SCATTERING AND THE ROLE OF OPERATORS IN BOHMIAN MECHANICS

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ABSTRACT

Using Bohmian mechanics, we analyze the problem of describing escape time, escape position and sojourn time—quantities for which the quantum formalism assigns no self-adjoint operator—for quantum systems. The large-scale behavior relevant to scattering theory is also discussed.

HOW DOES ONE HANDLE THIS?

Consider an electron with a localized initial wave function, with support inside a certain region G. Surrounding the electron are detectors, placed along the boundary of G, which measure the position and the time of "escape" of the electron from the region. What are the quantum mechanical predictions for the statistics of these quantities?

Predictions in quantum mechanics are based on a correspondence between operators and observable quantities, with the operators that correspond to classical observables arising as follows: The operators $\hat{\mathbf{q}}$, $\hat{\mathbf{p}}$ for position and momentum may be found by replacing the classical Poisson bracket by the commutator: $\{\ ,\ \} \to \frac{1}{i\hbar}[\ ,\ ]$. For a general classical observable, given by a function $f(\mathbf{q},\mathbf{p})$ on phase space, the rule is to replace $\mathbf{q},\mathbf{p}$ in f by the operators $\hat{\mathbf{q}}$, $\hat{\mathbf{p}}$. (This procedure is however ambiguous since it does not specify the order in which noncommmuting operators should appear in a product.) The spectral measure of the operator is then supposed to describe the statistics for the outcome of the measurement of the corresponding observable. This rule is trusted to yield the correct operators in the usual "measurement situations" where the observable is measured at a specific time chosen by the experimenter.

But what are the operators for the escape time and escape position? For a classical particle with trajectory $\mathbf{Q}(t)$, the escape time (the first exit time) and the corresponding escape position from the region G are given by

$$T_e := \inf\{t|\mathbf{Q}(t) \in G^c\} \tag{1}$$

and

$$\mathbf{Q}_e = \mathbf{Q}(T_e). \tag{2}$$

One should notice at once that these expressions are not "simple" functions $f(\mathbf{q}, \mathbf{p})$ on phase space, since they depend explicitly on the trajectory, i.e., on the classical dynamics. The simple rule of replacement mentioned above would presumably lead to grotesque ambiguities if applied to these quantities. Notice also that the moment of time at which the "counter clicks" is indeed random and is not a parameter chosen by the experimenter performing the measurement. Because of this "problem of continuous observation" (see, e.g., [2, 3]), some physicists have felt the need to generalize the quantum formalism so that it may be applied in such situations [1, 2, 3].

It is not at all clear what rule should in fact be used to find the "correct" operators. Moreover, the mere existence of an operator for "time" seems to conflict with general principles: From the sizable literature on the subject of "time operators" we may cite the argument of Pauli [4] that there can be no self-adjoint operator $\hat{t}$ which is canonically conjugate to the Hamiltonian H.[1] Furthermore it is shown in [1] that no orthogonal basis of arrival or escape time eigenstates exists,[2] and hence no corresponding self-adjoint time operator.

On the other hand, by being more flexible with the quantum rules various researchers have proposed solutions to some of these problems: Since $\|P_G\psi_t\|^2$ ($P_G\psi_t$ denotes the projection of ψ_t onto G) is the probability of finding the particle at time t in G, a natural guess for the probability density of the escape time is to define $\rho_e(t) = -\frac{d}{dt}\|P_G\psi_t\|^2$. Why is it natural? Imagine a classical picture in which the particle never returns to G once it leaves. In this case $\|P_G\psi_t\|^2$ would indeed be the probability that the particle is still in G at time t, which is (1−) the distribution function of the escape time. However, in general $\rho_e(t)$ may well be negative (the particle may return to G) and thus $\rho_e(t)$ cannot in general be interpreted as a probability density [2].

