Pre- and Post-selection paradoxes and contextuality in quantum mechanics

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Many seemingly paradoxical effects are known in the predictions for outcomes of intermediate measurements made on pre- and post-selected quantum systems. Despite appearances, these effects do not demonstrate the impossibility of a noncontextual hidden variable theory, since an explanation in terms of measurement-disturbance is possible. Nonetheless, we show that for every paradoxical effect wherein all the pre- and post-selected probabilities are 0 or 1 and the pre- and post-selected states are nonorthogonal, there is an associated proof of contextuality. This proof is obtained by considering all the measurements involved in the paradoxical effect – the pre-selection, the post-selection, and the alternative possible intermediate measurements – as alternative possible measurements at a single time.

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The study of quantum systems that are both pre- and post-selected was initiated by Aharonov, Bergmann and Lebowitz (ABL) in 1964 [1], and has led to the discovery of many counter-intuitive results, which we refer to as pre- and post-selection (PPS) effects [2], some of which have recently been confirmed experimentally [3].

These results have led to a long debate about the interpretation of the ABL probability rule [4]. An undercurrent in this debate has been the connection between PPS effects and contextuality. For instance, Bub and Brown [5] understood the paper of Albert, Aharonov and D’Amato [6] – which concerned a PPS effect known since as the “3-box paradox” – as a claim to a novel proof of contextuality, that is, as a version of the Bell-Kochen-Specker theorem [7, 8], and convincingly disputed this claim. Although the language of Ref. [5] does suggest such a reading, in Ref. [4] the authors clarified their position, stating that it was not their intention to conclude anything about hidden variable theories. Nonetheless, discussions of PPS paradoxes, that is, PPS effects of the 3-box paradox variety, continue to make use of a language that suggests implications for ontology [10] and the claim that certain PPS paradoxes are proofs of contextuality can be found in the literature [11]. Although we agree with Bub and Brown that this claim is mistaken, we show that there is nonetheless a close connection between the two phenomena.

This connection is expected to have interesting applications in quantum foundational studies. For instance, it has been suggested by some that Bell’s theorem [12] might be understood within a realist and Lorentz-invariant framework if one admits the possibility of a hidden variable theory that allows for backward-in-time causation [13]. A simple model has even been suggested by Kent [14]. The latter is closely connected to the fact that Bell correlations can be simulated using postselection, as shown in Bub and Brown [5]. This simulation by postselection is also the root of the detection-efficiency loophole in experimental tests of Bell’s theorem [15, 16]. Further investigations into the connection between proofs of nonlocality and PPS paradoxes would shed new light on these avenues of research. As nonlocality is a kind of contextuality (assuming separability [17]), the ubiquitous connection between contextuality and PPS paradoxes established in the present work is an important contribution to this project. Moreover, the fact that the phenomenon of contextuality itself might be understood by abandoning the traditional notion of causality, and the fact that its simulation by postselection will likely constitute a loophole for experimental tests of contextuality, makes this connection interesting in its own right.

Mermin [18] has already shown one connection between PPS effects and contextuality. His investigation concerned what is known as the “mean king’s problem” [19], which is a PPS effect that is qualitatively different from the paradoxical variety of PPS effect that we shall be considering. Moreover, Mermin demonstrated how one can obtain a type of mean king’s problem that is unsolvable starting from the measurements used in a proof of contextuality, whereas we demonstrate how one can obtain proofs of contextuality starting from the measurements used in a PPS paradox.

To be specific, we demonstrate the following: for every PPS paradox wherein all the PPS probabilities are 0 or 1 and the pre- and post-selection states are non-orthogonal, there is an associated proof of contextuality. The key to the proof is that measurements that are treated as temporal successors in the PPS paradox are treated as counterfactual alternatives in the proof of contextuality. This result suggests the existence of a subtle conceptual connection between the two phenomena that has yet to be fully understood. Thus, the present work contributes to the project of reducing the number of logically distinct quantum mysteries by revealing the connections between them.

