Inequivalence of stochastic and Bohmian arrival times in time-of-flight experiments

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Motivated by a recent prediction [Commun. Phys. **6**, 195 (2023).] that time-of-flight experiments with ultracold atoms could test different interpretations of quantum mechanics, this work investigates the arrival times predicted by the stochastic interpretation, whereby quantum particles follow definite but nondeterministic and nondifferentiable trajectories. The distribution of arrival times is obtained from a Fokker-Planck equation and confirmed by direct simulation of trajectories. It is found to be, in general, different from the distribution predicted by the Bohmian interpretation, in which quantum particles follow definite deterministic and differentiable trajectories. This result suggests that trajectory-based interpretations of quantum mechanics could be experimentally discriminated.

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I. INTRODUCTION

Do quantum particles follow definite trajectories? In the textbook presentations of quantum mechanics [1–4] following the standard Copenhagen interpretation of the theory or its statistical interpretation [5], emphasis is put on measurements as the only accessible elements of reality. Classical concepts such as trajectories are thus considered unnecessary or even inconsistent with observations. In this conception, a particle is only described by its quantum state in the absence of any observation, and "materializes" only at a certain position where it is observed by an experimental apparatus at a certain time.

However, it was shown long ago, prominently by Bohm [6,7], that the formalism of quantum theory is not inconsistent with the particles having definite trajectories in between measurements. This has led to the *de Broglie-Bohm theory* or *pilot wave theory*, which has been recognized as an alternative interpretation of quantum mechanics [8], in so far as it yields the same predictions as the standard interpretation. The Bohmian interpretation, however, has not gained much popularity, notably because it posits the seemingly unnecessary existence of hidden variables (the particles' positions at all times), and mainly because, like most interpretations of quantum mechanics, it does not seem to provide any new testable prediction.

It has long been known, however, that there are measurements for which the interpretations of quantum mechanics may lead to different predictions, namely, the measurements of arrival times [9]. While the quantum formalism gives the probabilities of a particle's position measurements at a given time through the square modulus $|\psi(\boldsymbol{x},t)|^2$ of its wave function, it does not provide explicit probabilities for the time t at which a particle arrives at a certain point $\boldsymbol{x}$. One could naïvely think that this probability distribution is still provided by the square modulus $|\psi(\boldsymbol{x},t)|^2$ at a fixed point $\boldsymbol{x}$, but a quick dimensional analysis shows that it cannot be so: $|\psi(\boldsymbol{x},t)|^2$ has the units of density, whereas the sought probability distribution should be a number per units of surface and time. The mathematical reason behind this difficulty is that time is only a parameter in standard quantum mechanics, whereas the conventional formalism requires measurable quantities to be described by a self-adjoint operator, and it is known that a self-adjoint operator cannot be constructed for time [10,11]. This problem has led to various efforts to find a plausible way to predict arrival times in quantum mechanics. Some of these works [12–18] either extend or reformulate the original formalism of quantum theory to obtain predictions, while others [19–30] have attempted to obtain predictions within the conventional framework of quantum theory (although this has been disputed [31–34]). On the other hand, in a trajectory-based interpretation of quantum mechanics such as the Bohmian interpretation, there is seemingly no difficulty to predict arrival times since the particle is assumed to follow a definite trajectory, with a definite arrival time at a certain point [35,36]. As a result, rather than a mere interpretation it becomes a falsifiable theory in its own right when applied to the arrival time problem. By measuring arrival times in time-of-flight experiments, it is therefore possible in principle to test the different formulations, extensions, and trajectory-based interpretations of quantum mechanics [37].

However, up to now, time-of-flight measurements have only been performed far from the particle's source of emission, in a regime where all theories give the same predictions, consistent with a classical motion of the particle near the detector. The situation may change, however, as a recent proposal [38] shows that it may be possible to discriminate these theories by measuring the arrival time distribution in a double-slit (or double-well) experiment.

In this context, it is of interest to revisit a rather little-known trajectory-based interpretation of quantum mechanics called *stochastic mechanics*. Stochastic mechanics started with the realization by Fényes [39] and then Nelson [40] that the Schrödinger equation naturally appears when considering a certain kind of frictionless Brownian motion. This led to an attempt to reconstruct quantum theory from the stochastic

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motion of particles induced by a hypothetical fluctuating ether [41]. Reference [42] gives a good account of the current status of stochastic mechanics. Although the original aim of deriving quantum theory from a more fundamental theory has not been achieved by stochastic mechanics, it allows for a given wave function to assign definite (but nondeterministic and nondifferentiable) trajectories to the corresponding particles in accordance with the predictions of quantum mechanics. From this perspective, it can be used as an alternative pilot wave theory. This theory may be regarded as a stochastic version of the de Broglie-Bohm pilot wave theory, and we call it the *stochastic pilot wave theory*, to distinguish it from the original stochastic mechanics.

Although the Bohmian and stochastic pilot wave theories are similar, there appear to have been no detailed comparisons between stochastic and Bohmian trajectories' arrival times. Previous results [43,44] suggest that stochastic trajectories and Bohmian trajectories lead to the same arrival time distribution. In this work, it is shown that they do in fact lead to different arrival time distributions, most notably in the case of the double-well experiment proposed in Ref. [38]. This opens the possibility to evidence, and even characterize, the trajectories of particles underlying the standard quantum theory. However, this requires the arrival times of such trajectories to be faithfully reported by a detecting apparatus, without any substantial error or perturbation from the detection scheme. The last section of this article discusses possible issues with actual measurements of these arrival times.

II. BOHMIAN AND STOCHASTIC TRAJECTORIES

The definitions of Bohmian and stochastic trajectories for a given wave function are closely related. Consider for simplicity, the case of a single nonrelativistic particle of mass m, described by a wave function $\psi(\boldsymbol{x}, t)$. One can define from the wave function the complex velocity $\boldsymbol{\mathcal{V}} = \frac{\hbar}{m}\nabla \ln \psi$ with real part $\boldsymbol{u}$ and imaginary part $\boldsymbol{v}$ called respectively *osmotic* and *average* velocities [40]. Accordingly, one obtains the two probability currents $\boldsymbol{i} = \rho\boldsymbol{u}$ and $\boldsymbol{j} = \rho\boldsymbol{v}$, where ρ is the probability density $|\psi|^2$. Note that $\boldsymbol{j}$ is the usual probability current $\frac{\hbar}{m}\text{Im}(\psi^*\nabla\psi)$ satisfying the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{j} = 0. \tag{1}$$

One may also define the forward and backward drifts

$$\boldsymbol{b} = \boldsymbol{v} + \boldsymbol{u}, \tag{2}$$

$$\boldsymbol{b}_* = \boldsymbol{v} - \boldsymbol{u}, \tag{3}$$

and the corresponding forward and backward currents

$$\boldsymbol{\mathcal{J}} = \rho\boldsymbol{b},$$
$$\boldsymbol{\mathcal{J}}_* = \rho\boldsymbol{b}_*.$$

The Bohmian trajectory starting from a point $\boldsymbol{x}_0$ at time t_0 is simply the trajectory that remains tangent to the average velocity field $\boldsymbol{v}$. Namely, the position $\boldsymbol{x}'$ at time $t' = t + dt$ is obtained from the position $\boldsymbol{x}$ at time t by the relation:

$$\boldsymbol{x}' = \boldsymbol{x} + \boldsymbol{v}(\boldsymbol{x}, t)dt. \tag{4}$$

Note that the trajectory is by construction differentiable, uniquely defined by the starting point, and never intersects any other trajectory starting from a different point at the same time.

