On the quantum probability flux through surfaces

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Abstract

We remark that the often ignored quantum probability current is fundamental for a genuine understanding of scattering phenomena and, in particular, for the statistics of the time and position of the first exit of a quantum particle from a given region, which may be simply expressed in terms of the current. This simple formula for these statistics does not appear as such in the literature. It is proposed that the formula, which is very different from the usual quantum mechanical measurement formulas, be verified experimentally. A full understanding of the quantum current and the associated formula is provided by Bohmian mechanics.

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I. INTRODUCTION

In Born's interpretation of the wave function ψ_t at time t of a single particle of mass m, $\rho_t(\mathbf{x}) = |\psi_t(\mathbf{x})|^2$ is the probability density for finding the particle at $\mathbf{x}$ at that time. The consistency of this interpretation is ensured by the continuity equation

$$\frac{\partial \rho_t}{\partial t} + \mathrm{div} \cdot \mathbf{j}^{\psi_t} = 0,$$

where $\mathbf{j}^{\psi_t} = \frac{1}{m}\mathrm{Im}\psi_t^* \nabla \psi_t$ is the quantum current ($\hbar = 1$).

The quantum current is usually not considered to be of any operational significance (see however [1]). It is not related to any standard quantum mechanical measurement in the way, for example, that the density ρ, as the spectral measure of the position operator, gives the statistics for a position measurement. Nonetheless, it is hard to resist the suggestion that the quantum current integrated over a surface gives the probability that the particle crosses that surface, i.e., that

$$\mathbf{j}^{\psi_t} \cdot d\mathbf{S}dt \tag{1}$$

is the probability that a particle crosses the surface element $d\mathbf{S}$ in the time dt. However, this suggestion must be taken "cum grano salis" since $\mathbf{j}^{\psi_t} \cdot d\mathbf{S}dt$ may be somewhere negative, in which case it cannot be a probability. But before discussing the situations where $\mathbf{j}^{\psi_t} \cdot d\mathbf{S}dt$ can be negative we want to consider first a regime for which we can expect this quantity to be positive, so that its meaning could in fact be the crossing probability, namely, the regime described by scattering theory.

II. STANDARD SCATTERING THEORY

In textbooks on quantum mechanics the principal objects of interest for scattering phenomena are nonnormalized stationary solutions of the Schrödinger equation with the asymptotic behavior

$$\psi(\mathbf{x}) \overset{x\to\infty}{\sim} e^{i\mathbf{p}_{in}\cdot\mathbf{x}} + f(\theta,\phi)\frac{e^{ipx}}{x},$$

where $e^{i\mathbf{p}_{in}\cdot\mathbf{x}}$ represents an incoming wave, $p = |\mathbf{p}_{in}|$, and $f(\theta,\phi)\frac{e^{ipx}}{x}$ is the scattered wave with angular dependent amplitude. $f(\theta,\phi)$ gives the probability for deflection of the particle in the direction specified by θ,ϕ by the well-known formula for the differential cross section

$$d\sigma = |f(\theta,\phi)|^2 \sin\theta d\theta d\phi \tag{2}$$

This representation of a scattering process is, however, not entirely convincing since Born's rule is not directly applicable to non-normalizable wave functions. More important, this picture is entirely time-independent whereas the physical scattering event is certainly a process in space and time. Indeed, according to some experts, the arguments leading to the formula (2) for the cross section "wouldn't convince an educated first grader" ([2], p. 97).