We begin with a curious prediction of the ABL rule known as the 3-box paradox. Suppose we have a particle that can be in one of three boxes. We denote the state where the particle is in box $j$ by $|j\rangle$. The particle is pre-selected in the state $|\phi\rangle = |1\rangle + |2\rangle + |3\rangle$ and post-
selected in the state \( |\psi\rangle = |1\rangle + |2\rangle - |3\rangle \) (states will be left unnormalized). At an intermediate time, one of two possible measurements is performed. The first possibility corresponds to the projector valued measure (PVM) \( \mathcal{E}_1 = \{ P_1, P_1^\perp \} \), where
\[
P_1 = |1\rangle \langle 1| \quad P_1^\perp = |2\rangle \langle 2| + |3\rangle \langle 3|.
\] (1)

The second possibility corresponds to the PVM \( \mathcal{E}_2 = \{ P_2, P_2^\perp \} \), where
\[
P_2 = |2\rangle \langle 2| \quad P_2^\perp = |1\rangle \langle 1| + |3\rangle \langle 3|.
\] (2)

Now note that \( P_1^\perp \) can also be decomposed into a sum of the projectors onto the vectors \( |2\rangle + |3\rangle \) and \( |2\rangle - |3\rangle \). However, the first of these is orthogonal to the post-selected state, while the second is orthogonal to the pre-selected state, so that the probability of the outcome \( P_1^\perp \) occurring, given that the pre- and post-selection were successful, must be 0. Consequently, the measurement of \( \mathcal{E}_1 \) necessarily has the outcome \( P_1 \). Similarly, \( P_2^\perp \) can be decomposed into a sum of the projectors onto the vectors \( |1\rangle + |3\rangle \) and \( |1\rangle - |3\rangle \), which are also orthogonal to the post- and pre-selected states respectively. Consequently, the measurement of \( \mathcal{E}_2 \) necessarily has the outcome \( P_2 \). Thus, if one measures to see whether or not the particle was in box 1, one finds that it was in box 1 with certainty, and if one measures to see whether or not it was in box 2, one finds that it was in box 2 with certainty!

This is reminiscent of the sort of conclusion that one obtains in proofs of the impossibility of a noncontextual hidden variable theory. Indeed, a proof presented by Clifton \cite{Clifton2003} makes use of the same mathematical structure, as we presently demonstrate.

Consider the eight vectors mentioned explicitly in our discussion of the 3-box paradox, but imagine that these describe alternative possible measurements at a single time (in contrast to what occurs in the 3-box paradox). In a noncontextual hidden variable theory, it is presumed that although all of these tests can be implemented simultaneously, their outcomes are determined by the values of preexisting hidden variables and are independent of the manner in which the test is made (the context). Thus each of these vectors is assigned a value, 1 or 0, specifying whether the associated test is passed or not. For any orthogonal pair, not both can receive the value 1, and for any orthogonal triplet, exactly one must receive the value 1. Representing the vectors by points and orthogonality between vectors by a line between points, these eight vectors above can be depicted as in Fig. 1.

Clifton’s proof is an example of a probabilistic proof of contextuality \cite{Clifton2004}, since it relies on assigning the states \( |\phi\rangle, |\psi\rangle \) probability 1 a priori. This is justified as follows: the state \( |\phi\rangle \) can be prepared, and if it is, then a subsequent test for \( |\phi\rangle \) will be passed with certainty, and a subsequent test for \( |\psi\rangle \) will be passed with nonzero probability (because \( \langle \psi | \phi \rangle \neq 0 \)). This implies that there must be some values of the hidden variables that assign value 1 to both. Consider such a hidden state. Since \( |1\rangle - |3\rangle \) and \( |2\rangle - |3\rangle \) are orthogonal to \( |\psi\rangle \), they must be assigned value 0 for this hidden state and since \( |1\rangle + |3\rangle \) and \( |2\rangle + |3\rangle \) are orthogonal to \( |\phi\rangle \), they must also be assigned value 0. But given that \( |1\rangle, |2\rangle + |3\rangle \), and \( |2\rangle - |3\rangle \) form an orthogonal triplet, it follows that \( |1\rangle \) must receive the value 1. Similarly, given that \( |2\rangle, |1\rangle + |3\rangle \), and \( |1\rangle - |3\rangle \) form an orthogonal triplet, it follows that \( |2\rangle \) must receive the value 1. However, \( |1\rangle \) and \( |2\rangle \) cannot both receive the value 1, since they are orthogonal. Thus, we have derived a contradiction.

To our knowledge, the connection between Clifton’s proof and the 3-box paradox has not previously been recognized.

We will demonstrate that this sort of connection is generic to PPS paradoxes. We begin with a short review of the ABL rule, hidden variable theories and contextuality.