On the other hand, a stochastic trajectory starting from a point $\boldsymbol{x}_0$ at time t_0 is defined as a stochastic diffusive process drifting along the forward velocity field $\boldsymbol{b}$. Namely, the position $\boldsymbol{x}'$ at time $t' = t + dt$ is obtained from the position $\boldsymbol{x}$ at time t by the relation

$$\boldsymbol{x}' = \boldsymbol{x} + \boldsymbol{b}(\boldsymbol{x}, t)dt + \boldsymbol{\xi}, \tag{5}$$

where $\boldsymbol{\xi}$ is a random vector with average zero and variance $\frac{\hbar}{m}dt$. Note that, in this case, the trajectories are nondeterministic, nondifferentiable, and may intersect.

It has be shown for both Bohmian [45] and stochastic [40,41] trajectories that when starting from an ensemble of points $\boldsymbol{x}_0$ at time t_0 distributed according to the initial density distribution $\rho(\boldsymbol{x}, t_0)$, the subsequent positions along the trajectories at a later time t are distributed according to the density $\rho(\boldsymbol{x}, t)$, in accordance with the predictions of standard quantum mechanics. This is illustrated in Figs. 1 and 2 for the case of an ensemble of particles initially confined in the ground state of a single harmonic well of oscillator lengths $\sigma_x, \sigma_y, \sigma_z \equiv \sigma$, with a wave function given by

$$\psi(\boldsymbol{x}, t) = G_{\sigma_x}(x, t)G_{\sigma_y}(y, t)G_{\sigma}(z, t), \tag{6}$$

and in the ground state of two degenerate harmonic wells separated by distance $2d$ in the vertical direction z, with wave function

$$\psi(\boldsymbol{x}, t) = G_{\sigma_x}(x, t)G_{\sigma_y}(y, t)\frac{G_\sigma(z - d, t) + G_\sigma(z + d, t)}{\sqrt{2}}, \tag{7}$$

where G_σ denotes the expanding Gaussian wave packet,

$$G_\sigma(x, t) = \frac{\exp\left(-\frac{x^2}{4\sigma s_t}\right)}{\left(2\pi s_t^2\right)^{1/4}} \text{ with } s_t = \sigma + \frac{i\hbar t}{2m\sigma}. \tag{8}$$

In both cases, it is assumed that the confining wells are immediately switched off at time $t = 0$, letting the particles free thereafter. In the case of the double well, it is assumed that the two wells are well separated ($d \gg \sigma$), so that the free expansion leads to an interference pattern in the density. One can check in Fig. 2 that this interference pattern is correctly reproduced by both the Bohmian and stochastic trajectories.

III. ARRIVAL TIME DISTRIBUTION

Now let us consider the arrival time of the particle on a detector. As mentioned earlier, the determination of arrival times is, in principle, straightforward since the particle's possible trajectories are known. Nevertheless, one is immediately faced with several important assumptions about the detector that can affect the measured arrival times. Is the detector localized around a single point, or a two-dimensional plane? Is the particle "destroyed" by the detector when it is detected (in the sense that it cannot be detected again)? Does the detector affect the particle's motion? If so, does it simply select trajectories guided by the wave function, or does it directly affect the wave function itself?

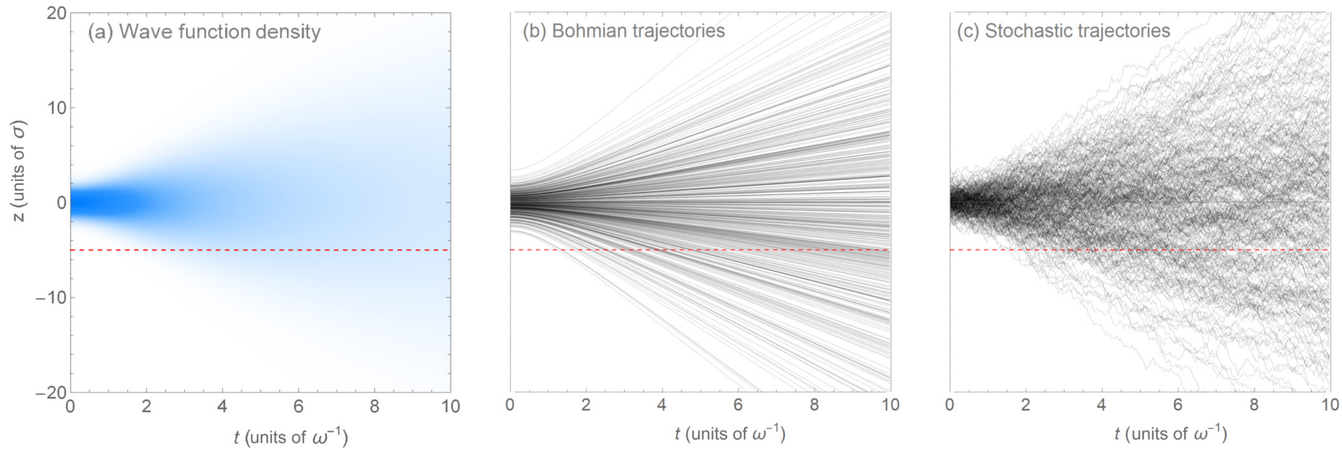

FIG. 1. Cloud of particles released from a single harmonic well of frequency $\omega = \hbar/2m\sigma^2$ and oscillator length σ. (a) Integrated density $\int dxdy|\psi(\boldsymbol{x}, t)|^2$ as a function of time. (b) z component of 400 Bohmian trajectories. (c) z component of 400 stochastic trajectories. The trajectories are calculated from Eqs. (4) and (5) with $dt = 1/(1600\omega)$. The red dashed line indicates the position of a detector at the distance $L = 5\sigma$ from the center of the well.

