Response to Pashby: Time operators and POVM observables in quantum mechanics.

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Abstract: I argue against a *general* time observable in quantum mechanics except for quantum gravity theory. Then I argue in support of *case specific* arrival time and dwell time observables with a cautionary note concerning the *broad* approach to POVM observables because of the wild proliferation available.

First, a terminological idiosyncracy of mine: I follow the admonitions (which will not be defended here) of Jean Marc Levy-Leblond [10] and Hans Christian von Bayer [22], to drop the term *particle* and call the bosons and fermions of the world, *quantons*.

1. Between Pashby and Hilgevoord

Back in 1998 professor Hilgevoord [9b], extensively referred to by Pashby [15], criticised a long paper I co-authored with Jeremy Butterfield [7], in which we discussed (among other things) Lorentz covariant 4-vector position operators, assigned to space-like hyperplanes, and with operator valued time components. Hilgevoord objected not only to the operator time components, but to the requirement of Lorentz covariance for the position operators as well! I did not then and do not now agree with these objections, for the time components were in no sense independent or general time operators, but supervened on the space components by being linear functions of them and this enabled the covariant transformation property. However, notwithstanding this episode, I think I am more sympathetic to Hilgevoord's objections [9c] to a *general* time operator in quantum mechanics (QM) than Pashby is. I will elaborate on this below.

On the other hand, I agree with Pashby's support of what I will call *case specific* time operators in QM, tentatively interpreted, when non self adjoint, as POVM observables. There are, however, delicate issues regarding the POVM interpretation of observables which I want to discuss in the context of such time operators. But first, my sympathies with Hilgevoord.

2. Time, observables and measurement

There are two brief arguments, other than Pauli's [16], that I would mount against a general, canonical, time operator in QM. They are first, and most importantly: In QM, space and time or space-time, are not, themselves, dynamical systems. QM is a theory of *temporally persistent dynamical systems*, indeed of *eternal* systems, which live in a fixed classical space-time. Unlike Quantum Gravity research or Quantum Cosmology, which seek a QM *of* space-time and must have general, operator valued, space - time observables *per se*, standard QM has no such need. The basic observables of standard QM, represented by self adjoint operators, are designed to answer questions about the possible values, or probabilities for values, of possible properties of persistent physical systems, *at specified times* (or, more relativistically, on specified space-like hypersurfaces). Even so-called unstable systems, which we normally think of as temporally transient, are included in this construal. We need only view the final decay products, the unstable parent quanton and the earlier formation progenitors as the final, middle and initial configurations, respectively, of a spontaneous internal transformation of *the* persistent system.

Second: I follow Ghirardi [8], Pearle [17], Penrose [18] and others in regarding primordial, stochastic state reduction (which we merely exploit in our measurements) as the really serious absentee in current QM. If and when this theoretical gap is filled, via improved versions of one or another of the already proposed schemes, or otherwise, I see it as only enhancing the special status of time in QM. For while state reductions (the exploited ones) can be tailored to specific observables and can have very varied relationships to spatial locations (think of reductions to near momentum eigenstates), they all occur at essentially *definite times,* either (the exploited ones) at times of our choosing or (the primordial ones) at wholly random times or, again, on space-like hypersurfaces. So there would be no question of measuring *when* the primordial reductions occur and trying to measure *just when* a measurement exploited reduction occurs (within the exploiting measurement) would be an instance of measuring a case specific time observable.

This conception of the reality of apparent state reductions may be wrong. If so, and *genuine* state reduction is replaced by an *illusion* induced by something like environmental decoherence [20]; well, that also is an ongoing temporal process which would not, I think, alter the special status of time in QM.