It is widely accepted that the stationary treatment is justified by an analysis of wave packets evolving with time. Using a normalized wave packet $\psi_t(\mathbf{x}) = e^{-iHt}\psi(\mathbf{x})$ one immediately obtains by Born's rule the probabilities for position measurements. But what are the relevant probabilities in a scattering experiment? In mathematical physics (e.g. [3], p. 356, and [4]) an answer to this is provided by Dollard's scattering-into-cones theorem [5]:

$$\lim_{t\to\infty}\int_C d^3x|\psi_t(\mathbf{x})|^2 = \int_C d^3p|\widehat{\Omega_-^\dagger\psi}(\mathbf{p})|^2.$$

This connects the asymptotic probability of finding the particle in some cone C with the probability of finding its asymptotic momentum $\mathbf{p}$ in that cone, where $\Omega_- = \text{s-}\lim_{t\to\infty} e^{iHt}e^{-iH_0t}$ is the wave operator ("s- lim" denotes the strong limit), $H = H_0 + V$, with $H_0 = -\frac{1}{2m}\nabla^2$, and $\hat{}$ denotes the Fourier transform. It is generally believed that the left hand side of the scattering-into-cones theorem is exactly what the scattering experiment measures, as if the fundamental cross section associated with the solid angle Σ (to be identified with a subset of the unit sphere) were

$$\sigma_{\text{cone}}(\Sigma) := \lim_{t\to\infty}\int_{C_\Sigma} d^3x|\psi_t(\mathbf{x})|^2,$$

where C_Σ is the cone with apex at the origin subtended by Σ (see Fig. 1). To connect this with (2), which is independent of the details of the initial wave function, one may invoke the right hand side of the scattering-into-cones theorem to recover the usual formula with additional assumptions on the initial wave packet (see [3] p. 356 for a discussion of this.)

So far the mathematics. But back to physics. The left hand side of the scattering-into-cones theorem is the probability that at some large but fixed time, when the position of the particle is measured, the particle is found in the cone C. But does one actually measure in a scattering experiment in what cone the particle happens to be found at some large but *fixed* time? Is it not rather the case that one of a collection of distant detectors surrounding the scattering center fires at some *random* time, a time that is not chosen by the experimenter? And isn't that random time simply the time at which, roughly speaking, the particle crosses the detector surface subtended by the cone?

This suggests that the relevant quantity for the scattering experiment should be the quantum current. If the detectors are sufficiently distant from the scattering center the current will typically be outgoing and (1) will be positive. We obtain as the probability that the particle has crossed some distant surface during some time interval the integral of (1) over that time interval and that surface. The integrated current thus provides us with a physical definition (see also [6], p. 164) of the cross section:

$$\sigma_{\text{flux}}(\Sigma) := \lim_{R\to\infty} \int_0^\infty dt \int_{R\Sigma} \mathbf{j}^{\psi_t} \cdot d\mathbf{S}, \tag{3}$$

where $R\Sigma$ is the intersection of the cone C_Σ with the sphere of radius R (see Fig. 1). As before, one would like to connect this with the usual formulas and hence we need the counterpart of the scattering-into-cones theorem—the flux-across-surfaces theorem—which provides us with a formula for σ_{flux}:

$$\lim_{R\to\infty} \int_0^\infty dt \int_{R\Sigma} \mathbf{j}^{\psi_t} \cdot d\mathbf{S} = \int_{C_\Sigma} d^3p |\widehat{\Omega_-^\dagger \psi}(\mathbf{p})|^2. \tag{4}$$

The fundamental importance of the flux-across-surfaces theorem was first recognized by Combes, Newton and Shtokhamer [7]. To our knowledge there exists no rigorous proof of this theorem, although the heuristic argument for it is straightforward. Let us consider first the "free flux-across-surfaces theorem," where $\psi_t := e^{-iH_0 t}\psi$:

$$\lim_{R\to\infty}\int_0^\infty dt\int_{R\Sigma}\mathbf{j}^{\psi_t}\cdot d\mathbf{S}=\int_{C_\Sigma}d^3p|\hat{\psi}(\mathbf{p})|^2 \tag{5}$$

(This free theorem, by the way, should be physically sufficient, since the scattered wave packet should in any case move almost freely after the scattering has essentially been completed (see also [7]).)

