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Logical pre- and post-selection paradoxes are proofs of contextuality

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If a quantum system is prepared and later post-selected in certain states, "paradoxical" predictions for intermediate measurements can be obtained. This is the case both when the intermediate measurement is strong, i.e. a projective measurement with Lüders-von Neumann update rule, or with weak measurements where they show up in anomalous weak values. Leifer and Spekkens [Phys. Rev. Lett. **95**, 200405] identified a striking class of such paradoxes, known as *logical* pre- and post-selection paradoxes, and showed that they are indirectly connected with contextuality. By analysing the measurement-disturbance required in models of these phenomena, we find that the strong measurement version of logical pre- and post-selection paradoxes actually constitute a direct manifestation of quantum contextuality. The proof hinges on under-appreciated features of the paradoxes. In particular, we show by example that it is not possible to prove contextuality without Lüders-von Neumann updates for the intermediate measurements, nonorthogonal pre- and post-selection, and 0/1 probabilities for the intermediate measurements. Since one of us has recently shown that anomalous weak values are also a direct manifestation of contextuality [Phys. Rev. Lett. **113**, 200401], we now know that this is true for both realizations of logical pre- and post-selection paradoxes.

1 Introduction

Can a ball be in two separate boxes at once, and does the answer to this question depend in any meaningful way upon quantum mechanics? Issues such as these have been raised by a series of colourfully described thought experiments involving pre- and post-selected quantum systems.

Suppose a quantum system is prepared in state $|\psi\rangle$, subjected to an intermediate projective measurement $\mathscr{M} = \{P_j\}$ with Lüders-von Neumann update rule[1], followed by a final projective measurement that includes the projector onto $|\phi\rangle$ as one of its outcomes. Assuming that no other evolution occurs, the joint probability for obtaining the outcome P_j and passing the post-selection is

$$\mathbb{P}(P_j, \phi | \psi, \mathscr{M}) = \left| \langle \phi \,|\, P_j \,|\, \psi \rangle \right|^2, \tag{1}$$

and the marginal probability for passing the post-selection is then

$$\mathbb{P}(\phi | \psi, \mathscr{M}) = \sum_j \mathbb{P}(P_j, \phi | \psi, \mathscr{M}) = \sum_j \left| \langle \phi \,|\, P_j \,|\, \psi \rangle \right|^2. \tag{2}$$

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[1] This is the traditional "projection postulate" where, upon obtaining the result P_j, the state of the system is updated to $P_j |\psi\rangle / \langle\psi| P_j |\psi\rangle$.

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From this, we can calculate the probabilities for the intermediate measurement conditioned on both the pre- and post-selection as

$$\mathbb{P}(P_j|\psi,\mathscr{M},\phi) = \frac{\mathbb{P}(P_j,\phi|\psi,\mathscr{M})}{\mathbb{P}(\phi|\psi,\mathscr{M})} = \frac{\left|\langle\phi\,|\,P_j\,|\,\psi\rangle\right|^2}{\sum_k \left|\langle\phi\,|\,P_k\,|\,\psi\rangle\right|^2}, \tag{3}$$

which is known as the "ABL rule" [1].

Various choices of $|\psi\rangle$, $\mathscr{M}$ and $|\phi\rangle$ have been shown to give counter-intuitive results, for example the "three-box paradox" [2], "quantum cheshire cats" [3] and recently the "quantum pigeonhole principle" [4].

For example, the three-box paradox involves a state space spanned by $\{|1\rangle, |2\rangle, |3\rangle\}$ representing a ball in box 1, 2, or 3 respectively. Consider a pre-selection $|\psi\rangle \propto |1\rangle + |2\rangle + |3\rangle$ and a post-selection $|\phi\rangle \propto |1\rangle + |2\rangle - |3\rangle$. If we "look in box 1", $\mathscr{M} = \{|1\rangle\langle 1|, |2\rangle\langle 2| + |3\rangle\langle 3|\}$, then whenever the post-selection succeeds we will have found the ball, $\mathbb{P}(|1\rangle\langle 1|\,|\psi,\mathscr{M},\phi) = 1$. But if instead we "look in box 2", $\mathscr{M}' = \{|1\rangle\langle 1| + |3\rangle\langle 3|, |2\rangle\langle 2|\}$, we also have $\mathbb{P}(|2\rangle\langle 2|\,|\psi,\mathscr{M}',\phi) = 1$. Hence the ball is in both boxes.

Or is it? In addition to general concerns about the interpretation of ABL probabilities for unperformed measurements (e.g. [5]), ontological models (without balls that are in more than one box) reproducing various aspects of the paradox have been proposed [6, 7, 8] and criticised [9]. The basic idea of such models is that the intermediate measurement can disturb the system, thus allowing the success of the post-selection to depend on which measurement was performed.

We believe the central question is this: does a given pre- and post-selection (PPS) phenomenon have a compelling classical explanation? And we believe the best way to make this question precise is: does the phenomena admit a non-contextual ontological model?

The most well-known obstruction to non-contextual models of quantum theory is the Kochen-Specker theorem [10]. The question of whether certain PPS paradoxes constitute proofs of the Kochen-Specker theorem has been discussed, and answered in the negative [11, 12, 13, 7]. Again the crucial issue is a non-contextual assignment of values to the intermediate measurement may appear contextual under post-selection, due to measurement disturbance.

