Quantum arrival-time problem: time observables vs. Bohmian trajectories

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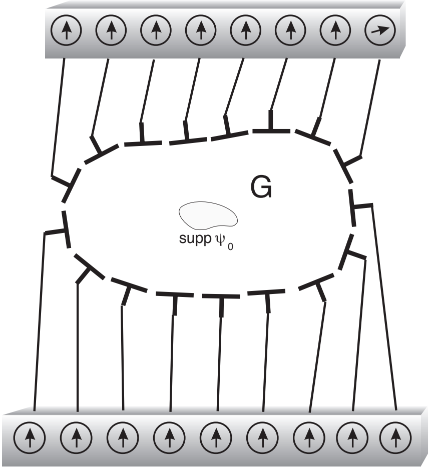
June 7, 2024

Arrival-time or Time-of-flight (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 $\Pi(t_f)$ as a functional depending on ψ_0 and on ∂G?
- $\Pi(t_f)\,dt_f$ is the probability that the particle is detected on ∂G between times t_f and $t_f + dt_f$.
- It follows that,

$$\int_0^\infty dt_f\;\Pi(t_f) + P(\infty) = 1.$$

A naive guess

Take the time-evolved wave function $\psi(\mathbf{r}, t)$ and let

$$\boxed{\Pi(t_f) \propto \int_{\partial G} d^3r \; |\psi(\mathbf{r}, t_f)|^2 \, ?}$$

[E. P. Wigner, in *Aspects of Quantum Theory*, ed. by A. Salam and E. P. Wigner (Cambridge University Press, 1972) pp. 237–247; C. R. Leavens, Phys. Lett. A 272, **160** (2000). L. Maccone and K. Sacha, Phys. Rev. Lett. **124**, 110402 (2020); R. Gambini and J. Pullin, New J. Phys. **24** 053011 (2022). K.-I. Aoki, A. Horikoshi, and E. Nakamura, Phys. Rev. A **62**, 022101 (2000); R. S. Bondurant, Phys. Rev. A **69**, 062104 (2004).]

A naive guess cont.

Take the tabletop free-particle Gaussian wave packet (∂G is the point $x = L$)

$$\psi(x,t) = \frac{1}{\pi^{1/4}\sqrt{1+it}} \exp\left[-\frac{x^2}{2(1+it)}\right]$$

proposal

$$\Pi(t_f) \propto |\psi(L,t_f)|^2$$

$$= \frac{1}{\sqrt{\pi\left(1+t_f^2\right)}} \exp\left[-\frac{L^2}{1+t_f^2}\right]$$

$$\sim \frac{t_f^{-1}}{\sqrt{\pi}}, \quad \text{as} \quad t_f \to \infty$$

A naive guess cont.: A lesson from Brownian motion

1D Brownian motion with single-time position density

$$\rho(x,t) = \frac{1}{\sqrt{4\pi D t}} \exp\left[-\frac{x^2}{4Dt}\right]$$

Solves the diffusion equation

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2}$$

First-passage time $t_f := \{t \geq 0 : X_t = L\}$ at a point L on a line is (*Levy's distribution*)

$$\boxed{\Pi(t_f) = \frac{L}{\sqrt{4\pi D t_f^3}} \exp\left[-\frac{L^2}{4Dt_f}\right] \sim C\, t_f^{-3/2}}$$

In general, ρ and Π are *not* related.

Quantum arrival-time problem

- Computation of $\Pi(t_f)$—which is empirically well-accessible—is one of the last areas where physicists disagree about what QM should predict.
- It has been claimed that
  - *"Wave mechanics cannot accommodate an exact and ideal arrival-time concept"*– Allcock (1969).
  - *"Time-of-arrival cannot be precisely defined and measured in quantum mechanics"*– Aharonov, Oppenheim, Popescu, Reznik, and Unruh (1998).
- But ToF experiments are endemic to atomic and particle physics.