In the following, it will be assumed that the detector is planar, destroys the particle as soon as it is detected, but does not affect its wave function (i.e., the wave function is assumed to remain the same as in the absence of detector). Let us say that the detector is placed at a certain distance L below the source of the particle. Then, according to our assumptions, the particle can only arrive from above the detector plane (assuming that the detector plane is large enough to prevent any trajectory from going around the detector and hitting it from below). For a statistical distribution of trajectories, the arrival time distribution is then simply proportional to the arrival flux of trajectories hitting the detector plane from above. Note that the motion in the three spatial directions are independent due to the separability of the wave functions (6) and (7), so that one can simply consider the motion along the z direction as far as the arrival times on the detector are concerned.

In the case of Bohmian trajectories, it has been shown [46] that the flux of trajectories through a plane is simply the flux of the probability current $\boldsymbol{j}$ through that plane. When all trajectories hit the detector plane from above, as in the case of a particle released from a single harmonic well [see Fig. 1(b)], the arrival flux $F(t)$ is thus the flux $-\int_P d\boldsymbol{S} \cdot \boldsymbol{j}(\boldsymbol{x}, t)$ of $\boldsymbol{j}$ through the detection plane P. Here, $d\boldsymbol{S} = dS\boldsymbol{n}$, where dS is the surface integration element and $\boldsymbol{n}$ the unit vector orthogonal to the detection plane and pointing out from the detecting side. Figure 3 confirms that the arrival flux of Bohmian trajectories numerically simulated from Eq. (4) (gray fill) coincides with the flux of the probability current $\boldsymbol{j}$ (dashed curve). As discussed in Ref. [38], the situation is more complicated in the case of the double well, because some trajectories may cross the detection plane three times [see Fig. 2(b)], thus hitting once the detector plane from below (a situation known as quantum reentry [47,48]). According to the assumption that the particle is destroyed as soon as it first hits the detector from above, the subsequent contributions from these trajectories to the flux of $\boldsymbol{j}$ through the plane should be discarded in the calculation of the arrival flux. This can only be achieved through the simulation of many trajectories, as shown in Fig. 4(a). One can see that the obtained arrival flux (gray fill) is zero at and, slightly after, the arrival times where

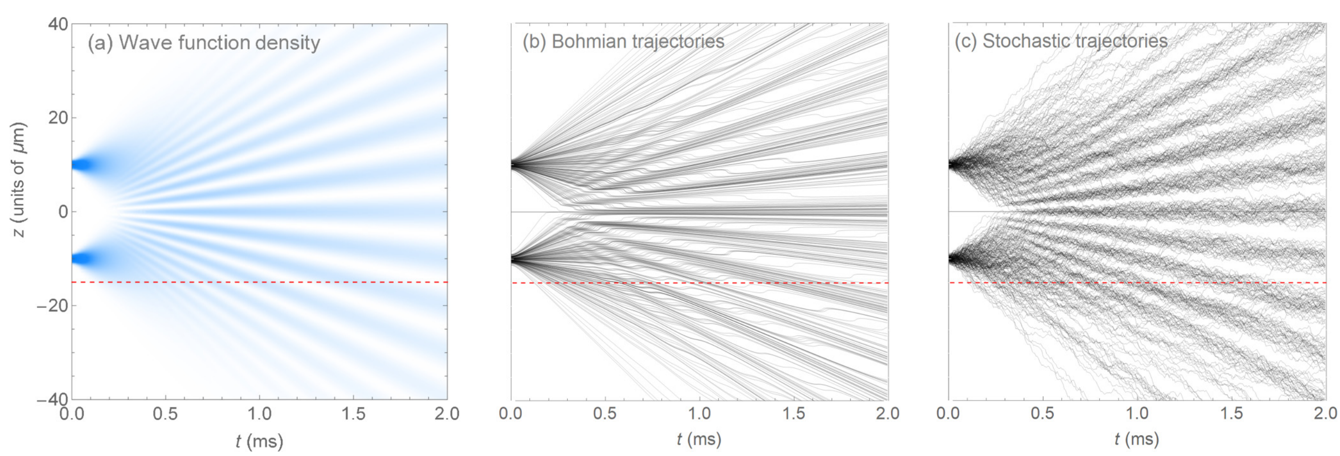

FIG. 2. Cloud of particles of mass $m = 4m_u$ released from two wells of oscillator length $\sigma = 0.5$ μm, separated by a distance $2d = 20$ μm along the z direction. The panels are similar to those of Fig. 1. The red dashed line indicates the position of a detector at the distance $L = 15$ μm from the center of the two wells.