The upshot is that I think Dirac, whether he miscalculated (as Pashby suggests) or not, was either lucky or wise in not sticking to his original guns [6a] of trying to formulate QM in the extended phase space with the extended Hamiltonian satisfying a constraint equation and with time emerging as an operator. For even without gravity to deal with, and notwithstanding the invaluable contribution of Dirac's later study of constrained dynamical systems [6b], I suspect that such an approach to QM in general would have encountered analogues to the kind of conceptual problems which plague quantum gravity research today. In quantum gravity research these conceptual problems must be faced; in the formulation of QM they would have been and were artificial.

3. Time-energy indeterminacy

While we do not have a general time observable in quantum mechanics, we do have a universal time-energy indeterminacy relation (TEIR) and it is striking how exactly opposite is our traditional interpretation of that relation from Heisenberg's early interpretation, as described by Pashby. While Heisenberg saw ΔT as an indeterminacy in a time of occurrence and ΔE was an *interval* between precise energy values, we now have ΔE as the standard deviation indeterminacy in the system energy while ΔT is the lower bound on the *intervals* defined by $\Delta T_X = \Delta X / |<\dot{X}>|$ for arbitrary observables, X. Derived by Mandelstam and Tamm [12] from the Robertson [19] general indeterminacy relations,

$$\Delta X \Delta E \geq (\hbar/2) |<\dot{X}>| \ , \qquad (1)$$

the ΔT of their TEIR, $\Delta T \Delta E \geq (\hbar/2)$, is the time one must wait for expectation values to change by amounts comparable to the corresponding standard deviations. This immediately yields the stationarity of energy eigenstates and, as Aharonov and Bohm [1] pointed out, it places no restriction at all on how quickly one can, in principle, perform an arbitrarily precise measurement of the energy of a physical system! However, for many states of interest, the standard deviation, ΔE, can be infinite and then (1) and the TEIR tell us nothing.

Accordingly, stronger indeterminacy relations have been derived with new time-energy relations among them [5]. Uffink and Hilgevoord [21a] have obtained one of the most interesting versions which I just mention here without further comment.

Let $\widehat{\Pi}(E)$ be the projection valued spectral resolution of the Hamiltonian, $\widehat{H} = \int E\, d\widehat{\Pi}(E)$. For unit norm states let $W_\alpha(\psi)$, where $0 < \alpha < 1$, be the size of the smallest energy interval, *I*, such that,

$$< \psi \,|\, \int_I d\widehat{\Pi}(E) \,|\, \psi > = \alpha \,. \tag{2}$$

Let, $\tau_\beta(\psi)$, where $0 < \beta < 1$, be the smallest time displacement such that,

$$< \psi \,|\, \exp\left(-\frac{i}{\hbar} \widehat{H} \tau_\beta(\psi) \right) |\, \psi > = \beta \,. \tag{3}$$

Then it can be shown that,

$$\tau_\beta(\psi) W_\alpha(\psi) \geq 2\hbar \arccos\left(\frac{\beta + 1 - \alpha}{\alpha} \right). \tag{4}$$

In particular, for α = 0.9 and $\beta = \sqrt{1/2}$, one obtains, $\tau_{\sqrt{1/2}} W_{0.9} \geq 0.9\hbar$ [9a].

4. Case specific time observables

Now I turn to case specific time observables where I agree with Pashby concerning both the possibility and the desirability of identifying and examining such observables in QM for various times of occurrence or durations.

Concepts of quantum observable times come in at least three forms: (1) times of occurrence (*arrival times*) of specified events, (2) intervals of time (*dwell times*) spent in specified regions or conditions or (3) (*relative times*) of occurrence of one event relative to a reference event. These are of a different nature from the ‘property’ observables for persistent systems. They acquire their objective indeterminacy from supervening on the property observables. They can be easily motivated within standard QM, beginning with the definition of case specific time operators. Until comparatively recent times such concepts have not received much attention, but are under intense examination now [13], and, as Pashby suggested, usually lead to non-self adjoint operators.

