Supplemental material of "What is nonclassical about uncertainty relations?"

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I. PROOF OF THE NONCONTEXTUAL BOUND

Consider an operational theory and a pair of measurements, denoted X and Z. Denote the real-valued vector representing outcome ± 1 of measurement X (respectively Z) by $\vec{e}_{\pm 1|X}$ (respectively $\vec{e}_{\pm 1|Z}$). For a preparation represented by the real-valued vector $\vec{s}$, the expectation values of X and Z are defined as

$$\begin{aligned}\langle X\rangle_{\vec{s}} &= (\vec{e}_{+1|X} - \vec{e}_{-1|X}) \cdot \vec{s}, \\ \langle Z\rangle_{\vec{s}} &= (\vec{e}_{+1|Z} - \vec{e}_{-1|Z}) \cdot \vec{s}.\end{aligned} \tag{1}$$

The X-predictability and Z-predictability for $\vec{s}$ are then defined as $|\langle X\rangle_{\vec{s}}|$ and $|\langle Z\rangle_{\vec{s}}|$.

Now consider a state $\vec{s}_1$ whose A_1^2-orbit is realizable, in the sense that one can identify states $\vec{s}_2$, $\vec{s}_3$, and $\vec{s}_4$ in the operational theory such that the quadruple satisfies Eqs. (10) and Eq. (11) of the main text. We here show that the assumption that these states and measurements admit of a noncontextual model (and hence satisfy Eq. (9) of the main text) implies that the X-predictability and Z-predictability must satisfy $|\langle X\rangle| + |\langle Z\rangle| \leq 1$ (Eq. (12) of the main text). We also show that this noncontextuality inequality is tight.

If $\vec{\mu}_1, \vec{\mu}_2, \vec{\mu}_3, \vec{\mu}_4$ denote the probability distributions over ontic states associated to the quadruple of operational states $\vec{s}_1, \vec{s}_2, \vec{s}_3, \vec{s}_4$, and $\vec{\xi}_{+1|X}$, $\vec{\xi}_{-1|X}$ (respectively $\vec{\xi}_{+1|Z}, \vec{\xi}_{-1|Z}$) are the conditional probability distributions associated to the +1 and -1 outcomes of the X measurement (respectively the Z measurement), then in an ontological model of these operational states and measurements, the expectation values of X and Z are defined as

$$\begin{aligned}\langle X\rangle &= (\vec{\xi}_{+1|X} - \vec{\xi}_{-1|X}) \cdot \vec{\mu}_1, \\ \langle Z\rangle &= (\vec{\xi}_{+1|Z} - \vec{\xi}_{-1|Z}) \cdot \vec{\mu}_1.\end{aligned} \tag{2}$$

Noting that the condition of equal-predictability counterparts, Eq. (10) of the main text, can equivalently be written as

$$\begin{aligned}&\mathbb{P}(+1|X,\vec{s}_1) = \mathbb{P}(-1|X,\vec{s}_2) = \mathbb{P}(-1|X,\vec{s}_3) = \mathbb{P}(+1|X,\vec{s}_4), \\ &\mathbb{P}(+1|Z,\vec{s}_1) = \mathbb{P}(+1|Z,\vec{s}_2) = \mathbb{P}(-1|Z,\vec{s}_3) = \mathbb{P}(-1|Z,\vec{s}_4),\end{aligned} \tag{3}$$

it follows that the ontological model must satisfy

$$\vec{\xi}_{+1|X} \cdot \vec{\mu}_1 = \vec{\xi}_{-1|X} \cdot \vec{\mu}_2 = \vec{\xi}_{-1|X} \cdot \vec{\mu}_3 = \vec{\xi}_{+1|X} \cdot \vec{\mu}_4, \tag{4}$$

$$\vec{\xi}_{+1|Z} \cdot \vec{\mu}_1 = \vec{\xi}_{+1|Z} \cdot \vec{\mu}_2 = \vec{\xi}_{-1|Z} \cdot \vec{\mu}_3 = \vec{\xi}_{-1|Z} \cdot \vec{\mu}_4. \tag{5}$$