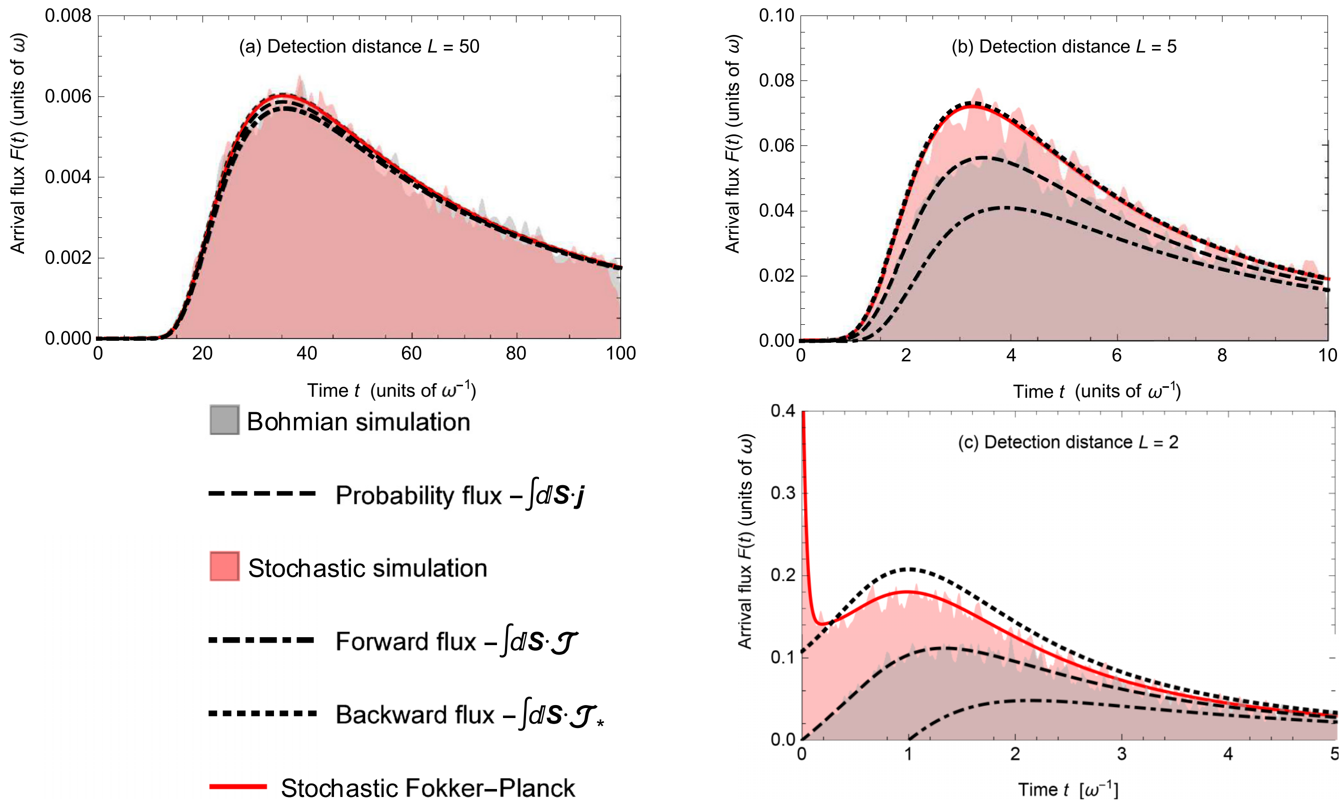

FIG. 3. Arrival flux of a cloud of particles released from a single well of frequency $\omega = \hbar/2m\sigma^2$ and oscillator length σ, onto a detector at different distances L from the well. (a) $L = 50\sigma$. (b) $L = 5\sigma$. (c) $L = 2\sigma$. The Bohmian (gray fill) and stochastic (red fill) arrival fluxes are obtained by sampling 32 000 trajectories propagated from Eqs. (4) and (5) with $dt = 1/(1600\omega)$.

the flux of $\boldsymbol{j}$ (dashed curve) is negative because the corresponding trajectories are blocked by the detector. Away from these specific arrival times, the arrival flux is well reproduced by the flux of $\boldsymbol{j}$.

In the case of stochastic trajectories, one could think by comparing Eqs. (4) and (5) that the arrival flux would be given by the forward current $\mathcal{J}$. However, that it is not the case. As shown in Fig. 3, the arrival flux of stochastic trajectories numerically simulated from Eq. (5) (red fill) is in fact better approached by the flux of the backward current $\mathcal{J}_*$ (dotted curve) than the forward current $\mathcal{J}$ (dot-dashed curve). This makes sense when one realizes that the backward current corresponds to the average current *arriving* at a given point, whereas the forward current corresponds to the average current *departing* from that point. Yet, the backward current only provides an approximation of the arrival flux.

It is actually possible to determine the arrival flux exactly by considering the density $\rho_L(\boldsymbol{x}, t)$ of trajectories *that do not reach the detection plane*. That is because once the density of such trajectories is known at a certain instant, one can calculate the number of those first reaching the plane at the next instant. As shown in Appendix D, the density ρ_L satisfies the following forward Fokker-Planck equation,

$$\frac{\partial \rho_L}{\partial t} + \nabla \cdot (\boldsymbol{b}\rho_L) - \frac{\hbar}{2m}\nabla^2 \rho_L = 0, \tag{9}$$

which is also known to be satisfied by the full density $\rho(\boldsymbol{x}, t)$ of all possible trajectories [40]. However, here it is complemented by the following Dirichlet boundary condition at the detection plane, $\rho_L(\boldsymbol{x}, t) = 0 \ \forall\, \boldsymbol{x} \in P$, which effectively implements the restriction that the underlying trajectories cannot reach the plane. It can be shown (see Appendix D) that the first-arrival flux $F(t)$ at the plane (for trajectories that do reach the plane) is then given by

$$F(t) = -\int_P d\boldsymbol{S} \cdot \frac{\hbar}{2m} \nabla \rho_L(\boldsymbol{x}, t). \tag{10}$$

Figures 3 and 4(b) show that the flux of Eq. (10) obtained by solving numerically the Fokker-Planck equation (9) (red curve) agrees within the sampling errors with the one calculated from the simulation of stochastic trajectories from Eq. (5) (red fill). Unlike the case of Bohmian trajectories, the arrival time distribution of stochastic trajectories can thus be obtained without resorting to a sampling of trajectories.

IV. EXPERIMENTAL OBSERVATION

Figures 3 and 4 clearly demonstrate that the arrival fluxes of Bohmian and stochastic trajectories are in general different. However, they may be difficult to distinguish experimentally. As found in Ref. [44], far from the source of particles, both the Bohmian and stochastic fluxes are indistinguishable from the flux of the probability current $\boldsymbol{j}$, as seen in Fig. 3(a). They become in principle distinguishable for detectors closer to the source, as shown in Fig. 3(b), but remain largely proportional to each other. Unless the initial number of particles is precisely known and the detection is 100% efficient, one could only extract the arrival time distribution from the detector's