Nevertheless it was found in [13] that certain PPS paradoxes, which were dubbed *logical* PPS paradoxes, may be converted into proofs of the Kochen-Specker theorem by considering a standard "prepare and measure" experiment (without post-selection) in which the intermediate measurements along with two additional measurements (based on what were the pre- and post-selection) are all considered as counterfactual alternatives. This leaves the status of the logical PPS paradox itself somewhat unclear.

Here we show that, by analysing the possible disturbance due to the intermediate measurement in a non-contextual model, the paradoxes, in their original form, are in fact proofs of contextuality in the sense of [14], which generalises Kochen-Specker non-contextuality to include preparations and Positive Operator Valued Measures (POVMs). Whilst previous discussions have centred on the *existence* of measurement disturbance, it turns out that the *amount* of disturbance permitted by non-contextuality (whilst non-zero) is insufficient to dissolve the paradox. Hence we will show

Theorem 1. *Every logical PPS paradox is a proof of contextuality.*

2 Logical pre- and post-selection paradoxes

From now on, we shall only consider ABL probabilities of the form $\mathbb{P}(P|\psi,\{P, I-P\},\phi)$ where the intermediate measurement has two outcomes and I is the identity operator. Since the projective measurement

$\{P, I-P\}$ is thus uniquely determined by P, we shall abbreviate $\mathbb{P}(P|\psi,\{P,I-P\},\phi)$ to $\mathbb{P}(P|\psi,\phi)$ and $\mathbb{P}(\phi|\psi,\{P,I-P\})$ to $\mathbb{P}(\phi|\psi)$.

Our definition of a logical PPS paradox is based on [13, 7]. Consider a Hilbert space, a choice of pre-selection $|\psi\rangle$ and post-selection $|\phi\rangle$, and a (finite) set of projectors $\mathscr{P}$ that is closed under complements, i.e. if $P \in \mathscr{P}$ then $I-P \in \mathscr{P}$. Suppose further that the ABL probabilities $\mathbb{P}(P|\psi,\phi)$ are either 0 or 1 for every $P \in \mathscr{P}$ (which is what leads to the terminology "logical").

Now consider the partial boolean algebra generated by $\mathscr{P}$, i.e. the smallest set of projectors $\mathscr{P}'$ that contains $\mathscr{P}$ and satisfies

- If $P \in \mathscr{P}'$ then $I-P \in \mathscr{P}'$.
- If $P,Q \in \mathscr{P}'$ and $PQ = QP$ then $PQ \in \mathscr{P}'$.

If we think of projectors as representing propositions, then these conditions ensure that we can take complements and conjunctions of compatible propositions.[2]

Finally, suppose that we try to extend the probability function $f(P) = \mathbb{P}(P|\psi,\phi)$ from $\mathscr{P}$ to $\mathscr{P}'$ such that the following *algebraic conditions* are satisfied[3]

(i) For all $P \in \mathscr{P}'$, $0 \leq f(P) \leq 1$.

(ii) $f(I) = 1, f(0) = 0$.

(iii) For all $P,Q \in \mathscr{P}'$ such that $PQ = QP$, $f(P+Q-PQ) = f(P)+f(Q)-f(PQ)$.

If it is not possible to do this then we say that the ABL predictions for $\mathscr{P}$ form a *logical PPS paradox*.

For example in the three-box paradox we have $f(|1\rangle\langle 1|) = \mathbb{P}(|1\rangle\langle 1||\psi,\phi) = 1$ and $f(|2\rangle\langle 2|) = \mathbb{P}(|2\rangle\langle 2||\psi,\phi) = 1$. Applying condition (iii) gives $f(|1\rangle\langle 1| + |2\rangle\langle 2|) = 2$ in violation of condition (i). Other examples can be found in [15, 16, 17, 4, 18].

The following simple proposition will be useful later.

Proposition 1. *In a logical PPS paradox, the pre-selection $|\psi\rangle$ and post-selection $|\phi\rangle$ are necessarily nonorthogonal.*

Proof. According to the definition of a logical PPS paradox, the ABL probabilities $\mathbb{P}(P|\psi,\phi)$ assigned to the projectors $P \in \mathscr{P}$ must be 0 or 1. However, if $|\psi\rangle$ and $|\phi\rangle$ are orthogonal, then no 0/1 probability assignments are possible. To see this, suppose that $\mathbb{P}(P|\psi,\phi) = 1$. Then, from eq. (3),

$$|\langle\phi|P|\psi\rangle|^2 = |\langle\phi|P|\psi\rangle|^2 + |\langle\phi|(I-P)|\psi\rangle|^2, \tag{4}$$

which implies $\langle\phi|(I-P)|\psi\rangle = 0$. This implies that

$$\langle\phi|P|\psi\rangle = \langle\phi|P|\psi\rangle + \langle\phi|(I-P)|\psi\rangle \tag{5}$$

$$= \langle\phi|(P+I-P)|\psi\rangle \tag{6}$$

$$= \langle\phi|\psi\rangle, \tag{7}$$

which is also zero if the pre- and post-selection are orthogonal. This means the post-selection never occurs, so there are no ABL rule probabilities and hence no paradox. A similar argument shows that the same is true for $\mathbb{P}(P|\psi,\phi) = 0$. □

[2] Since $P+Q-PQ = I-(I-P)(I-Q)$ we can also take disjunctions. We thank a referee for this simplification.

[3] [13, 7] gave an additional condition $f(P'Q') \leq f(P')$ when $P'Q' = Q'P'$. But this follows from condition (iii) with $P = P'Q'$ and $Q = P'(I-Q')$, and then using conditions (i) and (ii). Also note that conditions (ii) and (iii) give $f(I-P) = 1-f(P)$.