We only consider quantum systems with a finite dimensional Hilbert space and assume that no evolution occurs between measurements. We restrict our attention to sharp measurements, that is, those associated with PVMs. We also restrict attention to measurements for which the state updates according to \( \rho \rightarrow P_j \rho P_j / \text{Tr}(P_j \rho) \) upon obtaining outcome \( j \). This is known as the Lüders rule \cite{Luders1952}. We call this set of assumptions the standard framework for PPS effects. It includes all of the PPS “paradoxes” discussed in the literature to date. The extent to which our results can be generalized beyond this framework is a question for future research.

To describe pre- and post-selected systems, we imagine a temporal sequence of three sharp measurements. The initial, intermediate, and final measurements occur at times \( t_{\text{pre}}, t, \) and \( t_{\text{post}} \) respectively, where \( t_{\text{pre}} < t < t_{\text{post}} \). The only relevant aspects of the initial and final PVMs are the projectors associated with the outcomes specified by the pre- and post-selection. Let these be denoted by \( \Pi_{\text{pre}} \) and \( \Pi_{\text{post}} \) respectively, and let the PVM associated with the intermediate measurement be denoted by \( \mathcal{E} = \{ P_j \} \).

Assuming that nothing is known about the system prior to \( t_{\text{pre}} \), so that the initial density operator is \( I/d \),
where $I$ is the identity operator, the measurement at $t_{\text{pre}}$ prepares the density operator $\rho_{\text{pre}} = \Pi_{\text{pre}}/\text{Tr}(\Pi_{\text{pre}})$. By Bayes’ theorem, we can deduce that the probability of obtaining the outcome $k$ in the intermediate measurement is

$$p(P_k|\Pi_{\text{pre}}, \Pi_{\text{post}}, E) = \frac{\text{Tr}(\Pi_{\text{post}} P_k \Pi_{\text{pre}} P_k)}{\sum_j \text{Tr}(\Pi_{\text{post}} P_j \Pi_{\text{pre}} P_j)}.$$  

This is a special case of the most general version of the ABL rule [2], and we therefore refer to such probabilities as “ABL probabilities”. In the case where $\Pi_{\text{pre}}$ and $\Pi_{\text{post}}$ are rank-1 projectors onto states $|\phi\rangle$ and $|\psi\rangle$ respectively, this rule reduces to

$$p(P_k|\phi, \psi, E) = \frac{|\langle \psi | P_k |\phi\rangle|^2}{\sum_j |\langle \psi | P_j |\phi\rangle|^2}$$

which was implicitly used in our discussion of the 3-box paradox. We now implicitly used in our discussion of the 3-box paradox. A hidden variable theory is an attempt to understand quantum measurements as revealing features of pre-existing ontic states, by which we mean complete specifications of the state of reality. A particularly natural class of such theories are those that satisfy the following two assumptions [17]: measurement noncontextuality, which is the assumption that the manner in which the measurement is represented in the HVT depends only on the PVM and not on any other details of the measurement (the context); and outcome determinism for sharp measurements, which is the assumption that the outcome of a PVM measurement is uniquely fixed by the ontic state. We abbreviate these as MNHVTs. It follows that in an MNHVT, projectors are associated with unique pre-existing properties that are simply revealed by measurements [17].

Suppose we denote by $s$ the proposition that asserts that the property associated with projector $P$ is possessed. In an MNHVT the negation of $s$, denoted $\neg s$, is associated with $I - P$. Now consider a projector $Q$ that commutes with $P$, and denote the proposition associated with $Q$ by $t$. In an MNHVT the conjunction of $s$ and $t$, denoted $s \land t$, is associated with $PQ$ and the disjunction of $s$ and $t$, denoted $s \lor t$, is associated with $P + Q - PQ$ (the latter follows from the fact that $s \lor t = \neg (\neg s \land \neg t)$).

Let $p(s)$ denote the probability that the proposition $s$ is true. Classical probability theory dictates that

$$0 \leq p(s) \leq 1$$ (4)

$$p(\neg s) = 1 - p(s),$$ (5)

$$p(s \land \neg s) = 1, \quad p(s \land \neg s) = 0$$ (6)

$$p(s \lor t) \leq p(s), \quad p(s \lor t) \leq p(t)$$ (7)

$$p(s \lor t) = p(s) + p(t) - p(s \land t)$$ (8)

We therefore obtain the following constraints on an MNHVT.