Now the current should contribute to the integral in (5) only for large times, because the packet must travel a long time before it reaches the distant sphere at radius R. Thus we may use the long-time asymptotics of the free evolution. We split $\psi_t(\mathbf{x})=(e^{-iH_0t}\psi)(\mathbf{x})$ into

$$\begin{aligned}\psi_t(\mathbf{x}) &= (\frac{m}{2\pi it})^{3/2}\int d^3y e^{im\frac{|\mathbf{x}-\mathbf{y}|^2}{2t}}\psi(\mathbf{y})\\ &= (\frac{m}{it})^{3/2}e^{im\frac{x^2}{2t}}\hat{\psi}(\frac{m\mathbf{x}}{t})\\ &+ (\frac{m}{it})^{3/2}e^{im\frac{x^2}{2t}}\int\frac{d^3y}{(2\pi)^{3/2}}e^{-im\frac{\mathbf{x}\cdot\mathbf{y}}{t}}(e^{im\frac{y^2}{2t}}-1)\psi(\mathbf{y}).\end{aligned}$$

Since $(e^{im\frac{y^2}{2t}}-1)\to 0$ as $t\to\infty$, we may neglect the second term, so that as $t\to\infty$ we have that

$$\psi_t(\mathbf{x})\sim(\frac{m}{it})^{3/2}e^{im\frac{x^2}{2t}}\hat{\psi}(\frac{m\mathbf{x}}{t}). \tag{6}$$

(This asymptotics has long been recognized as important for scattering theory, e.g. [8,5].) From (6) we now find that

$$\mathbf{j}^{\psi_t}(\mathbf{x})=\frac{1}{m}\mathrm{Im}\psi_t^*(\mathbf{x})\nabla\psi_t(\mathbf{x})\approx\frac{\mathbf{x}}{t}(\frac{m}{t})^3|\hat{\psi}(\frac{m\mathbf{x}}{t})|^2. \tag{7}$$

(Note that by (7) the current is strictly radial for large times, so that $\mathbf{j}^{\psi_t}\cdot d\mathbf{S}$ is indeed positive.)

Using now the approximation (7) and substituting $\mathbf{p}:=m\frac{\mathbf{x}}{t}$ we readily arrive at

$$\int_0^\infty dt\int_{R\Sigma}\mathbf{j}^{\psi_t}\cdot d\mathbf{S}\approx\int_0^\infty dt\int_{R\Sigma}(\frac{m}{t})^3|\hat{\psi}(\frac{m\mathbf{x}}{t})|^2\frac{\mathbf{x}}{t}\cdot d\mathbf{S}$$

$$=\int_0^\infty dp p^2\int_\Sigma d\sigma|\hat{\psi}(\mathbf{p})|^2=\int_{C_\Sigma}d^3p|\hat{\psi}(\mathbf{p})|^2.$$

This heuristic argument for the free flux-across-surfaces theorem (5) is so simple and intuitive that one may wonder why it does not appear in any primer on scattering theory. (For a rigorous proof see [9]).

To arrive at the general result (4) one may use the fact that the long time behavior of $\psi_t(\mathbf{x}) := e^{-iHt}\psi(\mathbf{x})$ is governed by $e^{-iH_0t}\Omega_-^\dagger\psi$ (see, e.g., [5]) so that the asymptotic current is simply

$$\mathbf{j}^{\psi_t}(\mathbf{x}) = \mathrm{Im}\psi_t^*(\mathbf{x})\nabla\psi_t(\mathbf{x}) \approx \frac{\mathbf{x}}{t}(\frac{m}{t})^3|\widehat{\Omega_-^\dagger\psi}(\frac{m\mathbf{x}}{t})|^2,$$

yielding (4).

III. NEAR FIELD SCATTERING

We turn now to a much more subtle question (see also [12]): What happens if we place the detectors *not* too distant from the scattering center and prepare the wave function near the scattering center, i.e., what happens if we do not take the limit $R \to \infty$ so central to scattering theory? The detectors will of course again fire at some random time and position, but what now of the statistics? This question is not quite as innocent as it sounds; it concerns in fact one of the most debated problems in quantum theory: what we are considering here is the problem of time measurement, specifically the problem of escape time (and position at such time) of a particle from a region G. It is well known that there is no self-adjoint time observable of any sort and there is a huge and controversial literature on this and on what to do about it. (See [13,14] and references therein.) Note also that since the exit position is the position of the particle at a random time, it cannot be expressed as a Heisenberg position operator in any obvious way.