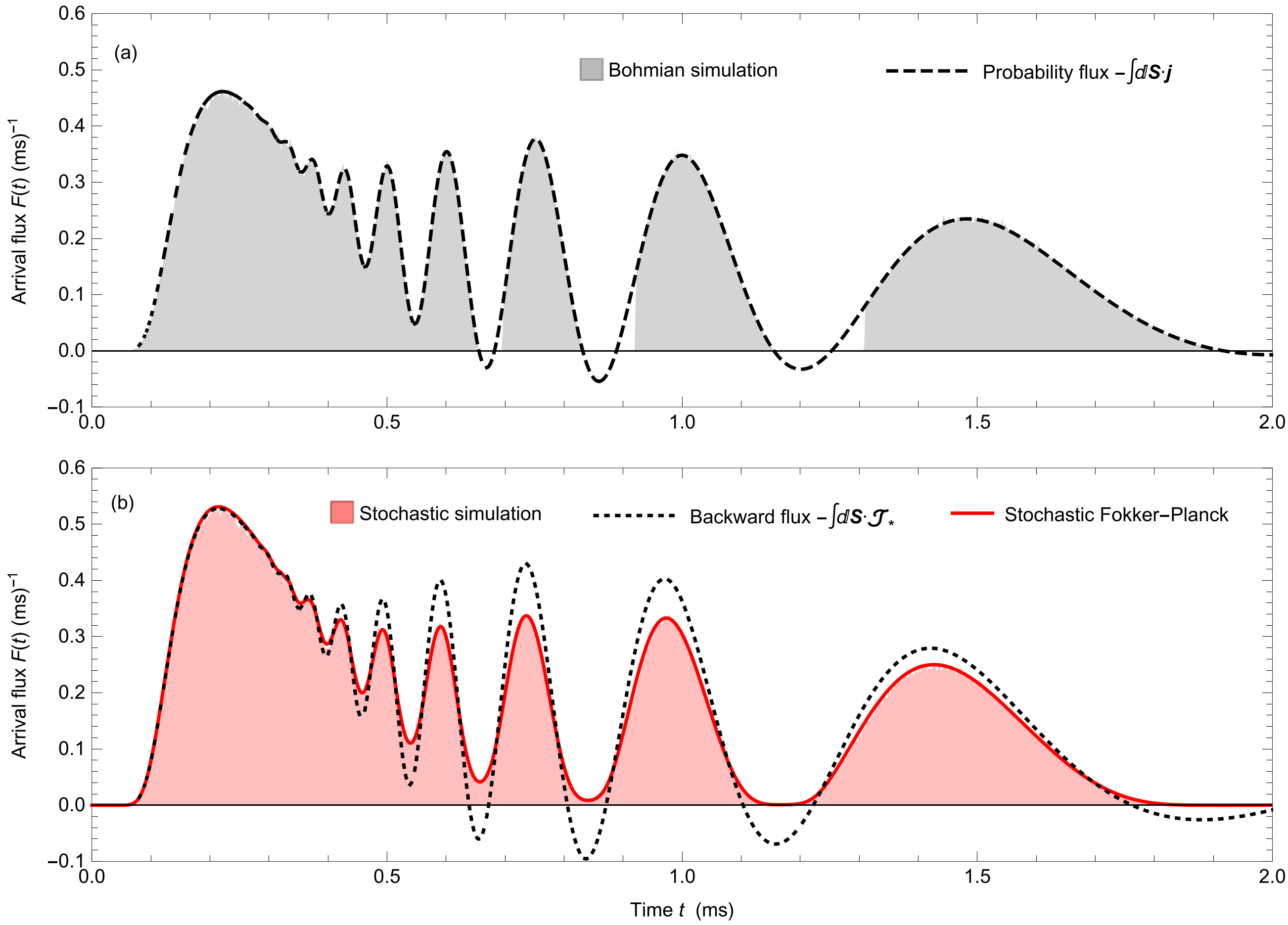

FIG. 4. Arrival flux of a cloud of particles released from a double well onto a detector at a distance $L = 15$ μm from the center of the two wells: (a) case of Bohmian trajectories; (b) case of stochastic trajectories. The fluxes are obtained by sampling 5×10^6 trajectories propagated from Eqs. (4) and (5) with $dt = 3.75$ μs.

counts, which would not be conclusive. Much closer to the source, as in Fig. 3(c) where the distance L is only twice the trap width σ, the arrival time distributions are predicted to be noticeably different. However, besides the technical issues with implementing such a close detector, the assumption that the detector does not alter the wave function is questionable in this case.

As advocated in Ref. [38], the double-well system with a detection plane perpendicular to the axis joining the two wells is more promising. The authors propose to confine a cloud of ultracold atoms in a double-well trap, release the trap and measure the arrival times of the atoms on a detector. At ultracold temperature, all atoms condense into the ground state of the trap. Each atom thus constitutes a realization of a single-particle time-of-flight experiment for the same wave function. The best candidate for this purpose is metastable ^{4}He, since it can be efficiently detected due to its high internal energy [49]. For easier comparison, the same parameters as those chosen in Ref. [38] have been taken in Figs. 2, 4, and 5, namely, $m = 4m_u$ (^{4}He mass, with m_u being the atomic mass unit), $d = 10$ μm, $\sigma = 0.5$ μm. Note that the horizontal initial velocity assumed in Ref. [38] to mimic a double-slit experiment does not affect the vertical motion and is irrelevant in a double-well experiment where atoms are simply released from their trap. For a detector at $L = 15$ μm from the center of the double well (thus at a distance 10σ from the nearest well), about 44% of the released atoms reach the detector within 6 ms. Their normalized arrival time distribution in that time frame is shown in Fig. 5, for both the Bohmian (gray) and stochastic trajectories (red). They are compared with the *Kijowski arrival time distribution* (black), which constitutes an important reference since it can be derived from different approaches to arrival time measurements, such as an axiomatic approach [23], an absorption potential model [21], a canonical quantization of the arrival time with the construction of a (generally non-self-adjoint) arrival-time operator [19,25], or a self-adjoint arrival-time operator that is not conjugate to the Hamiltonian [26].

One can see clear discrepancies between the three predicted distributions. In particular, trajectory-based interpretations of quantum theory both predict time frames where there are no arrivals, in contrast with the prediction of the Kijowski distribution. Observing a signal in these time frames would therefore invalidate these theories. To simulate the statistical noise, the Bohmian and stochastic distributions are calculated with the trajectories of 5×10^6 atoms, a number typically achieved in experiments. One can see that this noise is not an issue for distinguishing the curves. A major drawback is that to experimentally rule out any of these curves, the experimental data must be compared with a theoretical cal-

