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 the impossibility of a noncontextual hidden variable theory. This proof is obtained by considering all the measurements involved in the paradoxical effect—the preselection, 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. As first demonstrated by Albert, Aharonov, and D'Amato [5], using an effect now known as the "3-box paradox," the probability assigned to an outcome of a measurement given a pre- and a post-selection can depend not only on the projector associated with that outcome, but also on other details of the observable. This is a sort of context dependence. As such, it seems to undermine the significance of the Bell-Kochen-Specker theorem [6], which establishes the impossibility of a noncontextual hidden variable theory (HVT), since there is no reason to think that probabilities conditioned on the hidden variables should be noncontextual if quantum probabilities are themselves contextual. Bub and Brown [7] convincingly disputed this argument by giving an example for which similar reasoning would imply that quantum theory allowed superluminal signalling. As they showed, it is a mistake to think that a pre- and post-selected ensemble can be defined independently of the intermediate measurement. Although we agree that PPS paradoxes are not themselves proofs of the contextuality of HVTs, we show that there is nonetheless a close connection between the two.

This connection is expected to have interesting applications in quantum foundational studies. For instance, it has been suggested that Bell's theorem [8] might be understood within a realist and Lorentz-invariant framework if one admits the possibility of a HVT that allows for backward-in-time causation [9]. A simple model has even been suggested by Kent [10]. This is closely connected to the fact that Bell correlations can be simulated using post-selection, as shown in Ref. [7], which in turn is the root of the detection-efficiency loophole in experimental tests of Bell's theorem [11]. 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 [12]), the connection between contextuality and PPS paradoxes established in the present work is an important contribution to this project.

Mermin [13] has already shown one connection between PPS effects and contextuality. His investigation concerned what is known as the "mean king's problem" 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 the contextuality of HVTs, whereas we demonstrate how one can obtain proofs of contextuality starting from the measurements used in a PPS paradox.

To be specific, we show that for every PPS paradox wherein all the PPS probabilities are 0 or 1 and the pre- and post-selection states are nonorthogonal, there is an associated proof of the contextuality of HVTs. 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. Consider a particle that can be in one of three boxes. Denote the state where the particle is in box j by $|j\rangle$. The particle is preselected 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) [14] $\mathcal{E}_1 = \{P_1, P_1^\perp\}$, where $P_1 = |1\rangle\langle 1|$ and $P_1^\perp = |2\rangle\langle 2| + |3\rangle\langle 3|$. The second possibility corresponds to the PVM $\mathcal{E}_2 = \{P_2, P_2^\perp\}$, where $P_2 = |2\rangle\langle 2|$ and $P_2^\perp = |1\rangle\langle 1| + |3\rangle\langle 3|$.

Now note that $P_1^\perp$ can also be decomposed into a sum of the projectors onto the vectors $|2\rangle + |3\rangle$ and $|2\rangle - |3\rangle$. The first of these is orthogonal to the post-selected state, while the second is orthogonal to the preselected state, so 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 preselected 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 [15] makes use of the same mathematical structure, as we presently demonstrate.

Consider the eight vectors mentioned 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 HVT, it is presumed that although not 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 would be passed or not. Clearly, the following two rules must apply: (1) For any orthogonal pair, not both can receive the value 1, and (2) for any orthogonal triplet, exactly one must receive the value 1. Representing the vectors by points and orthogonality by lines, the eight vectors can be depicted as in Fig. 1.

Clifton's proof is an example of a *probablistic* proof of the contextuality of HVTs, since it relies on assigning the vectors $|\phi\rangle, |\psi\rangle$ probability 1 *a priori*. This is justified as

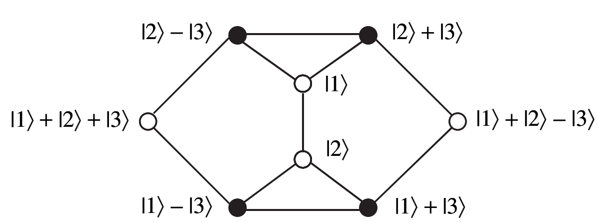

FIG. 1. The vectors in Clifton's proof of contextuality. White (black) represents the value 1 (0).