The obvious answer (see [15] for a one-dimensional version) is, of course, provided by (1), provided that the boundary of G is crossed at most once by the particle (whatever this is supposed to mean for a quantum particle), so that every crossing of the boundary of G is a first crossing, and provided of course that (1) is nonnegative.[1] Notice that the preceding provisos might well be expected to be intimately connected. We thus propose that (1) indeed gives the first exit statistics whenever the following current positivity condition (a condition on both the wave function and on the surface)

$$
\begin{aligned}
\mathrm{CPC}: \quad & \forall t > 0 \quad \text{and} \quad \forall \mathbf{x} \in \text{boundary of the region} \quad G \\
& \mathbf{j}^{\psi_t}(\mathbf{x}, t) \cdot d\mathbf{S} > 0
\end{aligned}
$$

is satisfied.

We predict that the statistics given by (1) will (approximately) be obtained in an experiment on an ensemble of particles prepared with (approximately) CPC wave function ψ which is initially well localized in some region G whenever the detectors around the boundary of G (see Fig. 2) are *sufficiently passive*, a condition that needs to be more carefully delineated but which should widely be satisfied. As to how widely the CPC is satisfied, this is not easy to say. We do note, however, that since whether or not it is satisfied depends upon the region G upon which we focus and around which we place our detectors, it may often be possible to suitably adjust the region G so that the CPC becomes satisfied, at least approximately, even if the CPC fails to be satisfied for our original choice of G.

A simple example of a situation where the CPC does hold and where one may easily compute the exit-time statistics is the following. A spherically symmetric Gaussian wave packet, with initial width σ, which is initially located at the center of G, a sphere with radius R, evolves freely. One readily finds for the exit time probability density $\rho(t) := \int \mathbf{j}^{\psi_t} \cdot d\mathbf{S}$ that

$$
\rho(t) \propto \frac{R^3 t}{\sigma^2}\left(\sigma^2 + \left(\frac{t}{2m\sigma^2}\right)^2\right)^{-5/2} e^{-\frac{1}{2\sigma^2}\frac{R^2}{1+\left(\frac{t}{2m\sigma^2}\right)^2}}.
$$

Of course, some important questions remain: The expression (1) is not a probability for

[1] The wave function ψ_t in (1) should of course be understood as referring to the Schrödinger evolution with no detectors present.

all wave functions—so what if anything does it physically represent in general? And what in the general case is the formula for the first exit statistics?

We stress again that the prediction (1) for the exit statistics is not of the standard form, as given by the quantum formalism, since it is not concerned with the measurement of an operator as observable.[2] However, no claim is made that the expression (1) and its interpretation cannot also be arrived at from standard quantum mechanics—it presumably can—e.g., by including the measurement devices in the quantum mechanical analysis. (See however [13].) After all, though there is no standard quantum observable (i.e., self-adjoint operator) to directly describe the escape time, the "pointer variable" for the detectors *is* a standard quantum observable, whose probability distribution after the experiment can in principle be computed in the standard way.

In the next section we shall explain how the current as the central object for escape and scattering phenomena arises naturally within Bohmian mechanics [17,18], where the physical meaning of (1) turns out to be the measure for the expected number of *signed* crossings, which of course can be negative.

IV. BOHMIAN MECHANICS

In Bohmian mechanics a particle moves along a trajectory $\mathbf{x}(t)$ determined by

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{v}^{\psi_t}(\mathbf{x}(t)) = \frac{1}{m}\mathrm{Im}\frac{\nabla\psi_t}{\psi_t}(\mathbf{x}(t)), \tag{8}$$

where ψ_t is the particle's wave function, evolving according to Schrödinger's equation. Moreover, if an ensemble of particles with wave function ψ is prepared, the positions $\mathbf{x}$ of the particles are distributed according to the quantum equilibrium measure $\mathbb{P}^\psi$ with density $\rho = |\psi|^2$ (ψ normalized) [18].