Meanwhile, the operational equivalence condition, Eq. (11) of the main text, together with an instance of the assumption of preparation noncontextuality, Eq.(9) of the main text, implies

$$\frac{1}{2}\vec{\mu}_1 + \frac{1}{2}\vec{\mu}_3 = \frac{1}{2}\vec{\mu}_2 + \frac{1}{2}\vec{\mu}_4. \tag{6}$$

It is this pair of constraints on the ontological model that implies a tradeoff relation between the X-predictability and the Z-predictability.

To derive an upper bound on $|\langle X\rangle_{\vec{s}_1}| + |\langle Z\rangle_{\vec{s}_1}|$ for any state $\vec{s}_1$ satisfying the A_1^2-orbit-realizability condition, it suffices to derive an upper bound on $\langle X\rangle_{\vec{s}_1} + \langle Z\rangle_{\vec{s}_1}$ (without the absolute values). The reason is that

$$\begin{aligned}&|\langle X\rangle_{\vec{s}_1}| + |\langle Z\rangle_{\vec{s}_1}| \\ &\quad = \max\Big\{\langle X\rangle_{\vec{s}_1} + \langle Z\rangle_{\vec{s}_1}, \langle X\rangle_{\vec{s}_1} - \langle Z\rangle_{\vec{s}_1}, \\ &\qquad - \langle X\rangle_{\vec{s}_1} + \langle Z\rangle_{\vec{s}_1}, -\langle X\rangle_{\vec{s}_1} - \langle Z\rangle_{\vec{s}_1}\Big\}.\end{aligned} \tag{7}$$

and this, together with the condition of having equal-predictability counterparts, Eq. (10) of the main text, implies that

$$\begin{aligned}&|\langle X\rangle_{\vec{s}_1}| + |\langle Z\rangle_{\vec{s}_1}| \\ &\quad = \max\Big\{\langle X\rangle_{\vec{s}_1} + \langle Z\rangle_{\vec{s}_1}, \langle X\rangle_{\vec{s}_4} + \langle Z\rangle_{\vec{s}_4}, \\ &\qquad \langle X\rangle_{\vec{s}_2} + \langle Z\rangle_{\vec{s}_2}, \langle X\rangle_{\vec{s}_3} + \langle Z\rangle_{\vec{s}_3}\Big\}. \\ &\quad \leq \max_{\vec{s}}(\langle X\rangle_{\vec{s}} + \langle Z\rangle_{\vec{s}}),\end{aligned} \tag{8}$$

where the maximization in the final expression is over all states satisfying the A_1^2-orbit-realizability condition, so that the final inequality is true by virtue of $\vec{s}_1$, $\vec{s}_2$, $\vec{s}_3$, and $\vec{s}_4$ being included in this set.

From this point onward, the basic structure of the argument follows the logic of Ref. [1]. The scenario involves just two binary-outcome measurements, so we can divide the ontic state space into four regions, corresponding to the four possible pairs of outcomes assigned to

these. Without loss of generality, therefore, we can consider only four ontic states, and the $\vec{\mu}$ and $\vec{\xi}$ vectors can consequently be taken to be vectors in a 4-dimensional real vector space. We adopt the convention that

$$\vec{\xi}_{+1|X} = (0,1,0,1), \tag{9}$$
$$\vec{\xi}_{+1|Z} = (1,1,0,0). \tag{10}$$

Normalization of states implies that $\vec{\xi}_{-1|X} \equiv \vec{u} - \vec{\xi}_{+1|X}$ and $\vec{\xi}_{-1|Z} \equiv \vec{u} - \vec{\xi}_{+1|Z}$, where $\vec{u} = (1,1,1,1)$ is the unit effect.