follows: the state $|\phi\rangle$ can be prepared, and if it is, then a subsequent test for $|\phi\rangle$ will be passed with certainty. Thus, for all valuations of the hidden variables consistent with the preparation of $|\phi\rangle, |\phi\rangle$ is assigned the value 1. Furthermore, after a preparation of $|\phi\rangle$ a test for $|\psi\rangle$ will be passed with nonzero probability (because $\langle\psi|\phi\rangle \neq 0$) and consequently *some* of the valuations of the hidden variables consistent with the preparation of $|\phi\rangle$ also assign value 1 to $|\psi\rangle$. Let λ denote a valuation that assigns 1 to both $|\phi\rangle$ and $|\psi\rangle$. Since $|1\rangle - |3\rangle$ and $|2\rangle - |3\rangle$ are orthogonal to $|\phi\rangle$, they must be assigned value 0 by λ and since $|1\rangle + |3\rangle$ and $|2\rangle + |3\rangle$ are orthogonal to $|\psi\rangle$, they must also be assigned value 0 by λ. But given that $|1\rangle$, $|2\rangle + |3\rangle$, and $|2\rangle - |3\rangle$ form an orthogonal triplet, by rule (2) it follows that $|1\rangle$ must be assigned the value 1 by λ. Similarly, given that $|2\rangle$, $|1\rangle + |3\rangle$, and $|1\rangle - |3\rangle$ form an orthogonal triplet, by rule (2) it follows that $|2\rangle$ must be assigned the value 1 by λ. However, by rule (1) $|1\rangle$ 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 show 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 $\rho \rightarrow P_j \rho P_j / \mathrm{Tr}(P_j \rho)$ upon obtaining outcome j. This is known as the Lüders rule. 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.

Now, consider a temporal sequence of three sharp measurements. The initial, intermediate, and final measurements occur at times t_{pre}, t, and t_{post} respectively. The only relevant aspects of the initial and final PVMs are the projectors associated with the outcomes specified by the pre- and post-selection. We denote these by Π_{pre} and Π_{post}, and we denote the PVM associated with the intermediate measurement by $\mathcal{E} = \{P_j\}$.

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

$$p(P_k|\Pi_{\mathrm{pre}}, \Pi_{\mathrm{post}}, \mathcal{E}) = \frac{\mathrm{Tr}(\Pi_{\mathrm{post}} P_k \Pi_{\mathrm{pre}} P_k)}{\sum_j \mathrm{Tr}(\Pi_{\mathrm{post}} P_j \Pi_{\mathrm{pre}} P_j)}. \quad (1)$$

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 $\Pi_{\rm pre}$ and $\Pi_{\rm post}$ are rank-1 projectors onto states $|\phi\rangle$ and $|\psi\rangle$ respectively, this rule reduces to the more familiar $p(P_k|\phi, \psi, \mathcal{E}) = |\langle\psi|P_k|\phi\rangle|^2/\sum_j|\langle\psi|P_j|\phi\rangle|^2$ which was implicitly used in our discussion of the 3-box paradox.

A hidden variable theory is an attempt to explain the outcomes of quantum measurements by a set of variables that are hidden to one who knows only the preparation procedure. We use the term *ontic state* to refer to a complete description of the real state of affairs according to the HVT. This includes a valuation of all the hidden variables, and may also include the quantum state vector if this has ontic (rather than epistemic) status in the HVT. A particularly natural class of HVTs are those that satisfy the following two assumptions [12]: *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, every projector is assigned a probability of 0 or 1 by an ontic state, independently of the nature of the measurement in which the projector appears, for instance, of what other projectors might be measured simultaneously with it. In other words, projectors are associated with unique preexisting properties that are simply revealed by measurement [12].

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 $s \wedge t$, is associated with PQ and the disjunction of s and t, denoted $s \vee t$, is associated with $P + Q - PQ$ (the latter follows from the fact that $s \vee t = \neg(\neg s \wedge \neg t)$).

Let $p(s)$ denote the probability that the proposition s is true. Classical probability theory dictates that $0 \leq p(s) \leq 1$, $p(\neg s) = 1 - p(s)$, $p(s \vee \neg s) = 1$, $p(s \wedge \neg s) = 0$, $p(s \wedge t) \leq p(s)$, $p(s \wedge t) \leq p(t)$, and $p(s \vee t) = p(s) + p(t) - p(s \wedge t)$. We therefore obtain the following constraints on an MNHVT.

Algebraic conditions.—For projectors P, Q such that $[P, Q] = 0$, we have $0 \leq p(P) \leq 1$, $p(I - P) = 1 - p(P)$, $p(I) = 1$, $p(0) = 0$, $p(PQ) \leq p(P)$, $p(PQ) \leq p(Q)$, and $p(P + Q - PQ) = p(P) + p(Q) - p(PQ)$.

The Bell-Kochen-Specker theorem shows that there are sets of projectors to which no assignment of probabilities 0 or 1 consistent with the algebraic conditions is possible. This demonstrates the impossibility of an MNHVT, or equivalently, the contextuality of HVTs of quantum mechanics [16].

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 [17].