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[2] Nor are they given by a positive-operator-valued measure (POV), which has been proposed as a generalized quantum observable, see [16]

In particular, the continuity equation for the probability shows that the probability flux $(|\psi_t|^2, |\psi_t|^2\mathbf{v}^{\psi_t})$ is conserved, since $|\psi_t|^2\mathbf{v}^{\psi_t} = \mathbf{j}^{\psi_t}$.

Hence, given ψ_t, the solutions $\mathbf{x}(t, \mathbf{x}_0)$ of equation (8) are random trajectories, where the randomness comes from the $\mathbb{P}^\psi$-distributed random initial position $\mathbf{x}_0$, ψ being the initial wave function.

Consider now, at time t=0, a particle with wave function ψ localized in some region $G \subset \mathbb{R}^3$ with smooth boundary. Consider the number $N(dS, dt)$ of crossings by $\mathbf{x}(t)$ of the surface element dS of the boundary of G in the time dt (see Fig. 3) . Splitting $N(dS, dt) =: N_+(dS, dt) + N_-(dS, dt)$, where $N_+(dS, dt)$ denotes the number of outward crossings and $N_-(dS, dt)$ the number of backward crossings of dS in time dt, we define the number of signed crossings by $N_s(dS, dt) =: N_+(dS, dt) - N_-(dS, dt)$.

We can now compute the expectation values with respect to the probability $\mathbb{P}^\psi$ of these numbers in the usual statistical mechanics manner. Note that for a crossing of dS in the time interval $(t, t + dt)$ to occur, the particle has to be in a cylinder of size $|\mathbf{v}^{\psi_t}dt \cdot d\mathbf{S}|$ at time t. Thus we obtain for the expectation value

$$\mathbb{E}^\psi(N(dS, dt)) = |\psi_t|^2|\mathbf{v}^{\psi_t}dt \cdot d\mathbf{S}| = |\mathbf{j}^{\psi_t} \cdot d\mathbf{S}|dt,$$

and similarly $\mathbb{E}^\psi(N_s(dS, dt)) = \mathbf{j}^{\psi_t} \cdot d\mathbf{S}dt$.

If we further introduce the random variables t_e, the first exit time from G, $t_e := \inf\{t \geq 0 | \mathbf{x}(t) \notin G\}$, and $\mathbf{x}_e$, the position of first exit, $\mathbf{x}_e = \mathbf{x}(t_e)$, we obtain a very natural and principled explanation of what we arrived at in a heuristic and suggestive manner in our treatment of scattering theory and the statistics of the first exit time and position. For Bohmian mechanics the CPC implies that every trajectory crosses the boundary of G at most once, and in this case we have

$$\mathbb{E}^\psi(N(dS, dt)) = \mathbb{E}^\psi((N_s(dS, dt)) =$$

$$0 \cdot \mathbb{P}^\psi(t_e \notin dt \text{ or } \mathbf{x}_e \notin dS) + 1 \cdot \mathbb{P}^\psi(\mathbf{x}_e \in dS \text{ and } t_e \in dt)$$

and we find for the joint *probability* of exit through dS in time dt

$$\mathbb{P}^{\psi}(\mathbf{x}_e \in dS \text{ and } t_e \in dt) = \mathbf{j}^{\psi_t} \cdot d\mathbf{S}dt. \tag{9}$$