Perhaps the very simplest (not to say simplistic) example, introduced by Aharonov and Bohm [1], and one of three examples considered by Brunetti et al [3a, c], among Pashby's sources, is the arrival time operator,

$$\hat{T}_0 = -\frac{1}{2}\left(\frac{m}{\hat{p}}\hat{x} + \hat{x}\frac{m}{\hat{p}}\right) . \tag{5}$$

With this operator one can, supposedly, calculate the average time of arrival, at the spatial origin of coordinates, of a free, non-relativistic quanton moving in one dimension. The position of the quanton at *parameter time*, $t = 0$ is represented by the operator, $\hat{x}$, and the momentum, by the operator, $\hat{p}$. Because 0 belongs to the spectrum of $\hat{p}$ and the 'inverse' of $\hat{p}$ appears in (5), $\hat{T}_0$, while symmetric, is not self adjoint. That 'inverse' restricts the domain of definition of $\hat{T}_0$. I think it is worth examining this toy model in some detail.

The motivation for the time operator construction, (5), is just the time dependence of the Heisenberg picture position operator for the free quanton,

$$\hat{x}(t) = \hat{x} + \frac{\hat{p}}{m}t . \tag{6}$$

The expectation value of position is zero at the precise time, $t_0 = -m < x > / < p >$, but this expectation value allows for contributing position eigenvalues that lie far afield from zero. There is no single, precise time for the quanton to arrive (be detected) exactly at $x = 0$, so the time operator, $\hat{T}$, that, hopefully, 'describes' the distribution of possible times is, perhaps naively, taken to satisfy the equation,

$$0 = \hat{x} + \frac{\hat{p}}{2m}\hat{T} + \hat{T}\frac{\hat{p}}{2m} , \tag{7}$$

where the symmetrized product allows for *momentum–time* incompatibility.

$\hat{T}_0$ of (5) is the solution to (7) and, indeed, it fails to commute with the quanton momentum and its position at $t = 0$.

$$[\hat{p}, \hat{T}_0] = i\hbar m\, \hat{p}^{-1}, \qquad [\hat{x}, \hat{T}_0] = (i\hbar m/2)(\hat{p}^{-2}\hat{x} + \hat{x}\,\hat{p}^{-2}) \tag{8}$$

The right hand commutator gives rise to the curious indeterminacy relation, in which the indeterminacy of the time of arrival at the spatial origin of coordinates, $x = 0$, competes with the indeterminacy of the quanton position at the parameter time, $t = 0$. Furthermore, the lower bound on the product of the standard deviations is governed by the expectation value of a function of position and momentum that could well diverge for many states!

From the left hand entry in (8), the momentum-time commutator, we do obtain the expected time-energy commutator,

$$[\hat{p}^2/2m, \hat{T}_0] = i\hbar\,, \tag{9}$$

but this does not conflict with Pauli's argument since the time operator is not self adjoint.

5. The POVM perspective

But just how shall we work with $\hat{T}_0$ in detail, given that it's not self adjoint? Brunetti et al tell us it is maximally symmetric with deficiency indices of 2 and 0. A more familiar account of the non-self adjoint character of $\hat{T}_0$ is provided by examining its continuous spectrum, generalized eigenstates. In the momentum representation they are given by,

$$\xi_t(p) = \sqrt{\frac{p}{mh}}\,\exp\left[\frac{i}{\hbar}\frac{p^2}{2m}t\right], \tag{10}$$

for the eigenvalue, t (that square root has to be handled carefully!). Notwithstanding the symmetry of $\hat{T}_0$, they are non-orthogonal, with the inner products,

$$<\xi_t\,|\,\xi_{t'}> = \delta(t-t') + \frac{i}{\pi}\frac{\mathrm{P}v}{t-t'}\;, \tag{11}$$

where $\mathrm{P}v$ denotes principal value. So $\hat{T}_0$ is not subject to a projection valued spectral analysis employing a projection valued measure (PVM). In its place a positive operator valued spectral analysis employing a positive operator valued measure (POVM) is available. Why is this fact useful in physics and how much difference does it make?