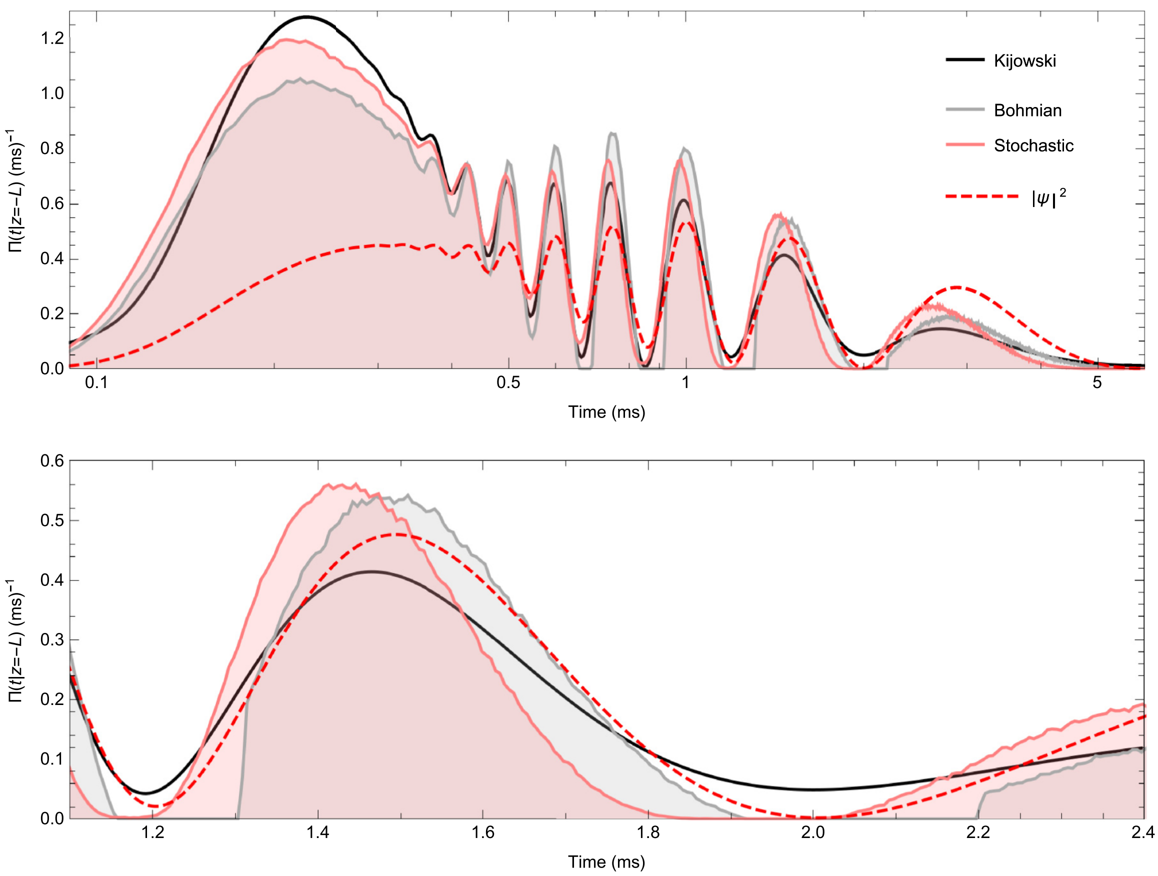

FIG. 5. (top) Arrival time distribution normalized over 6 ms, for different theories: the Kijowski arrival time distribution (black) obtained in several theories of the quantum arrival time [19,21,23,25,26], and the first-arrival time distributions obtained from Bohmian (gray) and stochastic (red) trajectories. The dashed curve shows the normalized distribution proportional to the wave-function density $|\psi(\boldsymbol{x},t)|^2$ integrated on the detection plane; this distribution corresponds to the multiple-arrival time distribution of stochastic trajectories, as well as the as the distribution obtained in the quantum clock proposal [37]. (bottom) Closeup of top panel around 2 ms, showing the time frames where the Bohmian and stochastic distributions vanish.

culation. Thus, very precise calibrations of all the parameters of the experiments, in particular the position of the detector, trap frequency, and time of release, are necessary. Nevertheless, the experimental discrimination appears to be feasible in principle.

It is important to note that the above conclusions are bound to the assumptions made in Sec. III. Let us briefly discuss what to expect if these assumptions are invalidated.

If one assumes that the detector does not necessarily detect the particle on its first arrival but has a certain probability distribution for detecting the particle at its various positions as it goes through the detector, the resulting arrival time distribution may be quite different, especially for stochastic trajectories. Indeed, while Bohmian trajectories are smooth and cross the detector plane at most three times, stochastic trajectories can enter the detector many times if the particle is not immediately destroyed. It was found numerically in Ref. [44] that taking into account these multiple counts through the detector gives a flux that is proportional to the density $|\psi(\boldsymbol{x},t)|^2$ on the detector plane. This result may sound surprising, since the density does not have the units of a flux, as stressed earlier. The proportionality coefficient must therefore have units of velocity. But what could be that constant velocity? Although the work of Ref. [44] did not address this question, it is in fact possible to express analytically the flux $F(t)$ of all stochastic trajectories through the detector plane (see Appendix E). It turns out that this flux is indeed proportional to the density, but the proportionality coefficient is formally infinite:

$$F(t) = \lim_{dt\to 0} 2\sqrt{\frac{\hbar}{2m\pi dt}} \int_P dS|\psi(\boldsymbol{x},t)|^2. \qquad (11)$$

This means that the stochastic trajectories cross the detector plane so many times that it results in an infinite flux. Physically, however, the proportionality coefficient should be finite due to the limited temporal resolution of the detector. Therefore, a detector detecting many passages of a single particle is expected to yield a finite number of counts proportional to the density. The first-arrival detection and multiple-passage detection constitute two opposite limits. For a detector detecting the particle with some delay probability distribution, the measured arrival time distribution is expected to be somewhere between these two limits. These limits are shown in Fig. 5 by the solid red curve (immediate detection of the first arrival) and the dashed red curve (multiple-passage detection). One can conclude from that figure that, even if the detector experiences delays and multiple counts, the distribution resulting from stochastic trajectories likely remains distinguishable from other predictions, although it is more complicated to predict. Incidentally, let us remark that the normalized distribution obtained from the flux of Eq. (11) coincides with the distribution obtained from the quantum clock proposal [37], according to which time measurement is obtained from the entanglement of the particle with a clock taken as a time reference.

Finally, there remains the question of whether the detector affects the wave function. Some works [50–53] have proposed that the wave function is affected by the detector through an absorbing boundary condition making the wave function proportional to its gradient through the detector,

$$\boldsymbol{n}\cdot\nabla\psi(\boldsymbol{x},t)=i\kappa\psi(\boldsymbol{x},t)\ \forall\,\boldsymbol{x}\in P, \tag{12}$$

where κ is an inverse length characterizing the detector. It is clear that this condition makes the current $\boldsymbol{n}\cdot\rho\boldsymbol{\mathcal{V}}=\frac{\hbar}{m}\psi^*\boldsymbol{n}\cdot\nabla\psi$ purely imaginary, i.e., $\boldsymbol{n}\cdot\boldsymbol{j}=\boldsymbol{n}\cdot\boldsymbol{\mathcal{J}}_*=\frac{\hbar}{m}\kappa\rho$. This situation is similar to that of Fig. 3(a), where $\boldsymbol{n}\cdot\boldsymbol{j}=\boldsymbol{n}\cdot\boldsymbol{\mathcal{J}}_*$. It was observed in that case that the stochastic and Bohmian trajectories lead to indistinguishable arrival time distributions. It is therefore likely that such a back effect of the detector on the wave function would make it difficult to distinguish the predictions of stochastic and Bohmian trajectories. However, it is presently unknown whether the detector affects the wave function in this way.

V. CONCLUSION

This work shows that two trajectory-based interpretations of quantum mechanics, the Bohmian and stochastic pilot wave theories, do not in general yield the same arrival times. It appears that these theories could be discriminated experimentally from other theories of arrival time, as well as from each other, using ultracold atoms released from a double well trap, as proposed in Ref. [38]. Although questions remain regarding the role of the detection scheme, it is an intriguing prospect that such experiments could shed some light on the longstanding question of the existence and nature of trajectories in quantum mechanics.

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APPENDIX A: STOCHASTIC MOTION

Let us consider a one-dimensional stochastic motion with forward drift $b(x,t)$ and diffusion coefficient $\mathcal{D}=\hbar/2m$. Namely, the position x' of the particle at time $t'=t+dt$ is obtained from its position x at time t by the relation:

$$x'=x+b(x,t)dt+\xi, \tag{A1}$$

where ξ is a random number with average zero and variance $2\mathcal{D}dt$. A realization of such motion is shown in Fig. 6.