**Algebraic conditions:** For projectors $P, Q$ such that $[P, Q] = 0$,

$$0 \leq p(P) \leq 1$$ (9)

$$p(I - P) = 1 - p(P),$$ (10)

$$p(I) = 1, \quad p(0) = 0,$$ (11)

$$p(PQ) \leq p(P), \quad p(PQ) \leq p(Q),$$ (12)

$$p(P + Q - PQ) = p(P) + p(Q) - p(PQ).$$ (13)

By the assumption of outcome determinism, the probability assigned to every projector for a particular ontic state is either 0 or 1. The Bell-Kochen-Specker theorem shows that there are sets of projectors to which no such assignment consistent with the algebraic conditions is possible.

A connection to PPS paradoxes is suggested by the fact that there exist sets of projectors for which an ABL probability assignment violates the algebraic constraints, while every projector receives probability 0 or 1. We call such a scenario a logical PPS paradox. The 3-box paradox is an example of this [33].

Now, if it were the case that in the HVT, the pre- and post-selection picked out a set of ontic states that was independent of the nature of the intermediate measurement, then the probability assigned by the ABL rule to a projector could also be interpreted as the probability assigned to it by these ontic states. But since the latter probabilities are required to satisfy the algebraic conditions in a MNHVT, the violation of these conditions would be a proof of contextuality. However, the set of ontic states picked out by the PPS need not be independent of the nature of the intermediate measurement in general. To see this, note that a measurement in an HVT need not be modelled simply by a Bayesian updating of one’s information, but may also lead to a disturbance of the ontic state, and the nature of this disturbance may depend on the nature of the intermediate measurement. Consequently, a PPS paradox is not itself a proof of contextuality. This is discussed in more detail in Ref. [23].

Despite these considerations, the main aim of this letter is to show that there is a connection between PPS paradoxes and contextuality, but it is significantly more subtle than one might have thought.

**Theorem.** For every logical PPS paradox within the standard framework for which the pre- and post-selection projectors are non-orthogonal, there is an associated proof of the impossibility of an MNHVT that is obtained by considering all the measurements defined by the PPS paradox – the pre-selection measurement, the post-selection measurement and the alternative possible intermediate measurements – as alternative possible measurements at a single time.

Our proof of this theorem generalizes the argument
presented for the 3-box paradox. We begin with two lemmas and a corollary.

Lemma 1. If $\Pi_{\text{pre}}, \Pi_{\text{post}}, P$ are projectors satisfying $\Pi_{\text{post}}(I - P)\Pi_{\text{pre}} = 0$, then there exists a pair of orthogonal projectors $Q$ and $R$ such that $I - P = Q + R$ where $\Pi_{\text{pre}}R = 0$ and $\Pi_{\text{post}}Q = 0$.

Proof. Let $R \equiv (I - P) \wedge (I - \Pi_{\text{pre}})$, where $P \wedge Q$ denotes the projector onto the intersection of the subspaces associated with $P$ and $Q$. This clearly satisfies $\Pi_{\text{pre}}R = 0$. Moreover, since $R$ is a subspace of $I - P$, the projector $Q \equiv (I - P) - R$ is orthogonal to $R$ and satisfies $I - P = Q + R$. Finally, $\Pi_{\text{post}}(I - P)\Pi_{\text{pre}} = 0$ entails that $\Pi_{\text{post}}$ is orthogonal to the projector onto $\text{ran}((I - P)\text{ran}(\Pi_{\text{pre}}))$, where $\text{ran}(X)$ denotes the range of $X$. But this projector is simply $(I - P) - (I - P) \wedge (I - \Pi_{\text{pre}}) = Q$. Thus, $\Pi_{\text{post}}Q = 0$ is satisfied.

Lemma 2. If under a pre-selection of $\Pi_{\text{pre}}$ and a post-selection of $\Pi_{\text{post}}$, the projector $P$ receives probability 1 in a measurement of some PVM $\mathcal{E}$, then in an MNHVT, if $\Pi_{\text{pre}}$ and $\Pi_{\text{post}}$ are assigned probability 1 by some ontic state $\lambda$, $P$ is also assigned probability 1 by the ontic state $\lambda$. Succinctly, if $p(P|\Pi_{\text{pre}}, \Pi_{\text{post}}, \mathcal{E}) = 1$ and $p(\Pi_{\text{pre}}|\lambda) = p(\Pi_{\text{post}}|\lambda) = 1$, then $p(P|\lambda) = 1$.