There is an obvious similarity between logical PPS paradoxes and the Kochen-Specker theorem. Briefly, a Kochen-Specker noncontextual model can be thought of as an assignment of values $v(P) \in \{0,1\}$ to projection operators such that the algebraic conditions are satisfied with $f(P) = v(P)$. The Kochen-Specker theorem shows that such an assignment is not possible in general. However, in the Kochen-Specker scenario, the value assignments represent the predictions of a hypothetical outcome-deterministic ontological model (or hidden variable theory if you prefer archaic terminology), which are supposed to reproduce the quantum predictions in an ordinary "prepare-and-measure" experiment (i.e. with no post-selection) when we average them over a probability measure. In contrast, the ABL probabilities represent the *quantum* predictions with both pre- and post-selection, and there is a possibility that the intermediate measurements may disturb the state of the system, changing the probability of whether the post-selection is successful. Thus, no direct inference from logical PPS paradoxes to Kochen-Specker contextuality is possible. To establish contextuality from logical PPS paradoxes, we shall therefore have to look deeper, employing the more general definition of non-contextuality from [14], which allows us to place constraints on the amount of disturbance that can occur in a non-contextual model.

3 Non-contextual ontological models

By a proof of contextuality, we mean a proof of the impossibility of a non-contextual ontological model, as defined in [14]. We will need two facets of the assumption of non-contextuality: *measurement non-contextuality* and *outcome determinism for sharp measurements*.

Briefly, a non-contextual ontological model associates a quantum system with a measurable space (Λ, Σ) where Λ is the set of "ontic states" and Σ is a σ-algebra, a preparation with a measure μ on (Λ, Σ), and POVM elements E with conditional probabilities $\text{Pr}(E|\lambda)$, such that $\sum_{E\in\mathscr{M}} \text{Pr}(E|\lambda) = 1$ for every POVM $\mathscr{M}$ and every $\lambda \in \Lambda$. Upon marginalising over the ontic states, the model is required reproduce the quantum probabilities:

$$\int_\Lambda \text{Pr}(E|\lambda) d\mu(\lambda) = \langle\psi|E|\psi\rangle \,. \tag{8}$$

where $|\psi\rangle$ is the prepared quantum state.

The assumption of measurement non-contextuality has already been made, namely that the conditional probability of obtaining outcome E, $\text{Pr}(E|\lambda)$, depends only on the POVM element E, and not on the other POVM elements in the POVM being measured nor on how it is measured (e.g which other POVM it was obtained from by coarse-graining).

Measurement non-contextuality has two consequences that we shall make use of in the proof of Theorem 1. Firstly, if a POVM $\{E_j\}$ can be obtained by coarse-graining a POVM $\{E_{jk}\}$, i.e. $E_j = \sum_k E_{jk}$, then

$$\text{Pr}(E_j|\lambda) = \sum_k \text{Pr}(E_{jk}|\lambda). \tag{9}$$

This is because one method of measuring the POVM $\{E_j\}$ is to measure the POVM $\{E_{jk}\}$ and then subsequenty marginalise over k, and all methods of measuring a POVM must give the same probabilities $\text{Pr}(E_j|\lambda)$. Secondly, for similar reasons, if a POVM $\{E_j\}$ is a mixture of two POVMs $\{E'_j\}$ and $\{E''_j\}$, i.e. $E_j = qE'_j + (1-q)E''_j$ for some $0 \leq q \leq 1$, then

$$\text{Pr}(E_j|\lambda) = q\text{Pr}(E'_j|\lambda) + (1-q)\text{Pr}(E''_j|\lambda). \tag{10}$$

This is because one method of measuring $\{E_j\}$ is to flip a biased coin with probability q of coming up heads, measure $\{E'_j\}$ if heads is obtained or $\{E''_j\}$ if tails is obtained, and then subsequently only recording the outcome j.

The assumption of outcome determinism for sharp measurements is that $\Pr(E|\lambda) \in \{0,1\}$ whenever E is a projector. Rather than being assumed, it can be derived from a version of non-contextuality for preparations, together with some basic facts about projective measurements in quantum theory. For the details of this argument see [14, 19].

It is straightforward to check that these assumptions imply that that the assignments $f(P) = \Pr(P|\lambda)$ have to satisfy the algebraic conditions. However, the possibility of measurement disturbance blocks a direct inference from the observed pre- and post-selected probabilities to the probabilities conditioned only on the pre-selection of an ontic state [7]. In order to prove Theorem 1, we therefore need to understand the type of disturbance caused by a projective measurement. It will turn out to be important that the channel induced by ignoring the outcome of such a measurement can also be implemented in a way that involves, with non-zero probability, doing nothing.

Lemma 1. *For each projective measurement $\{P_j\}$ there exists a non-zero probability q and a quantum channel (i.e. a completely-positive trace-preserving map) $\mathscr{C}$ such that*

$$\sum_j P_j \rho P_j = q\rho + (1-q)\mathscr{C}(\rho) \qquad \forall \rho. \tag{11}$$

Proof. Suppose j runs from 1 to n. Let $X = \{1,-1\}^n$, i.e. the set of all strings $x = (x_1, x_2, \ldots, x_n)$ where $x_j = \pm 1$. For $x \in X$ define

$$U_x = \sum_{j=1}^{n} x_j P_j \tag{12}$$

which is unitary since $U_x^\dagger U_x = \sum_{j,k=1}^{n} x_j x_k P_j^\dagger P_k = \sum_{j=1}^{n} {x_j}^2 P_j = \sum_{j=1}^{n} P_j = I$, where we have used that $\{P_j\}$ is a set of orthogonal projectors summing to the identity.