APPENDIX B: TEMPORAL DISTRIBUTION *F*

Let us define $F(x,t|x_0,t_0)dt$ as the probability for first reaching x between t and $t+dt$ starting from x_0 at time t_0.

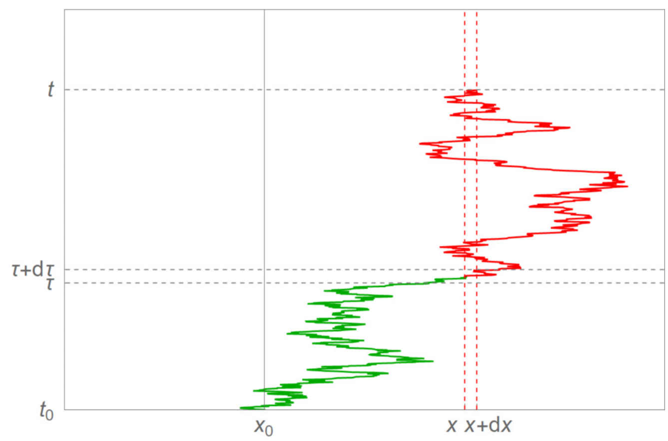

FIG. 6. Example of stochastic trajectory going from (x_0,t_0) and reaching t between x and $x+dx$. It first reaches x between time τ and $\tau+dt$ and then crosses x again several times between time $\tau+dt$ and t. The ensemble of all possible such trajectories determines the spatial probability distribution $R(x,t|x_0,t_0)$. The ensemble of all possible trajectories going from (x_0,t_0) and reaching x for the first time between τ and $\tau+dt$ (green section of the curve) determines the temporal probability distribution $F(x,\tau|x_0,t_0)$.

"First" means that x has not been crossed along the trajectory: the particle reaches x for the first time between t and $t+dt$ (see the green section of the curve in Fig. 6).

The probability for reaching x between time t_0 and t starting from x_0 is therefore

$$0\leqslant\int_{t_0}^{t}F(x,\tau|x_0,t_0)d\tau\leqslant 1. \tag{B1}$$

APPENDIX C: SPATIAL DISTRIBUTION *R*

Let us now define $R(x,t|x_0,t_0)dx$ as the probability for reaching t between x and $x+dx$, starting from x_0 at time t_0 (see the whole curve in Fig. 6).

1. Basic properties

Since the particle must be somewhere at any time t, one must have

$$\int_{-\infty}^{\infty}dx\,R(x,t|x_0,t_0)=1. \tag{C1}$$

Moreover, by summing the probabilities for all possible positions at an intermediate time τ, one obtains the following chain rule:

$$\int_{-\infty}^{\infty}dy\,R(x,t|y,\tau)R(y,\tau|x_0,t_0)=R(x,t|x_0,t_0). \tag{C2}$$

2. Fokker-Planck equation

The probability distribution R can be shown to satisfy the forward Fokker-Planck equation [54]

$$\frac{\partial R}{\partial t}+\frac{\partial}{\partial x}(bR)-\mathcal{D}\frac{\partial^2}{\partial x^2}R=0 \tag{C3}$$

with initial condition $R(x,t_0|x_0,t_0)=\delta(x-x_0)$. Thus for any density $\rho(x,t)$ satisfying the above Fokker-Planck equation with initial condition $\rho(x,t_0)=\rho_0(x)$, one can write $\rho(x,t)=\int dx_0 R(x,t|x_0,t_0)\rho_0(x_0)$. For this reason, $R(x,t|x_0,t_0)$ may be regarded as the propagator of the Fokker-Planck equation.

3. Relation between *F* and *R*

One can find a relation between F and R by summing the probabilities for all possible times at which the particle first reaches x before eventually reaching x again at the final time t:

$$\int_{t_0}^{t} d\tau R(x,t|x,\tau)F(x,\tau|x_0,t_0)=R(x,t|x_0,t_0). \tag{C4}$$

This relation is illustrated in Fig. 6.

APPENDIX D: DENSITY FROM TRAJECTORIES NOT REACHING *y*

The probability density for reaching (x,t) starting from (x_0,t_0) without having crossed y at any time $\tau\in[t_0,t]$ is given by

$$R_y(x,t|x_0,t_0)\equiv R(x,t|x_0,t_0)-\tilde{R}(x,t|y|x_0,t_0), \tag{D1}$$

where

$$\tilde{R}(x,t|y|x_0,t_0)=\int_{t_0}^{t} d\tau R(x,t|y,\tau)F(y,\tau|x_0,t_0) \tag{D2}$$

is the probability for reaching (x,t) from (x_0,t_0) and having crossed y at least once at some intermediate time τ. This implies that $R_y(y,t|x_0,t_0)=0$, owing to Eq. (C4).

Let us now calculate the following derivatives:

$$\frac{\partial}{\partial t}\tilde{R}=\underbrace{R(x,t|y,t)}_{\delta(x-y)}F(y,t|x_0,t_0)+\int_{t_0}^{t} d\tau\frac{\partial R(x,t|y,\tau)}{\partial t}F(y,\tau|x_0,t_0), \tag{D3}$$

$$\frac{\partial}{\partial x}(b\tilde{R})=\int_{t_0}^{t} d\tau\frac{\partial}{\partial x}[bR(x,t|y,\tau)]F(y,\tau|x_0,t_0), \tag{D4}$$

$$\frac{\partial^2}{\partial x^2}(\tilde{R})=\int_{t_0}^{t} d\tau\frac{\partial^2}{\partial x^2}[R(x,t|y,\tau)]F(y,\tau|x_0,t_0). \tag{D5}$$

By summing the above equations and using the fact that R satisfies the Fokker-Planck equation (C3), one arrives at

$$\frac{\partial}{\partial t}\tilde{R}+\frac{\partial}{\partial x}(b\tilde{R})-\mathcal{D}\frac{\partial^2}{\partial x^2}(\tilde{R})=\delta(x-y)F(y,t|x_0,t_0). \tag{D6}$$

Therefore, R_y satisfies the Fokker-Planck equation

$$\frac{\partial}{\partial t}R_y+\frac{\partial}{\partial x}(bR_y)-\mathcal{D}\frac{\partial^2}{\partial x^2}(R_y)=0 \tag{D7}$$

on $]-\infty,y[$ and $]y,\infty[$, with a discontinuity of the spatial derivative at $x=y$ given by

$$\left[\frac{\partial}{\partial x}R_y\right]_{x\to y^+}-\left[\frac{\partial}{\partial x}R_y\right]_{x\to y^-}=\frac{F(y,t|x_0,t_0)}{\mathcal{D}}. \tag{D8}$$