Now, define Λ to be the set (or ensemble) of ontic states that can obtain prior to the intermediate measurement given the pre- and post-selection. *If* Λ were 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 ontic states in Λ. But since the latter probabilities are required to satisfy the algebraic conditions in an MNHVT, the violation of these conditions would be a proof of the impossibility of an MNHVT. However, a measurement in an HVT need not be modeled simply by a Bayesian updating of one's information, but may also lead to a disturbance of the ontic state. Thus, to determine Λ we need to work backwards from the post-selection, asking what is the set Ω of ontic states that could obtain *after* the intermediate measurement given the post-selection, and then what ontic states could obtain *prior* to the intermediate measurement given Ω and given the nature of the disturbance. Since the disturbance may depend on the nature of the intermediate measurement, so too may Λ. Thus, the possibility of measurement disturbance blocks the conclusion that a PPS paradox is itself a proof of the contextuality of HVTs. This is discussed in more detail in Ref. [20].

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 nonorthogonal, 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 preselection, the post-selection, 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 $\Pi_{\rm pre}$, $\Pi_{\rm post}$, P are projectors satisfying $\Pi_{\rm post}(I - P)\Pi_{\rm pre} = 0$, then there exists a pair of orthogonal projectors Q and R such that $I - P = Q + R$ where $\Pi_{\rm pre}R = 0$ and $\Pi_{\rm post}Q = 0$.

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

Lemma 2.—If under a preselection of $\Pi_{\rm pre}$ and a postselection of $\Pi_{\rm post}$, the projector P receives probability 1 in a measurement of a PVM $\mathcal{E} = \{P, P_1^\perp, P_2^\perp, \ldots\}$ that appears in a logical PPS paradox, then in an MNHVT, if $\Pi_{\rm pre}$ and $\Pi_{\rm post}$ are assigned probability 1 by some ontic state λ, P is also assigned probability 1 by the ontic state λ. Succinctly, if $p(P|\Pi_{\rm pre}, \Pi_{\rm post}, \mathcal{E}) = 1$ and $p(\Pi_{\rm pre}|\lambda) = p(\Pi_{\rm post}|\lambda) = 1$, then $p(P|\lambda) = 1$.

Proof.—If $p(P|\Pi_{\rm pre}, \Pi_{\rm post}, \mathcal{E}) = 1$, it follows from the ABL rule that $\mathrm{Tr}(\Pi_{\rm pre}P_k^\perp \Pi_{\rm post}P_k^\perp) = 0$ for all k. Since $\mathrm{Tr}(A^\dagger A) = 0$ implies that $A = 0$, it follows that $\Pi_{\rm post}P_k^\perp \Pi_{\rm pre} = 0$ for all k and consequently that $\Pi_{\rm post}(I - P)\Pi_{\rm pre} = 0$. It then follows from lemma 1 that $I - P$ can be decomposed into a sum of projectors R and Q which are orthogonal to $\Pi_{\rm pre}$ and $\Pi_{\rm post}$ respectively. Given this orthogonality, for any λ in an MNHVT yielding $p(\Pi_{\rm pre}|\lambda) = p(\Pi_{\rm post}|\lambda) = 1$, we have $p(Q|\lambda) = p(R|\lambda) = 0$. The algebraic conditions then imply that $p(P|\lambda) = 1 - p(I - P|\lambda) = 1 - p(Q + R|\lambda) = 1$. □

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

Proof.—Given that each of the projectors $P, P_1^\perp, P_2^\perp, \ldots$ must receive value 0 or 1 in a logical PPS paradox, $p(P|\Pi_{\rm pre}, \Pi_{\rm post}, \mathcal{E}) = 0$ implies that $p(P_k^\perp|\Pi_{\rm pre}, \Pi_{\rm post}, \mathcal{E}) = 1$ for some k, which by lemma 2 implies that $p(P_k^\perp|\lambda) = 1$ for some k. It then follows from the algebraic constraints that $p(P|\lambda) = 0$. □

Proof of theorem.—By the assumption that $\Pi_{\rm pre}$ and $\Pi_{\rm post}$ are nonorthogonal, there exist ontic states λ such that $p(\Pi_{\rm pre}|\lambda) = p(\Pi_{\rm post}|\lambda) = 1$. 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 such λ. Since, by the assumption of a logical PPS paradox, the ABL probabilities violate the algebraic conditions, it follows that the probabilities conditioned on such λ 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 work is whether, in an arbitrary statistical theory (not just quantum theory), the existence of logical PPS paradoxes implies that this theory cannot be modeled by a noncontextual HVT. To answer this question, one must characterize PPS paradoxes and contextuality in a theory-independent manner. For an attempt to generalize the notion of contextuality to HVTs for arbitrary statistical theories, see Ref. [12]. No attempt at providing an operational characterization of logical PPS paradoxes has yet been made; however, the surprising features of the 3-box paradox have been reproduced within two simple toy theories, described in Refs. [20,21], and these toy theories can be understood in terms of a HVT that is noncontextual by the definition of Ref. [12]. Thus it seems that the existence of logical PPS paradoxes *does not* imply the impossibility of a noncontextual HVT. Nonetheless, there may be additional natural constraints that a general class of theories including quantum mechanics satisfy, under which this implication holds true. Further investigations into these issues are required.

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