Using similar ideas, one may also arrive at a "time-operator" for the total time spent in G, called the sojourn-time or dwell-time operator [2],[5]. For this particular "continuous observation," the generalization of the rule above is straightforward. The classical expression for the total time T_s spent by the particle in the region G is such that the position $\mathbf{Q}(t)$ can be unambigously replaced by the Heisenberg position operator

[1] $[\hat{t}, H] = i\hbar$ implies that the spectrum of both $\hat{t}$ and H is the whole real line, which conflicts with the semiboundedness of H.

[2] If, for example, "escape time eigenstates" $|t\rangle$ existed, states for which the electron would leave a certain region at an exactly specified time t, then any time-evolved eigenstate would have to be an eigenstate itself. That is, for times $t' > 0$, $e^{-iHt'}|t\rangle = |t - t'\rangle$, and this state must be orthogonal to $|t\rangle$. But the scalar product

$$\langle t|t - t'\rangle = \langle t|e^{-iHt'}|t\rangle$$

may be seen as a (distributional) boundary value from which it may be analytically continued (in t') into the lower half plane, Im $t' < 0$, (assuming $H \geq 0$). But by the unicity of the analytic continuation, the boundary value cannot be zero on a set of positive measure; otherwise it would have to be zero at $t' = 0$, which is surely not the case.

$\hat{\mathbf{q}}(t)$: With χ_G denoting the indicator function of the set G

$$T_s = \int_0^\infty \chi_G(\mathbf{Q}(t))dt. \tag{3}$$

This becomes

$$\hat{t}_s = \int_0^\infty P_G(t)dt \tag{4}$$

where $P_G(t)$ is the Heisenberg operator for the projection onto G. Note that formally $[\hat{t}_s, H] = i\hbar$ on the subspace of wave functions which are localized in G [2].

This operator gives a mean sojourn time which is in agreement with the classical result when $\|P_G\psi_t\|^2$ is the probability for the particle to be in G at time t (see the next section). However, in view of the negative result mentioned above,[3] there are doubts as to whether this operator yields more than the "correct" mean.

While little discussion seems to have been devoted to the problem of finding an operator for the escape position, the statistics for the escape position have received some attention, having been addressed in the "scattering-into-cones" theorem [6] and the "flux-across-surfaces" theorem [7]. We shall discuss these theorems later when we consider the large-scale behaviour typical of scattering theory.

We wish to focus on the question of how one handles situations where no self-adjoint operators exist for escape and sojourn time and escape position, i.e., where the usual quantum rules for predictions do not apply. What can be done?

We shall give a systematic discussion of this issue within the context of Bohmian mechanics, which is a theory of point particles in motion—in which particles have *trajectories*—and which is known to yield the same predictions as quantum mechanics whenever the latter is unambiguous [8, 9].

THE BOHMIAN WAY

In Bohmian mechanics a particle having wave function ψ moves along a trajectory $\mathbf{Q}(t)$ determined by

$$\frac{d}{dt}\mathbf{Q}(t) = \mathbf{v}_t(\mathbf{Q}(t)) = \frac{\hbar}{m}\mathrm{Im}\frac{\nabla\psi_t}{\psi_t}(\mathbf{Q}(t)) \tag{5}$$

where ψ_t is a solution of Schrödinger's equation

$$i\hbar\frac{\partial}{\partial t}\psi_t = (-\frac{\hbar^2}{2m}\nabla^2 + V)\psi_t. \tag{6}$$

The wave function $\psi \in L_2(\mathbb{R}^3)$ is supposed to be sufficiently smooth, so that the dynamics exists.[4] We do not wish to limit our discussion to free particle motion. Indeed we wish to include in the description the escape of the particle for scattering states. We may therefore think of the potential V as a typical scattering potential with scattering center lying in G.