Let us suppose that the starting point x_0 is on the left side of y. Since by construction the particle cannot cross y, $R_y(x,t|x_0,t_0)$ must be identically zero for $x\geqslant y$, and the first term in Eq. (D8) should vanish. Therefore, for an arbitrary initial density distribution $\rho_0(x)$ of points $x<y$, the density $\rho_L(x,t)\equiv\int_{-\infty}^{y} dx_0 R_y(x,t|x_0,t_0)\rho_0(x_0)$ is also identically zero for $x\geqslant y$ and satisfies the Fokker-Planck equation

$$\frac{\partial}{\partial t}\rho_L+\frac{\partial}{\partial x}(b\rho_L)-\mathcal{D}\frac{\partial^2}{\partial x^2}(\rho_L)=0 \tag{D9}$$

with the initial condition $\rho_L(x<y,t)\equiv\rho_0(x)$ and the boundary condition $\rho_L(y,t\geqslant t_0)=0$. The density ρ_L is the density resulting from trajectories not crossing y from the left, starting from an initial density ρ_0. The temporal distribution $F_L(y,t)$ for trajectories first reaching y from the left at time t is therefore $F_L(y,t)\equiv\int_{-\infty}^{y} dx_0 F(y,t|x_0,t_0)\rho_0(x_0)$. From Eq. (D8), one obtains

$$F_L(y,t)=-\mathcal{D}\left[\frac{\partial\rho_L(x,t)}{\partial x}\right]_{x\to y^-}. \tag{D10}$$

The formulation can be generalized to a three-dimensional stochastic motion. The density $\rho_L(\boldsymbol{x},t)$ of three-dimensional trajectories first reaching a plane P from a given side (say left), starting from an initial density $\rho_0(\boldsymbol{x})$, satisfies the three-dimensional Fokker-Planck equation

$$\frac{\partial\rho_L}{\partial t}+\nabla\cdot(\boldsymbol{b}\rho_L)-\mathcal{D}\nabla^2\rho_L=0, \tag{D11}$$

with the boundary condition $\rho_L(\boldsymbol{x},t)=0\;\forall\,\boldsymbol{x}\in P$. The flux of these trajectories through the plane is then given by

$$F(t)=-\int_P d\boldsymbol{S}\cdot\mathcal{D}\nabla\rho_L(\boldsymbol{x},t), \tag{D12}$$

where $d\boldsymbol{S}=dS\boldsymbol{n}$ is the elementary surface vector pointing from the left side of the plane.

APPENDIX E: FLUX FROM ALL TRAJECTORIES

Let us now go back to the one-dimensional motion and consider the flux of all (unblocked) trajectories through a certain point x_0 between time t and $t+dt$. The basic idea of the calculation is as follows: At time t, the probability density resulting from all unblocked trajectories is known to given by $\rho(x,t)$. For very small dt, the contributions to the flux between t and $t+dt$ are given by trajectories coming from the neighborhood of x_0, typically from the range $[x_0-b(x,t)dt-\sqrt{\mathcal{D}dt},x_0-b(x,t)+\sqrt{\mathcal{D}dt}]$ since the trajectories diffuse during a time dt within a typical distance $\approx 2\sqrt{\mathcal{D}dt}$. The number $d\mathcal{N}$ of such trajectories is therefore $\approx\rho(x_0,t)2\sqrt{\mathcal{D}dt}$, which gives a flux $d\mathcal{N}/dt\sim\rho(x_0,t)2\sqrt{\mathcal{D}/dt}$ that is proportional to the local density $\rho(x_0,t)$ but diverging as $dt^{-1/2}$.

Here is a more precise derivation. The total number $d\mathcal{N}$ of trajectories starting at time t from the density $\rho(x,t)$ and crossing the point x_0 (either from left or right) before time $t+dt$ is given by

$$d\mathcal{N}=\int_{-\infty}^{\infty} dx\,\rho(x,t)P_{x_0}(x'|x), \tag{E1}$$

where $P_{x_0}(x'|x)$ is the probability of crossing x_0 when starting from x and ending at x' given by the stochastic process of Eq. (A1). If the starting point x is smaller than x_0, it is the probability that $x'>x_0$ and if the starting point x is larger than

x_0, it is the probability that $x' < x_0$, namely,

$$P_{x_0}(x'|x) = \begin{cases} P(x' > x_0) & \text{for } x < x_0 \\ P(x' < x_0) & \text{for } x > x_0. \end{cases} \tag{E2}$$

From Eq. (A1), one has $x' = x + b(x,t)dt + \xi$, and since $\xi \sim \sqrt{\mathcal{D}dt}$, for sufficiently small dt one can neglect the term $b(x,t)dt$ with respect to ξ in the calculation of the probabilities. This gives

$$P_{x_0}(x'|x) = \begin{cases} P(\xi > x_0 - x) & \text{for } x_0 - x > 0 \\ P(\xi < x_0 - x) & \text{for } x_0 - x < 0. \end{cases} \tag{E3}$$

Even if the probability distribution of ξ is not normal at very small timescale, for dt larger than that timescale, it becomes normal due to the central limit theorem. Thus one can write

$$\begin{aligned} P_{x_0}(x'|x) &= P(\xi > |x_0 - x|) \\ &= \int_{|x_0-x|}^{\infty} \frac{1}{\sqrt{4\pi\mathcal{D}dt}} \exp\left(-\frac{\xi^2}{4\mathcal{D}dt}\right) d\xi \\ &= \frac{1}{2}\operatorname{erfc}\left(\frac{|x_0 - x|}{\sqrt{4\mathcal{D}dt}}\right). \end{aligned} \tag{E4}$$

Now one can make a Taylor expansion of $\rho(x,t)$ around x_0 by setting $x = x_0 + \epsilon$ in Eq. (E1):

$$d\mathcal{N} = \int_{-\infty}^{\infty} d\epsilon \left[\rho(x_0,t) + \epsilon \frac{\partial \rho}{dx}(x_0,t) + O(\epsilon^2)\right] P_{x_0}(x'|x). \tag{E5}$$

Performing the integration over ϵ using the explicit expression of P_{x_0} given by Eq. (E4), one arrives at

$$d\mathcal{N} = \sqrt{\frac{4\mathcal{D}dt}{\pi}}\rho(x_0,t) + 0 + O(dt^{3/2}). \tag{E6}$$

The total flux through x_0 at time t is therefore

$$\frac{d\mathcal{N}}{dt} = \sqrt{\frac{4\mathcal{D}}{\pi dt}}\rho(x_0,t) + O(dt^{1/2}) \tag{E7}$$

which is divergent in the limit of small dt.

The result is generalized to three dimensions for the adirectional flux through a surface S:

$$F = \sqrt{\frac{4\mathcal{D}}{\pi dt}} \int_S dS \rho(\boldsymbol{x},t). \tag{E8}$$

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