Now consider $\sum_{x\in X} x_j x_k$. If $j = k$ then this is $\sum_{x\in X} 1 = 2^n$. Otherwise, the number of strings with $(x_j, x_k) = (1,1)$, $(x_j, x_k) = (-1,-1)$, $(x_j, x_k) = (1,-1)$, and $(x_j, x_k) = (-1,1)$ are all equal, with the first two sets contributing 1 to the sum and the second to contributing -1. Hence $\sum_{x\in X} x_j x_k = 2^n \delta_{jk}$, and so

$$\frac{1}{2^n}\sum_{x\in X} U_x \rho U_x^\dagger = \frac{1}{2^n}\sum_{j,k=1}^{n}\sum_{x\in X} x_j x_k P_j \rho P_k = \sum_{j,k=1}^{n} \delta_{jk} P_j \rho P_k = \sum_j P_j \rho P_j. \tag{13}$$

.

Since $U_{\pm(1,\ldots,1)} = \pm I$ we have eq. (11) with $q = 2^{1-n}$ and $\mathscr{C}(\rho) \propto \sum_{x \neq \pm(1,\ldots,1)} U_x \rho U_x^\dagger$. □

Let us see the implication of this for the disturbance.

Lemma 2. *Let $\{E_k\}$ be a POVM, let $\{P_j\}$ be a projective measurement, and let $\mathscr{E}$ be the channel $\mathscr{E}(\rho) = \sum_j P_j \rho P_j$, corresponding to performing the measurement $\{P_j\}$ and not recording the outcome. In a measurement non-contextual model, if λ makes some outcome of $\{E_k\}$ possible, i.e. $\Pr(E_k|\lambda) > 0$ for some k, then $\Pr(\mathscr{E}^\dagger(E_k)|\lambda) > 0$, where $\mathscr{E}^\dagger$ is the adjoint channel to $\mathscr{E}$, i.e. λ also makes the kth outcome possible in the measurement procedure consisting of performing $\{P_j\}$ and not recording the outcome, followed by performing $\{E_k\}$.*

Proof. The effect of performing the measurement $\{P_j\}$ and not recording the outcome is given by the channel

$$\mathscr{E}(\rho) = \sum_j P_j \rho P_j. \tag{14}$$

If we apply this channel to a state ρ, then measure $\{E_k\}$, the probabilities are given by $\mathrm{Tr}(E_k \mathscr{E}(\rho)) = \mathrm{Tr}(\mathscr{E}^\dagger(E_k)\rho)$ where $\mathscr{E}^\dagger$ is the adjoint channel to $\mathscr{E}$ (for our channel $\mathscr{E}^\dagger = \mathscr{E}$ but it will useful to keep the conceptual distinction). So we can consider the overall procedure as a measurement of the POVM $\{\mathscr{E}^\dagger(E_k)\}$.

Now consider another procedure. With probability q we simply measure $\{E_k\}$, whereas with probability $1-q$ we measure $\{\mathscr{C}^\dagger(E_k)\}$, where $q>0$ and $\mathscr{C}$ are from Lemma 1. By eq. (10), in the ontological model this will correspond to $q\text{Pr}(E_k|\lambda)+(1-q)\text{Pr}\left(\mathscr{C}^\dagger(E_k)|\lambda\right)$.

But by Lemma 1 we have $\mathscr{E}^\dagger(E_k)=qE_k+(1-q)\mathscr{C}^\dagger(E_k)$, and so these two procedures correspond to the same POVM. By measurement non-contextuality, we therefore have

$$\text{Pr}\left(\mathscr{E}^\dagger(E_k)|\lambda\right)=q\text{Pr}(E_k|\lambda)+(1-q)\text{Pr}\left(\mathscr{C}^\dagger(E_k)|\lambda\right)\geq q\text{Pr}(E_k|\lambda), \tag{15}$$

so that $\text{Pr}(E_k|\lambda)>0$ implies $\text{Pr}\left(\mathscr{E}^\dagger(E_k)|\lambda\right)>0$. □

In other words, the measurement-disturbance of a projective measurement cannot make an outcome of a following measurement go from being possible to impossible.[4] Theorem 1 follows simply by showing that this is exactly the type of disturbance needed to dissolve a logical pre- and post-selection paradox.

In the case of a finite state space Λ, the proof would run as follows. By Proposition 1, when there is no intervening measurement, the post-selection can occur. Hence there exists some λ compatible with the preparation that makes the post-selection occur. Consider P with $\mathbb{P}(P|\psi,\phi)=1$. If $\text{Pr}(P|\lambda)=0$ then measurement-disturbance must always prevent the post-selection from occurring, in contradiction with Lemma 2. Hence outcome determinism for sharp measurements gives $\text{Pr}(P|\lambda)=1$. Repeating this for all other P with $\mathbb{P}(P|\psi,\phi)=1$, we find that $\text{Pr}(P|\lambda)=\mathbb{P}(P|\psi,\phi)$ for every $P\in\mathscr{P}$. But since $\text{Pr}(P|\lambda)$ must satisfy the algebraic conditions, we have a contradiction. We now present a formal proof that applies to an arbitrary space of ontic states.