There have been three main sources of the idea that POVMs comprise a valuable generalization of the standard concept of quantum observable. The earliest lies in the work of the physicist-philosopher, Gunther Ludwig [11], who anticipated the utility of POVMs in accounting for the probability distributions that could arise from innovative experimental procedures. Next came the recognition of POVMs as more adequately describing actual laboratory probability distributions due to technological limitations in attempts to implement ideal measurements of standard observables. The book, "Quantum Measurement" by Braginsky and Kahlili [2] is a good introduction to this source. Finally, there is a community of theorists who see in POVMs a vast source of valuable generalized observables that greatly extend our capacity for examining quantum systems. Paul Busch is a leader in this field and the books, "Operational Quantum Physics" [4a], which he co-edited, and "Time in Quantum Mechanics", to which he contributed [4b], are representative. The subject of POVM observables met with severe criticism in early days [21b] and calls for caution still occur [7b] (I will add to them shortly), but the field has weathered the criticism and is very active. The original mathematical work on POVMs is primarily due to Naimark [14].

A POVM for a single observable, X, is defined by a family of bounded, non-decreasing, positive operators, $\hat{P}(x)$, where, $-\infty \le x \le \infty$, satisfying the following conditions: for any, $x_1 \le x_2$,

$$0 = \hat{P}(-\infty) \le \hat{P}(x_1) \le \hat{P}(x_2) \le \hat{P}(\infty) = \hat{I} \ . \tag{12}$$

From these operators one can build the positive operator associated with any given member of a sigma field of Borel sets of the real line.

A PVM is the special case in which the $\hat{P}(x)$ are projection operators, $\hat{\Pi}(x)$, satisfying the further condition that,

$$\hat{\Pi}(x_1)\hat{\Pi}(x_2) = \hat{\Pi}(x_2)\hat{\Pi}(x_1) = \hat{\Pi}(x_1) \ . \tag{13}$$

If such a PVM comprises the spectral resolution for a standard observable, *X*, then the self adjoint operator, $\hat{X}$, for that observable, is just the first moment of the spectral resolution, i.e.,

$$\hat{X} := \int x \, d\hat{\Pi}(x) . \tag{14}$$

It follows from (13) that for any function, $f(x)$,

$$f(\hat{X}) = \int f(x) \, d\hat{\Pi}(x) . \tag{15}$$

In particular, for a unit step function,

$$\theta(x - \hat{X}) = \hat{\Pi}(x) , \tag{16}$$

and the PVM spectral resolution is recoverable from the first moment operator. Also any PVM provides the spectral resolution for some self adjoint operator.

Nothing of the kind holds for POVMs that are not PVMs! For such POVMs there is no condition analogous to (13). The positive operators in such a POVM need not even commute among themselves! Consequently, the POVM spectral resolution is usually *not recoverable* from the first moment operator!

Suppose we have a POVM, $\hat{P}_0(t)$, which provides a generalized spectral resolution for our time operator, $\hat{T}_0$. The mathematical meaning of this statement entails that two conditions must be satisfied. The first is that $\hat{T}_0$ and the first moment operator, $\int t \, d\hat{P}_0(t)$, have the same 'matrix elements', i.e.,

$$< \vartheta, \hat{T}_0 \, \psi > = \int t \; d < \vartheta, \hat{P}_0(t) \, \psi > , \tag{17}$$

for all ϑ and any ψ in the domain of definition for $\hat{T}_0$. The second condition for the POVM is that the squared norm of the action of $\hat{T}_0$ equals the expectation value of the *second moment* operator of the POVM, i.e.,

$$\left\| \hat{T}_0 \psi \right\|^2 = \int t^2 d < \psi, \hat{P}_0(t) \psi > . \tag{18}$$

In the QM application of POVMs , the probability for a measurement of $\hat{T}_0$ to yield a time lying between t_1 and t_2 would be given by,

$$\wp(t_1 \le t \le t_2) = < \int_{t_1}^{t_2} d\hat{P}_0(t) > = < (\hat{P}_0(t_2) - \hat{P}_0(t_1)) > . \tag{19}$$

The broadest use of POVMs in QM is not to provide generalized spectral resolutions for observables identified with non-self adjoint operators, as we are now considering, but to *define* generalized observables in terms of a POVM directly via (19) alone.