On the other hand,

- *“Perhaps the following points in the right direction of possible further progress. In the new theory [matrix mechanics], not all physically observable quantities really occur, namely, the time instants of the transition processes are still missing, which are certainly observable in principle (e.g., the instants of ejections of electrons in the photoelectric effect).”*– Pauli to Bohr (Nov. 1925).
- *“All measurements of quantum-mechanical systems could be made to reduce eventually to position and time measurements (e.g., the position of a needle on a meter or the time of flight of a particle).”*– Feynman and Hibbs (1965)

Present status

- Available ToF proposals are detailed in LoN Spring 2021 Series talk:

  "Can we fix quantum arrival times before 2026?"

- Several (~ 20) disparate ToF distributions have been proposed in the literature.
- Almost *all* of them are unsatisfactory; see, e.g.,
  - B. Mielnik & G. Torres-Vega, Concepts of Physics. II, **81** (2005).
  - C. R. Leavens, Phys. Lett. A **303**, 154 (2002); Phys. Lett. A **345**, 251 (2005).
  - S. Das & M. Nöth, Proc. R. Soc. A **477**, 20210101 (2021).
  - S. Das & W. Struyve, Phys. Rev. A **104**, 042214 (2021).
  - S. Goldstein, R. Tumulka, & N. Zanghì, arXiv:2405.04607.

This talk: A brief survey of *two* popular theoretical frameworks

- Quantum observables (self-adjoint operator, POVMs)
- Trajectory containing quantum theories (e.g., Bohmian mechanics)

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Times of arrival and gauge invariance

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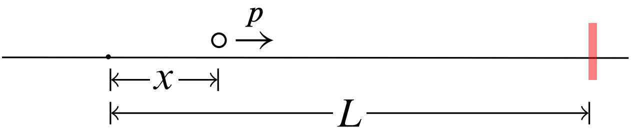
Research

Cite this article: Das S, Nöth M. 2021 Times of arrival and gauge invariance. *Proc. R. Soc. A* **477**: 20210101.
https://doi.org/10.1098/rspa.2021.0101

Received: 3 February 2021
Accepted: 4 May 2021

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

Aharonov-Bohm (1961), Paul (1962)



$$t_f^{\text{(cl)}} = m\,\frac{L-x}{p} \quad \rightarrow \quad \boxed{\hat{T}_{\mathsf{AB}} = \frac{m}{2}\Big[(L-\hat{x})\,\hat{p}^{-1} + \hat{p}^{-1}(L-\hat{x})\Big]}$$

- An application of the *correspondence principle*
- Formally,

$$\Big[\hat{T}_{\mathsf{AB}}, \frac{\hat{p}^2}{2m}\Big] = i\hbar\mathbb{1} \quad \Big(\overset{?}{\Rightarrow} \;\; \Delta E\, \Delta t_f \geq \hbar/2 \Big)$$

Arrival-time distribution

- Operators are not self-adjoint, have negative eigenvalues, never mind, ...
- Provide well-defined Positive Operator Valued Measure (POVM).
- In particular (setting $\hbar = m = \sigma = 1$)

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

- Freely moving particles, for which

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

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

$$\Pi_{\text{Kij}}(t_f) = F\!\left(e^{i\,p_x L}\,\langle \mathbf{p}|\psi_0\rangle\right)$$

Kijowski's derivation cont.

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

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

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.

- For generic wave functions, he *suggested*,

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

The devil is in the details

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

$$\langle \psi | \hat{T}_{\mathsf{AB}} | \psi \rangle = \frac{i}{4} \iint_{\mathbb{R}^2} dx\, dx' \; (2L - x - x') \; \boxed{\mathrm{sgn}(x - x')} \\ \times \; \psi_0^*(x)\, \psi_0(x'),$$

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

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

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

Serious Roadblocks for non-free motion

- Analogues of $t_f^{(\mathrm{cl})}$ seldom available.
- Even if available, it is extremely nonlinear. tunnelling situations or multiple crossings complicate matters. So, good luck with quantization.
- Detector geometries are very limited.
- External magnetic fields not accommodated yet (see later).