Note that we are here modelling the measurements using conditional probability distributions that give a deterministic outcome for each ontic state (such a response is said to be 'outcome deterministic' [2]). It was shown in Ref. [1] that this can always be done without loss of generality if there are no nontrivial operational equivalences among the measurement effects, as is the case here. The reason is as follows. The ontic states can be taken to be the convexly extremal points in the polytope of noncontextual assignments to the set of measurement effects. If there are no nontrivial operational equivalences among the measurement effects, however, then there are no constraints arising from noncontextuality and the polytope is simply the set of all logically possible assignments to the set of measurement effects. The convexly extremal elements of this polytope are outcome-deterministic.

Let the probability distribution over ontic states associated to the operational state $\vec{s}_1$ be parameterized as

$$\vec{\mu}_1 = (a,b,c,d), \tag{11}$$

with $a,b,c,d \in [0,1]$. By normalization of probability distributions, these four parameters are constrained by the equality

$$a+b+c+d = 1. \tag{12}$$

The probability distribution over ontic states associated to operational state $\vec{s}_2$ can be parameterized without loss of generality as follows

$$\vec{\mu}_2 = (b+\epsilon, a-\epsilon, d-\epsilon, c+\epsilon), \tag{13}$$

where ϵ is a real parameter satisfying

$$a-1 \le \epsilon \le a, \tag{14}$$
$$-b \le \epsilon \le 1-b, \tag{15}$$
$$-c \le \epsilon \le 1-c, \tag{16}$$
$$d-1 \le \epsilon \le d. \tag{17}$$

The proof that this parametrization is without loss of generality is as follows. Suppose $\vec{\mu}_2 = (b+\epsilon, a+\epsilon', d+\epsilon'', c+\epsilon''')$, which is clearly a generic parametrization. The fact that $\vec{s}_1$ and $\vec{s}_2$ have the same value of $\langle Z\rangle$ implies that $\vec{\mu}_1$ and $\vec{\mu}_2$ have the same sums over the first two components and the same sums over the second two components (via Eqs. (5) and (10)), which implies that $\epsilon' = -\epsilon$ and $\epsilon''' = -\epsilon''$. The fact that $\vec{s}_1$ and $\vec{s}_2$ have opposite values of $\langle X\rangle$ implies that the sum of the first and third components of $\vec{\mu}_2$ must be equal to the sum of the second and fourth components of $\vec{\mu}_1$ (via Eqs. (4) and (9)), which implies that $\epsilon'' = \epsilon$. Finally, the inequalities on ϵ follow from demanding that all of the components of $\vec{\mu}_2$ are valid probabilities.

The probability distribution over ontic states associated to operational state $\vec{s}_3$ can be parameterized without loss of generality as

$$\vec{\mu}_3 = (d-\gamma, c+\gamma, b+\gamma, a-\gamma), \tag{18}$$

where γ is a real parameter satisfying

$$a-1 \le \gamma \le a, \tag{19}$$
$$-b \le \gamma \le 1-b, \tag{20}$$
$$-c \le \gamma \le 1-c, \tag{21}$$
$$d-1 \le \gamma \le d. \tag{22}$$

The proof that this parametrization is without loss of generality is analogous to the case of $\vec{\mu}_2$.

Finally, the probability distribution over ontic states associated to operational state $\vec{s}_4$ can be parameterized without loss of generality as follows

$$\vec{\mu}_4 = (c+\delta, d-\delta, a-\delta, b+\delta), \tag{23}$$

where δ is a real parameter satisfying

$$a-1 \le \delta \le a, \tag{24}$$
$$-b \le \delta \le 1-b, \tag{25}$$
$$-c \le \delta \le 1-c, \tag{26}$$
$$d-1 \le \delta \le d. \tag{27}$$

Again, the proof is analogous to the one above.