But now consider the following *three parameter family* of POVMs, built upon some hypothetical $\hat{P}(t)$, where $0 \le a < 1$, $\lambda > a$ and τ, a time, is arbitrary,

$$\hat{P}_{a,\lambda,\tau}(t) := a\, \hat{P}(\lambda t + \tau) + (1-a)\, \hat{P}\left(\frac{\lambda(1-a)t - a\tau}{\lambda - a} \right) \tag{20}$$

If the $\hat{P}_{a,\lambda,\tau}(t)$ are all arrival time candidate POVMs, they must be time translationally covariant, i.e.,

$$\exp[(i/\hbar)\hat{H}\tau]\, \hat{P}_{a,\lambda,\tau}(t)\, \exp[-(i/\hbar)\hat{H}\tau] = \hat{P}_{a,\lambda,\tau}(t+\tau) \tag{21}$$

This can hold only if $\lambda = 1$. But both dwell time and relative time observables would be invariant under parameter time translation. Still, for dwell times we would want to require $\tau = 0$.

Regardless of the *kind* of time observable the POVM family, (20), is considered for, the first moment operators for *all* those POVMs are equal,

$$\int t\, d\hat{P}_{a,\lambda,\tau}(t) = \int t\, d\hat{P}(t) . \tag{22}$$

Consequently, if $\hat{P}_0(t)$ belongs to the family (20), they all have first moment operators with the same matrix elements as our $\hat{T}_0$! For any given quantum state, they all give the same answer to the question, ‘When is the average time of arrival at the origin?’.

The second moment operators of the various POVMs in (20) are not the same and their expectation values vary from the smallest, provided by $\hat{P}(t)$, to larger values that increase without bound as $a \to 1$. So under our assumption about $\hat{P}_0(t)$, that it belongs to the family in (20), at most a few members of the family will satisfy (18) while all members satisfy (17). In fact, since our time operator is *maximally* symmetric, it is known that only the one member of (20), $\hat{P}_0(t)$, will satisfy (18). While this is good news for our time operator, because of uniqueness, it also means that all the other POVMs in the family can not provide generalized spectral resolutions for any symmetric operator, whatsoever!

To see that, let the state vectors, η_k be an orthonormal basis in the state space. Then satisfying both (17) and (18) requires,

$$\Sigma_k \left| < \eta_k , \int t \, d\hat{P}_0(t) \psi > \right|^2 = < \psi , \int t^2 \, d\hat{P}_0(t) \psi > . \qquad (23)$$

All the members of (20) yield the same left hand side. Only $\hat{P}_0(t)$, among them, yields the correct right hand side. So only $\hat{P}_0(t)$ provides a spectral resolution of the time operator, $\hat{T}_0$, or of any symmetric operator. Note that if $\hat{P}_0(t)$ was a PVM instead of just a POVM, (23) would not be a *requirement* at all, it would be an identity!

Notwithstanding the fact that within the family, (20), only $\hat{P}_0(t)$ can, satisfy (23), we can still, tentatively, regard the POVMs as defining time observables, $T_{a,\lambda,\tau}$, in the broad sense. The squared standard deviation for these observables would be defined by,

$$(\Delta T_{a,\lambda,\tau})^2 := < \int t^2 \, d\hat{P}_{a,\lambda,\tau}(t) > - < \int t \, d\hat{P}_{a,\lambda,\tau}(t) >^2 \qquad (24)$$