Theorem (Groenewold-Van Hove theorem) Any procedure associating

- every classical phase-space function $f(x, p)$ to a quantum operator F, in particular,
- x and p to the usual position and momentum operators of QM, and simultaneously
- classical Poisson brackets to quantum commutators: $\{f, g\} \mapsto (1/i\hbar)[F, G]$,

as Dirac envisioned, *cannot* exist [A. Carosso, Studies in History and Philosophy of Science **96**, 35 (2022)]

- suggested by Baute, Egusquiza, and Muga 2000s

$$\Pi_{\mathsf{STD}}(t_f) = \frac{1}{2\pi}\sum_{\alpha=\pm}\int_{\mathbb{R}^2} dp_y\, dp_z \left| \int_{-\infty}^{\infty} dp_x\, \theta(\alpha p_x) \times \sqrt{|p_x|}\; \langle \mathbf{p} | \exp\left(-i\, t_f\, \hat{H}\right) |\psi_0\rangle \right|^2$$

- new problems pop up...

- "the significance of the [quantum observables] has been exaggerated, in the sense that elements entering as useful mathematical techniques have been raised to the level of fundamental concepts in the physical theory" [D. Bohm, Prog. Theor. Phys. **9**, 273 (1953).]
- "If anyone tells me that 'to every observable there corresponds a Hermitian operator for which the eigenvalues correspond to observed values,' I will defeat him! I will cut his feet off!" [R. Feynman reported in D. Hestenes, in Annales de la Fondation Louis de Broglie, Vol. 28 (Fondation Louis de Broglie, 2003) p. 367.]

ToF predictions via particle trajectories

- Quantum theories featuring particle trajectories are naturally suited for handling arrival- and tunneling-time problems; this has long been recognized.
- Against this background, the value of such theories, whose framework offers a starting point completely different from relying on guessing a self-adjoint operator or POVM, becomes evident.

The de Broglie-Bohm pilot-wave theory or Bohmian mechanics

- In standard QM, the physical state of a system is assumed to be *completely specified* by its wave function.
- The possibility that there exist further dynamical variables determining the actual behavior of each individual system at the quantum level is rejected.
- Whereas, in Bohmian mechanics (de Broglie-Bohm or pilot-wave theory)[1] there are both particles *and* waves.

$$\boxed{\mathbf{R}_1(t),\ \mathbf{R}_2(t),\dots,\ \mathbf{R}_N(t)} \qquad \text{and} \qquad \boxed{\psi(\mathbf{r}_1,\mathbf{r}_2,\dots,\mathbf{r}_N;t).}$$

- Particles move under the influence of the wave function.

[1] At least in the nonrelativistic theory

Equations of motion

- Wave equation (Schrödinger, Pauli, Dirac, Proca ...)

$$\boxed{i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N;t) = H\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N;t)}$$

- Guiding equation (de Broglie, Bohm, Bell, Slater, Madulong ...)

$$\boxed{\dot{\mathbf{R}}_i(t) = \mathbf{v}_i^{\psi}\big(\mathbf{R}_1(t),\mathbf{R}_2(t),\ldots,\mathbf{R}_N(t);t\big).}$$

- First order differential equations (unlike Newton's mechanics!)
- Deterministic dynamics: Initial wave function and initial particle positions fix the future completely.
- Specification of H and the velocity fields $\mathbf{v}_i^{\psi}$ depends on particle spin and on whether the dynamics is "relativistic" or non-relativistic.

Reconciling determinism with Heisenberg's uncertainty and the Born Rule

- With chaos theory and nonlinear dynamics so fashionable, it is not astonishing for apparent randomness emerging from a deterministic dynamical system.
- QM makes well-tested statistical predictions but is unable to describe *individual* quantum processes without bringing in unsatisfactory assumptions, e.g., the (observation-induced) collapse of the wave function.
- *"The statistical quantum theory would, within the framework of future physics, take an approximately analogous position to the statistical mechanics within the framework of classical mechanics. I am rather firmly convinced that the development of theoretical physics will be of this type."- Einstein (1949)*

Bohmian mechanics of spin-0 particles

- Guidance Eq. for spin-0 particles:

$$\boxed{\frac{d\mathbf{R}(t)}{dt} = \frac{\hbar}{m}\,\mathrm{Im}\left[\frac{\boldsymbol{\nabla}\psi(\mathbf{R}(t),t)}{\psi(\mathbf{R}(t),t)}\right]}$$

- $\psi(\mathbf{r},t)$ solves Schrödinger's Eq.