We start by noting that this parameterization, together with Eq. (6), implies

$$a+d = b+c+(\epsilon+\gamma+\delta). \tag{28}$$

Combining this constraint with the normalization condition, Eq. (12), we obtain

$$a+d = \frac{1}{2} + \frac{\epsilon+\gamma+\delta}{2} \tag{29}$$
$$b+c = \frac{1}{2} - \frac{\epsilon+\gamma+\delta}{2}. \tag{30}$$

For brevity, we drop the $\vec{s}_1$ subscript from the expectation values of X and Z. Given Eqs (2), (9), (10) and (11), it follows that

$$\langle X\rangle = b+d-a-c,$$
$$\langle Z\rangle = a+b-c-d, \tag{31}$$

which in turn implies that

$$\langle X\rangle + \langle Z\rangle = 2(b-c). \tag{32}$$

We can now evaluate the upper bound on the latter equation,

$$\begin{aligned}\langle X\rangle + \langle Z\rangle =& 2\,(b-c) = 2\,(b+c) - 4c \\ =& 1 - (\epsilon+\gamma+\delta) - 4c \\ \leq& 1 + 3c - 4c = 1 - c \leq 1,\end{aligned} \tag{33}$$

where, in the second line we have used Eq. (30), and in the third line we have used the inequalities (16), (21), and (26) to minimize $(\epsilon+\gamma+\delta)$. This concludes the proof.

The single nonlinear inequality $|\langle X\rangle| + |\langle Z\rangle| \leq 1$ that we have proven can be expressed equivalently as four inequalities on linear combinations of $\langle X\rangle$ and $\langle Z\rangle$, namely,

$$\langle X\rangle + \langle Z\rangle \leq 1, \tag{34a}$$
$$\langle X\rangle - \langle Z\rangle \leq 1, \tag{34b}$$
$$-\langle X\rangle + \langle Z\rangle \leq 1, \tag{34c}$$
$$-\langle X\rangle - \langle Z\rangle \leq 1. \tag{34d}$$

In the space of possible values of $\langle X\rangle$ and $\langle Z\rangle$, these describe a diamond, depicted in Fig. 1.

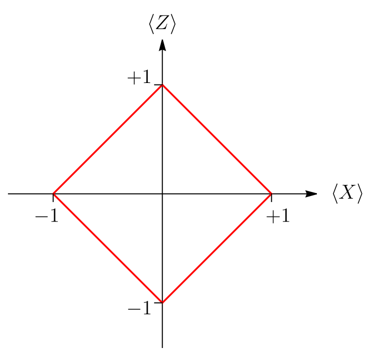

FIG. 1. The noncontextually realizable expectation values of X and Z for states that satisfy the A_1^2-orbit realizability condition.

As an aside, we note that *unlike* the absolute values of expectation values (such as $|\langle X\rangle|$ and $|\langle Z\rangle|$), the expectation values themselves (such as $\langle X\rangle$ and $\langle Z\rangle$) are not measures of predictability. As such, the four inequalities in Eq. (34) do not individually express constraints on predictabilities of measurements. However, one can still view each of these inequalities as a kind of *fine-grained* uncertainty relation, insofar as it expresses constraints on the outcome statistics of a pair of measurements achievable by a single state.[1]

We now turn to demonstrating that the noncontextuality inequality we have derived is tight by exhibiting an example of a noncontextual model that can achieve any point on the bounding curve.

It is clear from the last inequality in Eq. (33) that to saturate this upper bound, we must set $c = 0$. Setting $\epsilon = 0$, $\gamma = 0$ and $\delta = 0$ as well, we can infer that $b = 1/2$ via Eq. (30). In this example, the four probability distributions over ontic states take the following simple form:

$$\vec{\mu}_1 = (1/4+u, 1/2, 0, 1/4-u), \tag{35}$$
$$\vec{\mu}_2 = (1/2, 1/4+u, 1/4-u, 0), \tag{36}$$
$$\vec{\mu}_3 = (1/4-u, 0, 1/2, 1/4+u), \tag{37}$$
$$\vec{\mu}_4 = (0, 1/4-u, 1/4+u, 1/2), \tag{38}$$