The initial position $\mathbf{Q}$ of the particle with initial wave function ψ is distributed according to the probability density $\rho = |\psi|^2$ (ψ is assumed to be normalized). The continuity equation (quantum flux equation) shows that the flux

$$(|\psi_t|^2, \mathbf{j}_t) = (|\psi_t|^2, |\psi_t|^2\mathbf{v}_t,)$$

[3] The argument above does not directly apply in general to the sojourn time since the particle may leave the region G and return to it, but in cases of no return the escape time and sojourn time are the same.

[4] For the "existence of dynamics" see [11] and the contribution of K. Berndl in this volume.

is conserved, implying *equivariance*, i.e., that under the motion (5) the time-evolved probability density $\rho_t = |\psi_t|^2$ at all times.

We may now discuss our problem—in accordance with the title of this conference—on three levels.

Level 1: microscopic

The escape time T_e, the escape position $X(T_e)$ and the sojourn time T_s ((1)–(3)) are in Bohmian mechanics random variables on the probability space $\Omega = G$, the set of initial positions, equipped with the probability measure $\mathbb{P}$ given by the density $|\psi|^2$. Thus, in principle, all the statistics can be computed.

As we remarked above, the mean of T_s is readily computed from (3) applying Fubini's theorem and using equivariance (see also [10]):

$$\mathbb{E}(T_s) = \int_0^\infty \|P_G(t)\psi\|^2 dt. \tag{7}$$

As we have said, this connects with (4) since

$$\mathbb{E}(T_s) = (\psi, \hat{t}_s \psi). \tag{8}$$

The *distribution* of T_s, however, will depend in a rather complicated manner on ψ; in particular, there is no reason to expect it to be given by the the spectral measure of $\hat{t}_s$.

Level 2: mesoscopic

In general, the particle may well return to G after the first-exit time T_e. By the "mesoscopic level" we have in mind the situation where the particle never returns to G once it leaves. This is guaranteed by the following current positivity condition (CPC):

$$\text{CPC}: \quad \forall t \geq 0 \quad \text{and} \quad \forall \mathbf{q} \in \partial G, \qquad \mathbf{j}(\mathbf{q}, t) \cdot \mathbf{n}(\mathbf{q}) \geq 0, \tag{9}$$

where $\mathbf{n}(\mathbf{q})$ denotes the outward normal. This ensures that a trajectory may cross the surface ∂G of G at most once. For a given surface ∂G, the CPC is of course a condition on the wave function. Under the CPC, the product of the current and the surface-time element $d\sigma dt$ is the joint distribution for escape time and position:

$$\mathbb{P}((\mathbf{Q}_e, T_e) \in (d\sigma, dt)) = \mathbf{j}(\mathbf{q}, t) \cdot \mathbf{n}(\mathbf{q}) d\sigma dt \tag{10}$$

For the sake of proper normalization, we assume that the particle leaves the region G with certainty, i.e., that

$$\lim_{t\to\infty} \|P_G(t)\psi\|^2 = 0. \tag{11}$$

(This holds, for example, for a wave function whose spectral decomposition has only an absolutely continuous component [12].)

Integrating (10) over the surface and applying Gauss' theorem yields, by virtue of the continuity equation (the quantum flux equation), the escape-time density

$$\rho_e(t) = -\frac{d}{dt}\|P_G(t)\psi\|^2. \tag{12}$$

This is now completely clear since the CPC implies that if the particle is in G at time t, it did not leave G before time t, i.e., that $\mathbb{P}(t_e > t) = \|P_G(t)\psi\|^2$.

We may introduce in (12) the self-adjoint operator

$$Z(t) = -\frac{d}{dt}P_G(t) = -\frac{i}{\hbar}[H, P_G(t)] \tag{13}$$

so that

$$\rho_e(t) = (\psi, Z(t)\psi). \tag{14}$$

$Z(t)$ is clearly a positive operator on a linear subspace of wave functions satisfying the CPC.