Proof of Theorem 1. The proof works by showing that in order to reproduce the ABL probabilities, there must exist ontic states λ such that $\text{Pr}(P|\lambda)=\mathbb{P}(P|\psi,\phi)$ for every $P\in\mathscr{P}$. Since $\text{Pr}(P|\lambda)$ must satisfy the algebraic conditions on $\mathscr{P}'$, and there is no extension of $\mathbb{P}(P|\psi,\phi)$ that does so, this is a contradiction, so no measurement noncontextual model is possible.

It suffices to prove this for those $P\in\mathscr{P}$ such that $\mathbb{P}(P|\psi,\phi)=1$, since if $\mathbb{P}(P|\psi,\phi)=0$ then $\mathbb{P}(I-P|\psi,\phi)=1$ and, in the ontological model, we necessarily have $\text{Pr}(P|\lambda)+\text{Pr}(I-P|\lambda)=1$.

We start by reproducing the reasoning that led to eq. (3) at the ontological level. For concreteness, suppose that the post-selection works by making the projective measurement $\{|\phi\rangle\langle\phi|, I-|\phi\rangle\langle\phi|\}$ and selecting the cases where the $|\phi\rangle\langle\phi|$ outcome is obtained. A projective measurement $\{P,I-P\}$ with Lüders-von Neumann update followed by a measurement of $\{|\phi\rangle\langle\phi|, I-|\phi\rangle\langle\phi|\}$ is a method of measuring the POVM $\{E_{P,\phi},E_{P,\bar{\phi}},E_{\bar{P},\phi},E_{\bar{P},\bar{\phi}}\}$, where

$$E_{P,\phi}=P|\phi\rangle\langle\phi|P \qquad E_{P,\bar{\phi}}=P(I-|\phi\rangle\langle\phi|)P \tag{16}$$

$$E_{\bar{P},\phi}=(I-P)|\phi\rangle\langle\phi|(I-P) \qquad E_{\bar{P},\bar{\phi}}=(I-P)(I-|\phi\rangle\langle\phi|)(I-P), \tag{17}$$

so we can calculate the joint probabilities in the ontological model as

$$\mathbb{P}(P,\phi|\psi)=\int_\Lambda \text{Pr}(E_{P,\phi}|\lambda)d\mu(\lambda), \tag{18}$$

[4]It is worth noting that the proof features an additional measurement $\mathscr{C}^\dagger(E_k)$, which does not appear in definition of the paradox. But this is merely a device for getting an operational handle on the measurement-disturbance, and no particular facts about $\mathscr{C}^\dagger(E_k)$ or its representation in the ontological model (other than it's non-negativity) are used.

and the marginal for passing the post-selection as

$$\mathbb{P}(\phi|\psi) = \int_\Lambda \Pr(E_{P,\phi}|\lambda)d\mu(\lambda) + \int_\Lambda \Pr(E_{\bar{P},\phi}|\lambda)d\mu(\lambda), \tag{19}$$

and so the probability for P conditional on both pre- and post-selection is

$$\mathbb{P}(P|\psi,\phi) = \frac{\mathbb{P}(P,\phi|\psi)}{\mathbb{P}(\phi|\psi)} = \frac{\int_\Lambda \Pr(E_{P,\phi}|\lambda)d\mu(\lambda)}{\int_\Lambda \left(\Pr(E_{P,\phi}|\lambda) + \Pr(E_{\bar{P},\phi}|\lambda)\right)d\mu(\lambda)}. \tag{20}$$

Now, if $\mathbb{P}(P|\psi,\phi) = 1$ then eq. (20) implies

$$\Pr(E_{P,\phi}|\lambda) = \Pr(E_{P,\phi}|\lambda) + \Pr(E_{\bar{P},\phi}|\lambda), \tag{21}$$

on a set Ω_P such that $\mu(\Omega_P) = 1$. Let $\Lambda^\phi = \{\lambda \in \Lambda | \Pr(|\phi\rangle\langle\phi||\lambda) = 1\}$. We proceed by coarse-graining $\{E_{P,\phi}, E_{P,\bar{\phi}}, E_{\bar{P},\phi}, E_{\bar{P},\bar{\phi}}\}$ in two different ways, applying eq. (9) each time.

Firstly, since $E_{P,\phi} + E_{\bar{P},\phi} = \mathscr{E}^\dagger(|\phi\rangle\langle\phi|)$, the RHS of eq. (21) equals $\Pr(\mathscr{E}^\dagger(|\phi\rangle\langle\phi|)|\lambda)$, and therefore so does the LHS, $\Pr(E_{P,\phi}|\lambda)$. Hence given that $\Pr(|\phi\rangle\langle\phi||\lambda) = 1$ on $\Omega_P \cap \Lambda^\phi$, by Lemma 2 $\Pr(E_{P,\phi}|\lambda) = \Pr(\mathscr{E}^\dagger(|\phi\rangle\langle\phi|)|\lambda) > 0$ on this set also.

Secondly, $E_{P,\phi} + E_{P,\bar{\phi}} = P$ gives $\Pr(E_{P,\phi}|\lambda) + \Pr(E_{P,\bar{\phi}}|\lambda) = \Pr(P|\lambda)$ and thus $\Pr(P|\lambda) \geq \Pr(E_{P,\phi}|\lambda) > 0$ on $\Omega_P \cap \Lambda^\phi$. By outcome determinism for sharp measurements, in fact $\Pr(P|\lambda) = 1$ on $\Omega_P \cap \Lambda^\phi$.