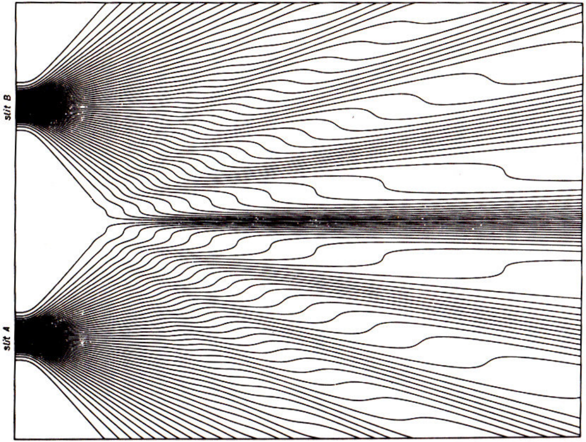
$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\mathbf{r},t)\psi}$$

- Given $\mathbf{R}(0)$ and $\psi(\mathbf{r},0)$, the particle's path is uniquely determined.
- In the presence of magnetic fields $\boldsymbol{\nabla} \mapsto \boldsymbol{\nabla} + \frac{q}{i\hbar}\mathbf{A}$.
- Many-body and spin-aware generalizations are available [S. Das, arXiv:2404.17646]

Making contact with quantum phenomena

- Bohmian trajectories for benchmark QM problems, e.g., diffraction, two-slit interference (with and without monitoring), barrier tunneling, EPR correlations, etc., "remain among the most striking illustrations so far of the insight provided by this theory into quantum phenomena."
- In all fairness, while operators as quantum observables play no role in the formulation of BM, their effectiveness as empirical shorthands is best appreciated through a Bohmian lens [D. Dürr, S. Goldstein, and N. Zanghì, J. Stat. Phys. **116**, 959 (2004).]

Typical Bohmian trajectories for the double-slit experiment



Double-slit trajectories were first presented in [C. Philippidis, C. Dewdney, and B. Hiley, IL Nuov Cim B **52**, 15 (1979)].

A customary Bell quote

"Is it not clear from the smallness of the scintillation on the screen that we have to do with a particle? *And is it not clear, from the diffraction and interference patterns, that the motion of the particle is directed by a wave?* De Broglie showed in detail how the motion of a particle, passing through just one of two holes in screen, could be influenced by waves propagating through both holes. And so influenced that the particle does not go where the waves cancel out, but is attracted to where they cooperate." [J. S. Bell, *Six Possible Worlds of Quantum Mechanics* (1986)]

A few takeaways

- It follows that one could have particle trajectories and still account for interference experiment.
- *"It is clear that [the double-slit experiment] can in no way be reconciled with the idea that electrons move in paths. ... In quantum mechanics there is no such concept as the path of a particle."* [Landau & Lifshitz, Vol. 3, p. 2]
- *"Many ideas have been concocted to try to explain the curve for P_{12} [the interference pattern] in terms of individual electrons going around in complicated ways through the holes. None of them has succeeded."* [Feynman Lectures, Vol. III, Sec. 1.5]

From pictures to predictions: Back ot ToF experiments

- Impact positions and arrival (or hitting) times of Bohmian trajectories are always well-defined for any ∂G.
- Bohmian trajectories are widely used for discussing arrival- (and tunneling-) time problems [S. Das, arXiv:2309.15815]
- For any Bohmian trajectory [Leavens, DDGZ, Grübl, ...]

$$\boxed{T_f(\mathbf{R_0}) = \inf\left\{t \geq 0 \,|\, \mathbf{R}(t) \in \partial G,\, \mathbf{R}(0) = \mathbf{R_0}\right\}}$$

  gives the *first* arrival-time on ∂G.
- A quantity that has no counterpart in standard quantum theory (also spontaneous collapse and MW theories).