The expression for the probability that the escape time is within an arbitrary set Δ

$$\mathbb{P}(T_e \in \Delta) = (\psi, Z(\Delta)\psi) := (\psi, \int_\Delta Z(t)dt\psi) \tag{15}$$

leads us now to the map $\Delta \mapsto Z(\Delta)$, which is a positive-operator-valued measure (POV) [13]. A POV is a generalization of a projection-valued measure (PV) in the sense that the operators $(Z(\Delta))$ need not be projections.[5]

As in the spectral theorem, we may associate with a POV a self-adjoint operator, namely its first moment. This association is, however, many-to-one, and the operator itself is of rather limited value: We may define $\hat{t}_e$ by

$$\hat{t}_e = \int_0^\infty tZ(t)dt = \int_0^\infty P_G(t)dt, \tag{16}$$

where the second equality follows from (13). Thus $\hat{t}_e = \hat{t}_s$ (cf.(4)) as, of course, it must. But in general the $Z(\Delta)$ are not projections ($Z(\Delta)^2 \neq Z(\Delta)$ in general) and hence they do not define the spectral resolution of $\hat{t}_e$. Therefore the spectral measure for $\hat{t}_e$ does not in general describe the escape time distribution. (Of course this operator does yield the correct mean.)

We obtain the distribution of the escape position in the mesoscopic regime by integrating (10) over t:

$$\rho_e(\mathbf{q}) = \int_0^\infty \mathbf{j}(\mathbf{q}, t) \cdot \mathbf{n}(\mathbf{q})dt, \quad \mathbf{q} \in \partial G. \tag{17}$$

As with the escape time, one may extract from (17) a POV,[6] which will in general not be a PV.

Level 3: macroscopic

By the macroscopic level we have in mind the "scattering regime," in which the surface ∂G is very far from the scattering center so that the large-time asymptotic behavior becomes relevant.

While on the mesoscopic level we have assumed by definition that the CPC holds, we may expect that on the macroscopic level the CPC must hold for scattering states (i.e. states for which (11) holds). However, to be sure, we still assume the CPC.

For simplicity, we assume that G is the ball K_r of radius r centered at the origin, which coincides with the scattering center. Let C be a concentric cone and let $\Delta_r^C := \partial K_r \cap C$ be the surface defined by the intersection of the surface of the ball and the cone. What is the probability that the particle escapes through Δ_r^C in the limit as $r \to \infty$? For this we need to integrate (17) over Δ_r^C and take the limit. One easily finds heuristically that

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[5] What we call a POV is in [3] called a "generalized resolution of identity" (GRI). It is introduced there in connection with the problem of the escape time operator.

[6] (17) as well as (10) indeed define a POV [15].

$$\lim_{r\to\infty} \mathbb{P}(\mathbf{Q}_e \in \Delta_r^C) = \lim_{r\to\infty} \int_{\Delta_r^C} \int_{t=0}^{\infty} \mathbf{j}_t \cdot d\sigma dt = \lim_{t\to\infty} \|P_C(t)\psi\|^2. \tag{18}$$

Together with Dollard's "scattering-into-cones theorem"[6] (which assumes the existence of the wave operators $\Omega_\pm := s - \lim_{t\to\mp\infty} e^{iHt}e^{-iH_0 t}$)

$$\lim_{t\to\infty} \|P_C(t)\psi\|^2 = \|P_C \mathcal{F}\Omega_-^\dagger \psi\|^2, \tag{19}$$

this yields the flux-across-surfaces theorem:

$$\lim_{r\to\infty} \int_{\Delta_r^C} \int_{t=0}^{\infty} \mathbf{j}_t \cdot d\sigma dt = \|P_C \mathcal{F}\Omega_-^\dagger \psi\|^2. \tag{20}$$

Here $\mathcal{F}$ denotes the Fourier transform.