Proof. If $p(P|\Pi_{\text{pre}}, \Pi_{\text{post}}, \mathcal{E}) = 1$, then by the ABL rule

$$\frac{\text{Tr}(\Pi_{\text{pre}}P\Pi_{\text{post}})}{\text{Tr}(\Pi_{\text{pre}}P\Pi_{\text{post}}) + \text{Tr}(\Pi_{\text{pre}}(I - P)\Pi_{\text{post}}(I - P))} = 1$$

which implies that $\text{Tr}(\Pi_{\text{pre}}(I - P)\Pi_{\text{post}}(I - P)) = 0$, and since $\text{Tr}(A^\dagger A) = 0$ implies that $A = 0$, it follows that $\Pi_{\text{post}}(I - P)\Pi_{\text{pre}} = 0$. It then follows from lemma 1, that $I - P$ can be decomposed into a sum of projectors $R$ and $Q$ which are orthogonal to $\Pi_{\text{pre}}$ and $\Pi_{\text{post}}$ respectively.

Given this orthogonality, for any $\lambda$ in an MNHVT that yields $p(\Pi_{\text{pre}}|\lambda) = 1$, and $p(\Pi_{\text{post}}|\lambda)$, we have $p(Q|\lambda) = p(R|\lambda) = 0$. It then follows from the algebraic conditions that $p(P|\lambda) = 1 - p(I - P|\lambda) = 1 - p(Q + R|\lambda) = 1 - p(Q|\lambda) - p(R|\lambda) = 1$.

Corollary. If $p(P|\Pi_{\text{pre}}, \Pi_{\text{post}}, \mathcal{E}) = 0$ and $p(\Pi_{\text{pre}}|\lambda) = p(\Pi_{\text{post}}|\lambda) = 1$, then $p(P|\lambda) = 0$.

Proof. $p(P|\Pi_{\text{pre}}, \Pi_{\text{post}}, \mathcal{E}) = 0$ implies $p(I - P|\Pi_{\text{pre}}, \Pi_{\text{post}}, \mathcal{E}) = 1$, which by lemma 2 implies $p(I - P|\lambda) = 1$. It then follows from the algebraic constraints that $p(P|\lambda) = 0$.

Proof of theorem. By the assumption that the PPS projectors are nonorthogonal, there exist ontic states $\lambda$ such that $p(\Pi_{\text{pre}}|\lambda) = p(\Pi_{\text{post}}|\lambda) = 1$. This, together with lemma 2 and its corollary, implies that whatever probability assignments to $\{P\}$ arise from the ABL rule also arise in any MNHVT as the probability assignment to $\{P\}$ for those ontic states $\lambda$ yielding $p(\Pi_{\text{pre}}|\lambda) = p(\Pi_{\text{post}}|\lambda) = 1$. Since, by the assumption of a logical PPS paradox, the ABL probabilities violate the algebraic conditions, it follows that the probabilities conditioned on this $\lambda$ in an MNHVT also violate the algebraic conditions. However, probability assignments in an MNHVT must satisfy these conditions, therefore an MNHVT is ruled out.

A question that has not been addressed in the present paper is whether the existence of logical PPS paradoxes in a theory implies measurement contextuality. To answer this question, one must characterize each of these features in a theory-independent manner, and examine whether every theory that exhibits the former also exhibits the latter. For an attempt to provide an operational characterization of logical PPS paradoxes has yet been made, but in [23], Kirkpatrick has proposed an analogue of the 3-box paradox in the context of a model with playing cards [23], and we have proposed a similar analogue in the context of a simple partitioned-box model in [23]. These models are measurement noncontextual by the definition of [17]. Thus if one agrees that either the 3-box paradox of Kirkpatrick or that of [23] is indeed a logical PPS paradox, then one can conclude that logical PPS paradoxes do not imply contextuality.

Nonetheless, the toy theory of [26], which is in many respects more similar to quantum theory than the models of [25] or [23], seems unable to reproduce the logical PPS paradoxes. Moreover, one of the most conspicuous phenomena that this toy theory fails to reproduce is contextuality (where again we appeal to the operational definition of contextuality provided in [17]). All of this suggests that there may be a natural set of conditions that quantum theory, classical probability theory with Bayesian updating and the toy theory of [26] satisfy, but that Kirkpatrick’s model and the partitioned box model of [23] do not satisfy, under which logical PPS paradoxes can only arise if there is contextuality. Further investigations into these issues are required.

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[32] A PVM is a set of projectors that sum to the identity operator
[33] Another example is the “failure of the product rule” discussed in [27, 28]. By our results, this is related to the contextuality proofs discussed in [24, 31, 31].