In principle one could compute the first exit statistics also when the CPC fails to be satisfied. These are in fact given by the same formula (9) as before, provided one replaces $\mathbf{j}^{\psi_t}$ by the truncated probability current $\tilde{\mathbf{j}}$ arising from killing the particle when it reaches the boundary of G. This is simply given, on the boundary of G, by

$$\tilde{\mathbf{j}}^{\psi_t}(t, \mathbf{x}) = \begin{cases} \mathbf{j}^{\psi_t}(\mathbf{x}) & \text{if } (t, \mathbf{x}) \text{ is a first exit from } G \\ 0 & \text{otherwise} \end{cases} \tag{10}$$

where $(t, \mathbf{x})$ is a first exit from G if the Bohmian trajectory passing through $\mathbf{x}$ at time t leaves G at this time, for the first time since $t = 0$. Thus, we have generally that

$$\mathbb{P}^{\psi}(\mathbf{x}_e \in dS \text{ and } t_e \in dt) = \tilde{\mathbf{j}}^{\psi_t} \cdot d\mathbf{S}dt. \tag{11}$$

However, there is an important difference between the CPC probability formula (9), involving the usual current, and the formula (11), involving the truncated current. The usual current is well defined in orthodox quantum theory, even if it is true, as we argue, that its full significance can only be appreciated from a Bohmian perspective. The truncated current cannot even be *defined* without reference to Bohmian mechanics, since whether or not $(t, \mathbf{x})$ is a first exit from G depends upon the full and detailed trajectory up to time t. (In particular, a different choice of dynamics, as for example given by stochastic mechanics [10,11], would yield a different truncated current. It is natural to wonder whether the truncated current given by Bohmian mechanics provides in the general case the best fit to the measured escape statistics expressible without reference to the measuring apparatus.)

Finally, we note that in the context of scattering theory our definition (3) of σ_{flux} captures exactly what it should once one has real trajectories, namely the asymptotic probability distribution of exit positions,

$$\sigma_{\text{flux}}(\Sigma) = \lim_{R \to \infty} \mathbb{P}^{\psi}(\mathbf{x}_e \in R\Sigma).$$

This follows from the fact that the expected number of backward crossings of the sphere of radius R vanishes as $R \to \infty$ (see [9]).

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FIGURES

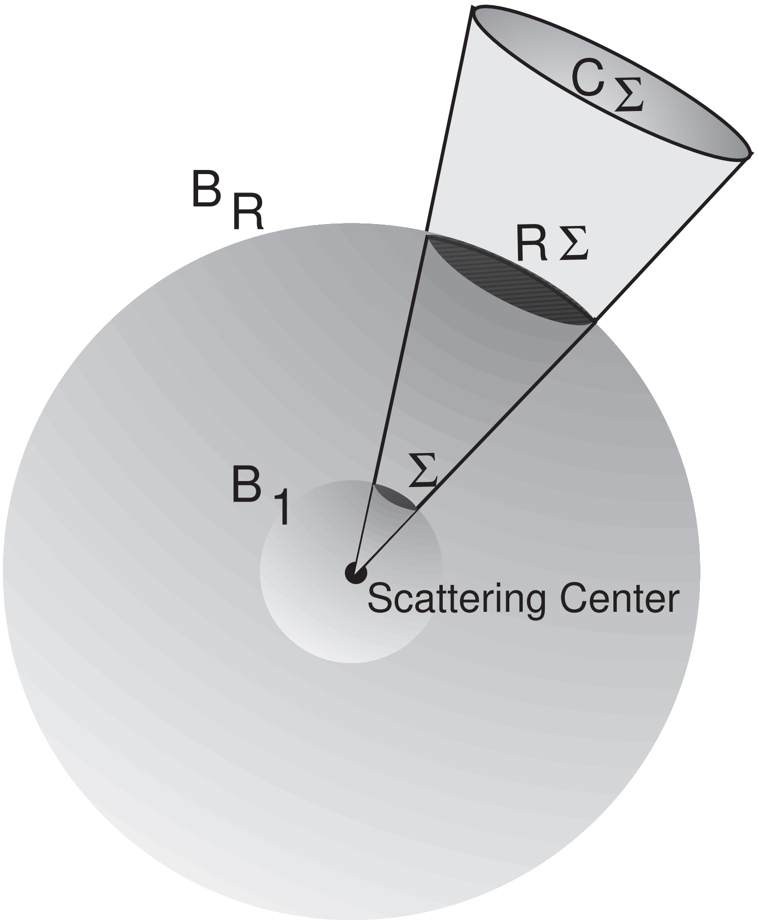

FIG. 1. The geometry of the scattering-into-cones and the flux-across-surfaces theorems.