Repeating this argument for every $P \in \mathscr{P}$ such that $\mathbb{P}(P|\psi,\phi) = 1$, we have that, for every such P, there exists a set $\Omega_P \subseteq \Lambda$ such that $\mu(\Omega_P) = 1$ and $\Pr(P|\lambda) = 1$ on $\Omega_P \cap \Lambda^\phi$.

Finally, notice that outside Λ^ϕ, outcome determinism for sharp measurements gives $\Pr(|\phi\rangle\langle\phi||\lambda) = 0$. By Proposition 1, $|\psi\rangle$ and $|\phi\rangle$ are nonorthogonal, which means that $\mu(\Lambda^\phi) > 0$:

$$0 < |\langle\phi|\psi\rangle|^2 = \int_\Lambda \Pr(|\phi\rangle\langle\phi||\lambda)d\mu(\lambda) = \int_{\Lambda^\phi} d\mu(\lambda) = \mu(\Lambda^\phi). \tag{22}$$

Now, $\Omega = \cap_{P\in\mathscr{P}}\Omega_P$ is also measure one according to μ because it is the intersection of a finite number of measure one sets. Thus $\mu(\Omega \cap \Lambda^\phi) = \mu(\Lambda^\phi) > 0$, in particular $\Omega \cap \Lambda^\phi$ is nonempty. Recall that on this set $\Pr(P|\lambda) = 1$ for $P \in \mathscr{P}$ such that $\mathbb{P}(P|\psi,\phi) = 1$. Since these assignments cannot be extended to $\mathscr{P}'$ without violating the algebraic conditions, this contradicts the assumption that the model is non-contextual. □

4 The connection to weak values

Similar conclusions can be reached for an alternative version of PPS paradoxes based on weak measurements. Without going into details, an observable A can be measured by coupling the system to a continuous variable pointer system via a Hamiltonian $H = gA \otimes p$, where g is the coupling constant, A is the observable to be measured, and p is the momentum of the pointer. If the parameters are chosen such that $gt \ll \Delta x$, where t is the duration of the measurement interaction and Δx is the initial position uncertainty of the pointer, then this is called a “weak measurement”.

If the system is pre- and post-selected, with a weak measurement in the middle, then, to first order in gt, the position distribution of a suitably prepared pointer simply shifts by an amount $gtw(A|\psi,\phi)$, where

$$w(A|\psi,\phi) = \mathrm{Re}\left(\frac{\langle\phi|A|\psi\rangle}{\langle\phi|\psi\rangle}\right), \tag{23}$$

and $w(A|\psi,\phi)$ is called the *weak value* of A. Weak values can lie outside the eigenvalue range of the operator A, in which case they are called *anomalous* weak values.

It is easy to check that the weak values assigned to a partial boolean algebra of projection operators always satisfy the algebraic conditions (ii) and (iii) with $f(P) = w(P|\psi,\phi)$. This is because, unlike the ABL probabilities, the denominator of $w(P|\psi,\phi)$ does not depend on which projector we are measuring. However, anomalous weak values mean that condition (i) is sometimes violated, i.e. $w(P|\psi,\phi)$ can be negative or greater than 1.

It is also easy to verify that if $\mathbb{P}(P|\psi,\phi)$ is 0 or 1 then $w(P|\psi,\phi) = \mathbb{P}(P|\psi,\phi)$ [2]. This means that, whenever there is a logical PPS paradox for $\mathscr{P}$, there is some projector in the partial boolean algebra $\mathscr{P}'$ that has an anomalous weak value. This is because, by definition, there is no extension of the ABL probabilities to $\mathscr{P}'$ that satisfies all of the algebraic conditions, and condition (i) is the only one that can be violated by weak values. Therefore, logical PPS paradoxes will always show up as anomalous weak values in the weak measurement version of the experiment.

For example, in the three-box paradox, we have $w(|1\rangle\langle 1| + |2\rangle\langle 2|\,|\psi,\phi) = 2$ and $w(|3\rangle\langle 3|\,|\psi,\phi) = -1$.

Because weak measurements do not disturb the state of the system to first order in gt, strange behaviour of weak values is often thought to be more puzzling than strange behaviour of ABL probabilities. However, weak values should be interpreted with caution because they are not probabilities, but rather small shifts in the distribution of pointer position. Nonetheless, it has recently been shown [20] that anomalous weak values are proofs of contextuality, Combined with our results above, this means logical PPS paradoxes are proofs of contextuality in both their strong and weak measurement versions.

5 Important features of the paradoxes

Theorem 1 establishes that logical PPS paradoxes are proofs of contextuality. However, classical analogues of violation of the algebraic conditions have been reproduced by classical toy theories [6, 7, 8], which do not appear to be contextual. In light of this, it is worth discussing the additional features of logical PPS paradoxes that are essential to our proof, but do not appear in the toy models.

5.1 The importance of Lüders-von Neumann updates

If we allow more general update rules for the intermediate measurement, then we can obtain similar predictions to a logical PPS paradox, but with orthogonal pre- and post-selection and without contextuality.

For example, consider a qubit pre-selected in the state $|0\rangle$ and post-selected in the state $|1\rangle$. At an intermediate time, we make a projective measurement $\{|+\rangle\langle +|, |-\rangle\langle -|\}$, where $|\pm\rangle \propto |0\rangle \pm |1\rangle$, in one of two different ways.