Setting $\lambda = 1$ for an arrival time observable, detailed examination of (20) results in,

$$(\Delta T_{a,1,\tau})^2 \geq (\Delta T_{a,1,0})^2 + a\tau^2 / (1-a) . \qquad (25)$$

The POVM, $\hat{P}_{a,1,\tau}(t)$, yields no eigenstates at all for the observable, $T_{a,1,\tau}$ unless $a = 0$ or $\tau = 0$! Since $\hat{T}_0$ does have continuous spectrum eigenstates (see (10)) it follows that $\hat{P}_0(t)$, belonging to (20), must equal

$$\hat{P}_{a,1,0}(t) = \hat{P}_{0,1,\tau}(t) = \hat{P}(t) . \qquad (26)$$

Regarding the others, $\widehat{P}_{a,1,\tau}(t)$; is it physically reasonable to admit, as observables, POVMs that have *no* (generalized) eigenstates throughout the state space? For the affirmative, see three paragraphs below.

The dwell time case, in which λ may vary but τ = 0, leads to a similar result in which $T_{a,\lambda,0}$ can only have an eigenstate for the eigenvalue, 0, unless a = 0 or λ = 1. The relative time case is more nuanced.

Before dismissing these examples as merely bizarre curiosities, bear in mind that I just cobbled (20) together for this workshop and, very probably, it just scratches the surface of ways in which one can build POVMs, all of which share the same first moment operator. If there are much more varied ways of doing that, it seems likely to lead to instances of the query, "Which one?". The definition of $\widehat{T}_0$ via (7) was tentative, after all.

From PVM observables one can extract *everything* from the first moment operator, even the eigenstates. From a POVM observable, interpreted broadly, one can not even know, from the first moment operator, if there *are* eigenstates! This makes me wary of the broad approach to POVM observables. The POVM theoretical community, however, regards a particular subclass of POVMs devoid of eigenstates as very important. Called *informationally complete*, these POVMs yield probability distributions that distinguish between any two distinct quantum states [4a]. No PVM can do that.

Returning to Pashby and Brunetti et al: the latter, as indicated by Pashby, explicitly construct the POVM that corresponds to $\widehat{T}_0$, according to (17,18)[3a], and their construction, while natural and physically plausible, would not be uniquely compelling, if they hadn't known what operator, $\widehat{T}_0$, they were after (see Pashby's footnote 11 for differing interpretations of the POVM construction). Elsewhere they show [3b] that time translationally covariant POVMs lead to an indeterminacy relation for arrival time observables alone! Not a time-energy indeterminacy relation, but a *time* indeterminacy relation. The standard deviations of their time observables are never less than a universal constant divided by the *expectation value* of the system energy! Accordingly, the $\widehat{T}_0$ generalized eigenstates, mentioned above, (10), are the limits of finite norm states with energy expectation values that grow without bound in the limit.

As case specific time observables gain importance from the POVM approach to time in QM, issues of the sort considered here will have to be further clarified. An approach to these issues may have recourse to Naimark's theorem [14] , which Brunetti et al exploit in their constructions, and Pashby mentioned. Naimark showed that every POVM is the projection from a larger Hilbert space of a PVM. This PVM would be the spectral resolution of a self adjoint operator in the larger Hilbert space which is then projected down to our first moment operator. Usually the larger Hilbert space is regarded as having mathematical significance only, but it can take the form of an Hilbert space for a supersystem containing the system of interest as a subsystem. I suspect that it would be advantageous to be able to interpret the supersystem and the larger Hilbert space, physically. Still, each of my $\widehat{P}_{a,\lambda,\tau}(t)$ POVMs would lead to different PVMs in (different?) larger Hilbert spaces and different, self adjoint, 'time' operators, all of which would project down to a first moment operator with the same matrix elements as our $T_{\mathrm{a},\lambda,\tau}$. So again the question looms: "Which one?".

For both case specific time observables and others, many theorists are enamored of POVMs because of the panoramic garden of delights they seem to offer. While delights there may be, the garden is not without weeds!

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