where the parameter $u \in [-1/4, 1/4]$ determines how a and d share the probability 1/2 between them. Notice that, with this form of the $\vec{\mu}$s, the expectation values of X and Z take the form $\langle X\rangle = 1-u'$ and $\langle Z\rangle = u'$, for $u' = 1/2 + 2u \in [0,1]$, which means that varying among all the values of u (and so u'), one can achieve any point that saturates the inequality $\langle X\rangle + \langle Z\rangle \leq 1$. By virtue of the A_1^2 symmetry of the problem, one can construct examples that saturate the other inequalities in Eq. (34) as well. We conclude that one can achieve any point saturating the noncontextuality inequality of Eq. (12) in the main text, establishing that the latter is tight.

Fig. 7 depicts some examples of the four distributions of Eqs. (35)-(38) for different values of u', and illustrates the point on the noncontextual bound that each corresponds to.

II. ALTERNATIVE WAY OF OBTAINING THE NONCONTEXTUALITY INEQUALITIES

The complete set of noncontextuality inequalities that hold for two binary-outcome measurements and four preparations that have the operational equivalence relation of Eq. (11) of the main text have been worked out previously in Ref. [1]. This is a relaxation of the problem considered here, since in Ref. [1], the four preparations are not required to satisfy the A_1^2-symmetry condition.

Defining the eight parameters $\mathbb{P}_{ts} \equiv \mathbb{P}(+1|t,s)$, where t labels the measurement setting and s labels the preparation, the noncontextuality inequalities derived in Ref. [1]

[1] One does not need to express uncertainty relations in terms of traditional measures of unpredictability such as variance or entropy. If the probability distributions over the outcomes of two measurements are denoted by vectors $\vec{p}_1$ and $\vec{p}_2$, any tradeoff relation of the form $f(\vec{p}_1,\vec{p}_2) \leq C$ for some function f and constant C can express an uncertainty relation. Examples of this general form of uncertainty relation, where the function f is linear, have been presented, for example, in Ref. [3] under the name of *fine-grained uncertainty relations*.

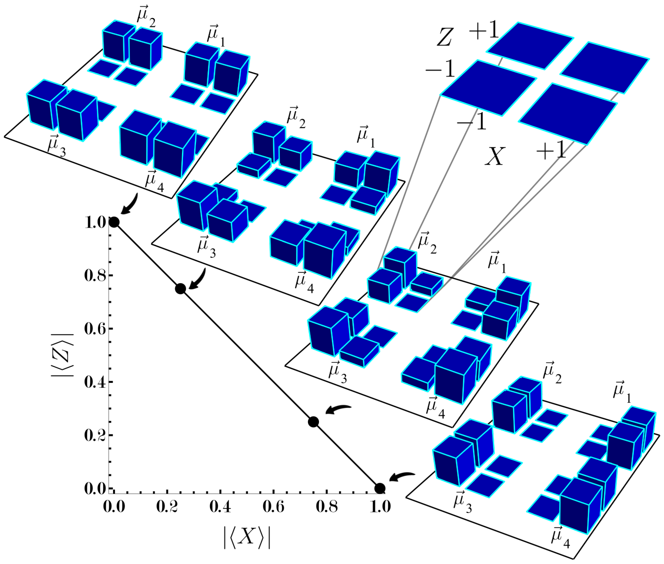

FIG. 2. Four quadruples of probability distributions over ontic states that satisfy the A_1^2-orbit-realizability condition and that saturate the linear tradeoff between the Z-predictability and the X-predictability. Note that the condition that the state has equal-predictability counterparts is manifest in the shapes of these distributions (see the legend regarding the labelling of the ontic states in terms of the X and Z measurement outcomes they predict). Similarly, the operational equivalence of the equal mixture of the two distributions on one diagonal ($\vec{\mu}_1$ and $\vec{\mu}_3$) and the two on the opposite diagonal ($\vec{\mu}_2$ and $\vec{\mu}_4$) is also easily verified by eye.