We would like to emphasize that while (20) may conceivably be satisfied even without the CPC's holding (in some appropriate asymptotic sense), the CPC is crucial if we are to regard (20) as the probability that the particle first exits through Δ_r^C. Thus the CPC, together with the flux-across-surfaces theorem, appears to be the basis of scattering theory. The importance of (20) for scattering was recognized in [7], but the proof was only given for the free evolution.[7]

We wish next to point out that the POV structure of (17) characteristic of the mesoscopic regime has become, in the macroscopic regime, a PV structure: We may readily recognize on the r.h.s. of (20) the PV defined by the (direction of the) "asymptotic momentum" $\hat{\mathbf{p}}^+ = \Omega_- \hat{\mathbf{p}} \Omega_-^\dagger$, i.e., by $C \mapsto \chi_C(\hat{\mathbf{p}}^+)$.

We can also of course write down the differential cross section $\frac{d\sigma}{d\omega}$ by introducing angular variables θ_e, ϕ_e and the solid angle $d\omega$ and by writing the PV on the r.h.s. of (20) as

$$Z(d\omega) := \Omega_- \mathcal{F}^{-1} P_{C_{d\omega}} \mathcal{F} \Omega_-^\dagger = \chi_{C_{d\omega}}(\hat{\mathbf{p}}^+) \tag{21}$$

where $C_{d\omega}$ is the cone spanned by $d\omega$. Then

$$d\sigma := \lim_{r\to\infty} \mathbb{P}(\theta_e, \phi_e \in d\omega) = (\psi, Z(d\omega)\psi) \tag{22}$$

is the probability that the particle escapes asymptotically within the solid angle $d\omega$.

WHAT CAN BE OBSERVED?

The reader may now well ask the "Gretchenfrage"[8]: "Can one measure all the random variables of levels 1, 2, and 3? Can one do realistic experiments, involving apparatuses as measuring devices, which actually record the escape time and position as computed from the theory; in other words, can one *observe* these random variables?"

The answer is provided by the following straightforward and completely general result of Bohmian mechanics [15]: The statistics of quantities which are measured in an experiment are *always* given by a POV. Thus we may say the following concerning the measurability of the random variables $T_e, \mathbf{Q}_e$ and T_s:

- Level 1, microscopic, the CPC is not assumed to hold.

[7] For the general proof see [14].

[8] "Nun sag, wie hast du's mit der Religion?
Du bist ein herzlich guter Mann
Allein ich glaub du hälst nicht viel davon." (Faust I, Goethe)

In general, the random variables are not distributed according to a POV and there can be no experiment to measure them.

As a side remark, we mention that measurements of the mean sojourn time have been discussed in connection with the so-called Larmor clock: In the limit of an infinitely small magnetic field localized in G, it can be shown that the precession angle of the spin of the particle is proportional to the mean of the sojourn time [5].

- Level 2, mesoscopic, the CPC holds.

  As we have seen, in this case the statistics are always given by POV's. Moreover, the detectors around the boundary should accurately measure the random variables under discussion. (An analysis of the experiment and a discussion of the accuracy of the measurement is contained in [1].)

- Level 3, macroscopic.

  The statistics of the escape position are given by (the PV associated with) the asymptotic momentum, which of course can be measured.

WHAT ROLE DO OPERATORS PLAY?

We have remarked that Bohmian mechanics yields in very natural situations a description of what goes on which cannot be directly verified through measurements. But that turns out to be a strength rather than a weakness of the (indeed of any *complete*) theory: In Bohmian mechanics the act of measurement can be analyzed in as much detail as one wishes; in particular, Bohmian mechanics tells us precisely which quantities can be measured and which physical processes qualify as measurements of whatever it is that can be measured. This analysis reveals the status of operators in the description of nature, and allows a clear view of the range of applicability of the usual quantum mechanical formulas. The particular example of escape statistics exemplifies the general situation [15], namely, that operators as "observables" appear merely as computational tools in the phenomenology of certain types of experiments—those for which the statistics of the result are governed by a PV. However, they have no fundamental significance and do not at all reflect what, on the microscopic level, is really going on.

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