}(\lambda) = (\hat{\mathbf{p}} - q\nabla\lambda)^2/(2m) - q\partial\lambda/\partial t$. A self-consistent free-motion TOF distribution, $\Pi_\lambda(\tau) = F(\psi_\tau^{(\lambda)}, \lambda)$, given by some positive functional F, and a solution $\psi_\tau^{(\lambda)}(\mathbf{x})$ of Schrödinger's equation with Hamiltonian $\hat{H}(\lambda)$, would be expected to have a vanishing functional derivative, i.e. $\delta\Pi_\lambda(\tau)/\delta\lambda = 0$. In addition, one could require that $\Pi_\lambda(\tau)$ reproduce $\Pi_{\mathrm{Kij}}(\tau)$ whenever $\lambda(\mathbf{x}, t)$ is a constant, for which $\hat{H}(\lambda) = \hat{\mathbf{p}}^2/(2m)$. It is an interesting question whether such a Π_λ could be associated with a POVM and, if so, what general POVM structures would be compatible with it.

Data accessibility. We declare that all the information required to reproduce the paper are contained within the paper.

Authors' contributions. S.D. suggested investigating the importance of gauge for arrival-time predictions. Both authors reviewed the literature, conducted analytical calculations, and drafted the manuscript. Both authors gave final approval for publication and agree to be held accountable for the work performed therein.

Competing interests. We declare we have no competing interests.

[12]From a Bohmian perspective, this is not a showstopper since the notion of an observable is absent in the fundamental posits of this theory (see also [89]). In this context, one could even argue 'that the significance of the [observables] has been exaggerated, in the sense that elements entering into useful mathematical techniques have been raised to the level of fundamental concepts entering into the physical theory' [90].