Bohmian trajectory arrival-time distribution

- Given suitable statistical hypotheses about the initial conditions $\mathbf{R_0}$ and ψ_0, the distribution of $T_f(\mathbf{R_0})$ can be defined.

- In a sequence of identically prepared ToF experiments with a fixed initial wave function ψ_0, the $\mathbf{R_0}$s are typically $|\psi_0|^2$-distributed [Dürr, Goldstein, Zanghì, 1992]

- In this case, the (Bohmian) ToF distribution can be written as

$$\boxed{\Pi_{\text{BM}}(t_f) = \int_{\text{supp}(\psi_0)} d^3R_0\ \delta\Big(t_f - T_f(\mathbf{R_0})\Big)\,|\psi_0(\mathbf{R_0})|^2,}$$

where $\delta(\cdot)$ is Dirac's delta function.

Bohmian trajectory arrival-time distribution cont.

- For completeness, we have the *non-detection probability*

$$P_{\text{BM}}(\infty) = \int_{T_f^{-1}(\infty)} d^3R_0 \, |\psi_0(\mathbf{R}_0)|^2$$

- Scope of applicability is insanely broad!
- Can be easily adapted to instances where ψ_0 is chosen at random from a statistical mixture encoded in a density matrix.
- Not to forget multi-particle generalisations.

Is this on the right track?

- In general, it is difficult to compute, except when it reduces to the quantum flux distribution

$$\boxed{\Pi_{\text{BM}}(t_f) = \int_{\partial G} \mathbf{J}(\mathbf{r}, t_f) \cdot d\mathbf{s},}$$

in scattering situations, where

$$\mathbf{J}(\mathbf{r}, t) = \frac{\hbar}{m} \mathrm{Im}\big[\psi^*(\mathbf{r}, t) \boldsymbol{\nabla} \psi(\mathbf{r}, t)\big] - \frac{q}{m} \mathbf{A}(\mathbf{r}, t) |\psi(\mathbf{r}, t)|^2.$$

- Reproduces known statistics for ToF-momentum spectroscopy experiments [S. Das, arXiv:2404.17646] and scattering cross sections.

- Spin-0 particle of mass m and charge q, with

$$\mathbf{r} \equiv (\rho, \phi, z), \quad \rho = \sqrt{x^2 + y^2},$$

- moving in a uniform magnetic field $\mathbf{B}(\mathbf{r}) = 2B_0\,\hat{\mathbf{z}}$
- We will consider two vector potentials,

$$\boxed{\mathbf{A}(\mathbf{r}) = B_0\,\rho\,\hat{\phi}}, \quad \text{and} \quad \boxed{\mathbf{A}'(\mathbf{r}) = \mathbf{A}(\mathbf{r}) - \eta\, z\,\hat{\mathbf{z}}},$$

- that yield $\boldsymbol{\nabla} \times \mathbf{A} = \boldsymbol{\nabla} \times \mathbf{A}' = \mathbf{B}$
- η is a free (real) parameter that can be changed without altering the physical magnetic field under consideration.

- Reporting masses lengths and times in the units of m, $\sqrt{\hbar/qB_0}$, and m/qB_0, respectively,
- A simple Gaussian wave packet solution is

$$\begin{aligned}\psi(\mathbf{r},t) &= \psi'(\mathbf{r},t)\, e^{i\eta z^2/2} \\ &= \frac{e^{-it}}{\pi^{3/4}\sqrt{1+it}} \exp\left[-\frac{r^2}{2} - \frac{z^2}{2(1+it)}\right].\end{aligned}$$

- For this, $\Pi_{\text{BM}}(t_f)$ and $\Pi_{\text{STD}}(t_f)$ can be calculated in closed-form.

An illustrative example cont.

- $$\Pi_{\mathsf{BM}}(t_f) = \frac{L}{\sqrt{\pi}} \frac{t_f}{\left(1+t_f^2\right)^{3/2}} \exp\left[-\frac{L^2}{1+t_f^2}\right]$$

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

  where

  $$\frac{1}{\sigma(t)} = \frac{1}{1+it} + i\eta.$$

An illustrative example cont.