In the first method, upon obtaining outcome $|+\rangle\langle +|$, we apply the projection postulate as usual, but if the $|-\rangle\langle -|$ outcome is obtained then we reset the system to the $|0\rangle$ state. This is a valid state-update rule, as it corresponds to the quantum instrument[5]

$$\mathscr{E}_+(\rho) = |+\rangle\langle +|\rho|+\rangle\langle +| \qquad \mathscr{E}_-(\rho) = |0\rangle\langle -|\rho|-\rangle\langle 0|. \tag{24}$$

[5]Given a POVM $\{E_j\}$, a quantum instrument is a set of CP maps $\{\mathscr{E}_j\}$ such that $\mathscr{E}_j^\dagger(I) = E_j$ and $\sum_j \mathscr{E}_j$ is trace-preserving. For any such instrument, it is possible to measure the POVM in such a way that the state update rule is $\rho \to \mathscr{E}_j(\rho)/\mathrm{Tr}(E_j\rho)$. See [21] for details.

Clearly, if the post-selection succeeds, then the outcome of the intermediate measurement must have been $|+\rangle\langle+|$, since otherwise the state of the system prior to post-selection would still be orthogonal to $|1\rangle$, so we have $\mathbb{P}(|+\rangle\langle+|\,|\,|0\rangle,\{\mathscr{E}_+,\mathscr{E}_-\},|1\rangle)=1$.

In the second method, we do the opposite, applying the projection postulate on obtaining the $|-\rangle\langle-|$ outcome and resetting the the system to the $|0\rangle$ state otherwise, which corresponds to the instrument

$$\mathscr{E}'_+(\rho)=|0\rangle\langle+|\rho|+\rangle\langle0| \qquad\qquad \mathscr{E}'_-(\rho)=|-\rangle\langle-|\rho|-\rangle\langle-|. \tag{25}$$

By the same reasoning, we can conclude that $\mathbb{P}(|-\rangle\langle-|\,|\,|0\rangle,\{\mathscr{E}'_+,\mathscr{E}'_-\},|1\rangle)=1$.

If we allow ourselves to combine the probabilities for different intermediate measurements in the same way that we did for logical PPS paradoxes, setting $f(|+\rangle\langle+|)=\mathbb{P}(|+\rangle\langle+|\,|\,|0\rangle,\{\mathscr{E}_+,\mathscr{E}_-\},|1\rangle)$ and $f(|-\rangle\langle-|)=\mathbb{P}(|-\rangle\langle-|\,|\,|0\rangle,\{\mathscr{E}'_+,\mathscr{E}'_-\},|1\rangle)$, then this would violate the algebraic conditions. However, this is not a proof of contextuality as it can be easily accounted for by measurement-disturbance in a non-contextual ontological model.

Specifically, it occurs in a suitably modified version of Spekkens' toy theory [22] in which we modify the measurement-disturbance slightly in order to model the "resetting" that occurs for one of the outcomes.

Briefly, the Spekkens' toy bit has four ontic states, which we label 1, 2, 3, 4. The $|0\rangle$ state is modelled by a uniform distribution over 1 and 2, the $|1\rangle$ state by a uniform distribution over 3 and 4, the $|+\rangle$ state by a uniform distribution over 1 and 3, and the $|-\rangle$ state by a uniform distribution over 2 and 4. The post-selection consists of checking whether the ontic state is 3 or 4 and rejecting if it is not.

For a projective measurement of $\{|+\rangle\langle+|,|-\rangle\langle-|\}$ with Lüders-von Neumann update, we output $|+\rangle\langle+|$ if the ontic state is 1 or 3 and then disturb the system by doing nothing with probability $1/2$ and swapping 1 and 3 with probability $1/2$, and we output $|-\rangle\langle-|$ if the ontic state is 2 or 4 and then disturb the system by doing nothing with probability $1/2$ and swapping 2 and 4 with probability $1/2$.

For the modified update rule $\{\mathscr{E}_+,\mathscr{E}_-\}$, the only thing we change is that, upon obtaining the $|-\rangle\langle-|$ outcome, we swap 1 and 2 instead of 2 and 4. Similarly for $\{\mathscr{E}'_+,\mathscr{E}'_-\}$, upon obtaining the $|+\rangle\langle+|$ outcome, we swap 1 and 2 instead of 1 and 3. It is easy to see that this setup predicts the same probabilities as quantum theory. Indeed, when the post-selection succeeds, only the $|+\rangle\langle+|$ outcome can occur when the instrument $\{\mathscr{E}_+,\mathscr{E}_-\}$ is used, as this is the only way the system can end up in 3 or 4 if it starts out in 1 or 2, and similarly only the $|-\rangle\langle-|$ outcome can occur when the instrument $\{\mathscr{E}'_+,\mathscr{E}'_-\}$ is used.

The model just described is very similar to the toy model for logical PPS paradoxes introduced in [7], with the exception that, instead of modifying the measurement-disturbance, the model of [7] eliminates it for the intermediate measurement outcome that is supposed to have probability 0.

What we learn from this is that, in order to imply contextuality, it is not enough to just have a set of predictions for intermediate measurements that violate the algebraic conditions. It is important that the intermediate measurements have Lüders-von Neumann update, because this allows us to infer that the pre- and post-selection must be nonorthogonal, and that the intermediate measurement cannot make the post-selection go from being possible to being impossible. Both of these were needed for the proof of Theorem 1. This explains why, although violations of the algebraic conditions have been found in various toy models, there are no true logical PPS paradoxes in noncontextual theories when we attempt to faithfully model Lüders-von-Neumann updates.