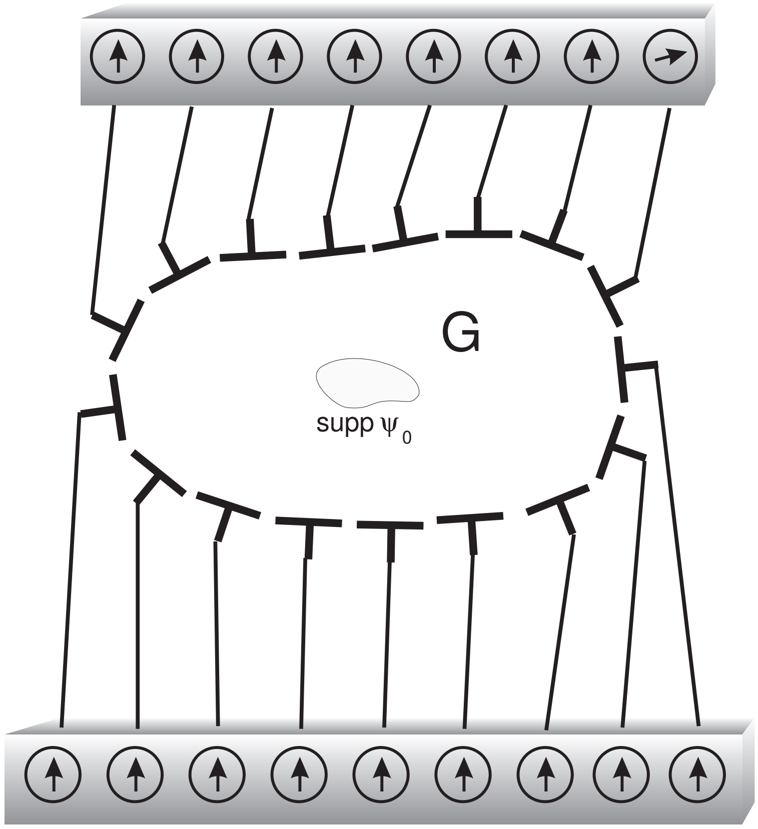

FIG. 2. Escape experiment: A region G is defined by an array of detectors, which surround a smaller region, supp ψ_0, in which a particle's wave function is initially localized. The detectors record the time at which they fire. Typically only one of the detectors will fire, and the position of this detector yields the measured exit position.

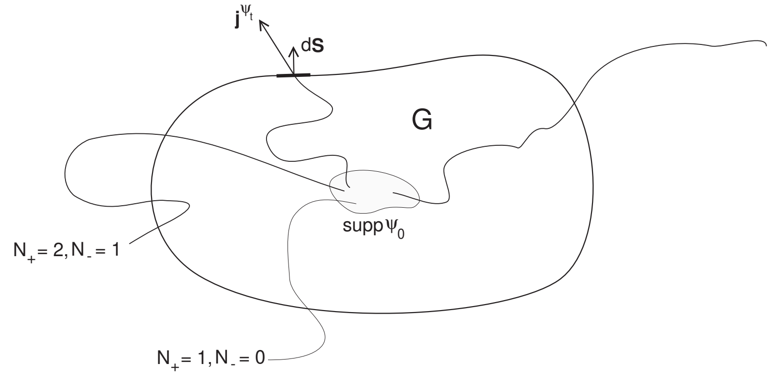

FIG. 3. In Bohmian mechanics the flow lines of the current represent the possible trajectories of the Bohmian particle. Some Bohmian trajectories leaving G are drawn (for the Schrödinger evolution without detectors, see footnote 1).