5.2 The importance of 0/1 probabilities

Another important aspect of logical PPS paradoxes is that we demanded that the probabilities of the intermediate measurement outcomes should all be 0 or 1. Dropping this requirement can yield probabilities that violate the algebraic conditions, but nonetheless still have a noncontextual model.

An example of this is the "quantum cheshire cat" [3]. In this experiment, we have a two qubit system which is pre-selected in the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle, \tag{26}$$

and post-selected in the state

$$|\phi\rangle = \frac{1}{\sqrt{2}}(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle). \tag{27}$$

Now, the ABL probabilities satisfy $\mathbb{P}(|1\rangle\langle 1| \otimes I|\psi,\phi) = 0$, but $\mathbb{P}(|1\rangle\langle 1| \otimes |+\rangle\langle +||\psi,\phi) = \mathbb{P}(|1\rangle\langle 1| \otimes |-\rangle\langle -||\psi,\phi) = 1/6$. This is a violation of the algebraic conditions because $|1\rangle\langle 1| \otimes I = |1\rangle\langle 1| \otimes |+\rangle\langle +| + |1\rangle\langle 1| \otimes |-\rangle\langle -|$, so we should have $f(|1\rangle\langle 1| \otimes I) = f(|1\rangle\langle 1| \otimes |+\rangle\langle +|) + f(|1\rangle\langle 1| \otimes |-\rangle\langle -|)$. However, all of the states and measurements in this experiment are correctly modelled by Spekkens' toy theory so, without going into detail, we can conclude that this does not establish contextuality. Thus, the condition that logical PPS paradoxes should involve $0/1$ probabilities is essential. A violation of the algebraic conditions on its own is not enough to establish contextuality.

Interestingly though, the weak measurement version of the quantum cheshire cat does establish contextuality, because it involves anomalous weak values. Since an ABL probability of 0 implies a weak value of zero, we have $w(|1\rangle\langle 1| \otimes I|\psi,\phi) = 0$, but we also find that $w(|1\rangle\langle 1| \otimes |+\rangle\langle +||\psi,\phi) = 1/2$ and $w(|1\rangle\langle 1| \otimes |-\rangle\langle -||\psi,\phi) = -1/2$. These satisfy the condition $w(|1\rangle\langle 1| \otimes I|\psi,\phi) = w(|1\rangle\langle 1| \otimes |+\rangle\langle +||\psi,\phi) + w(|1\rangle\langle 1| \otimes |-\rangle\langle -||\psi,\phi)$, as weak values always do, but the value $-1/2$ lies outside the eigenvalue range of the projector $|1\rangle\langle 1| \otimes |-\rangle\langle -|$, so it is anomalous. It is rather intriguing that an experiment that can be modelled non-contextually in its strong measurement version can nonetheless become contextual when the measurements are weakened. It would be interesting to know if violations of the algebraic conditions for non-0/1 ABL probabilities always imply anomalous weak values in this way.

6 Conclusion

In conclusion, we outline what Theorem 1 tells us about logical pre- and post-selection paradoxes. We follow the three-pronged approach of the conclusions in [20], where broadly similar techniques were used to show that anomalous weak values are also proofs of contextuality.

Firstly, the proof enables a classification of possible interpretations of a logical pre- and post-selection paradox. Suppose that, despite Theorem 1, we demanded an ontological model for, say, the three-box paradox. Then at least one of the requirements of non-contextuality must be violated. It could be the algebraic conditions, i.e. the ball really is in two boxes at once. But it could instead be the outcome determinism of sharp measurements, i.e. there could be no fact about which box the ball is in until the measurement. Finally it could be that the intermediate measurement *always* disturbs the post-selection, in violation of the measurement non-contextuality of the post-selection. Since we view any form of contextuality as a deficiency in the explanation offered by an ontological model, we see no particular reason to privilege one of these possibilities over the others. A sensible option is to reject the ontological models framework entirely, but without a replacement it is impossible to say anything rigorous about what lies behind these paradoxes.

Secondly, the proof suggests that several aspects of these paradoxes are crucial to preventing a compelling classical explanation, despite having received little attention thus far. If the intermediate measurements were not projective, then the pre- and post-selected states need not overlap, and then there would be no reason to think that the post-selection could occur in the absence of a disturbance. There would also be no reason to think that the intermediate measurements were reading out a pre-defined value. If the state update rule for the intermediate measurement was something other than Lüders-von Neumann rule, or Lemma 1 was not a feature of quantum theory, then there would be no reason to think that the intermediate measurement sometimes has no effect on the post-selection.

Finally, the proof helps to identify the issues that would have to be addressed in order to turn a logical pre- and post-selection paradox into an experimental proposal for demonstrating non-classicality (i.e. a proposal that doesn't render the experiment redundant by simply assuming all of quantum theory *a priori*). For example, one would first need an experimental version of the argument from preparation non-contextuality to outcome determinism for sharp measurements, for example by using the predictability of the intermediate measurements on states that overlap with the original preparation [23]. One would need an analysis of how close to the unrealistic 0 and 1 probabilities of the pre- and post-selected values the experiment would have to come. Finally one would need an operational method of testing that the post-selection measurement is the same (to some appropriate level of approximation) whether preceded by an intermediate projective measurement or the mixture of channels in Lemma 1.

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