are:

$$\mathbb{P}_{12} + \mathbb{P}_{22} - \mathbb{P}_{23} - \mathbb{P}_{14} \leq 1\,, \tag{39a}$$
$$\mathbb{P}_{12} + \mathbb{P}_{22} - \mathbb{P}_{13} - \mathbb{P}_{24} \leq 1\,, \tag{39b}$$
$$\mathbb{P}_{22} + \mathbb{P}_{13} - \mathbb{P}_{12} - \mathbb{P}_{24} \leq 1\,, \tag{39c}$$
$$\mathbb{P}_{12} + \mathbb{P}_{23} - \mathbb{P}_{22} - \mathbb{P}_{14} \leq 1\,, \tag{39d}$$
$$\mathbb{P}_{22} + \mathbb{P}_{14} - \mathbb{P}_{12} - \mathbb{P}_{23} \leq 1\,, \tag{39e}$$
$$\mathbb{P}_{23} + \mathbb{P}_{14} - \mathbb{P}_{12} - \mathbb{P}_{22} \leq 1\,, \tag{39f}$$
$$\mathbb{P}_{12} + \mathbb{P}_{24} - \mathbb{P}_{22} - \mathbb{P}_{13} \leq 1\,, \tag{39g}$$
$$\mathbb{P}_{13} + \mathbb{P}_{24} - \mathbb{P}_{12} - \mathbb{P}_{22} \leq 1\,. \tag{39h}$$

Note that probabilities for the $s = 1$ preparation do not appear here. This is because it was possible to eliminate these using the operational equivalence relation, Eq. (11) of the main text. (We note also that the $\mathbb{P}_{12}$ term in the sixth inequality was mistakenly written as $\mathbb{P}_{21}$ in Ref. [1].) Together with the requirement that

$$\forall t, s: \qquad 0 \leq \mathbb{P}_{ts} \leq 1,$$

these fully characterize the polytope of noncontextually realizable correlations.

Associating the measurement setting $t = 1$ to Z and the setting $t = 2$ to X, so that

$$\mathbb{P}_{1s} = \frac{\langle Z\rangle_s + 1}{2}, \qquad \mathbb{P}_{2s} = \frac{\langle X\rangle_s + 1}{2}, \tag{40}$$

we can simplify the noncontextuality inequalities of Eq. (39) using the A_1^2-symmetry condition (Eq. (10) of the main text) and then re-express them in terms of $\langle Z\rangle \equiv \langle Z\rangle_s$ and $\langle X\rangle \equiv \langle X\rangle_s$. Doing so, one finds that the eight linear inequalities of Eq. (39) reduce to the four linear inequalities of Eq. (34), and consequently to the single nonlinear inequality of Eq. (12) of the main text.

III. EXTENSION OF RESULTS TO THE CASE OF THREE MEASUREMENTS

It is useful to consider the generalization of our results to *three* measurements, corresponding in the qubit theory to X, Y and Z Pauli observables. We have already noted that in the qubit theory, there is a nontrivial tradeoff among these, given in Eq. (2) of the main text and termed the quantum XYZ-uncertainty relation. The XYZ-uncertainty relations of our other four foil theories are as follows:

$$\text{qubit stabilizer:}\;\; |\langle X\rangle| + |\langle Y\rangle| + |\langle Z\rangle| \leq 1, \tag{41}$$
$$\eta\text{-depolarized qubit:}\;\; \langle X\rangle^2 + \langle Y\rangle^2 + \langle Z\rangle^2 \leq (1-\eta)^2, \tag{42}$$
$$\text{gbit:}\;\; |\langle X\rangle| \leq 1, |\langle Y\rangle| \leq 1, |\langle Z\rangle| \leq 1 \tag{43}$$
$$\text{simplicial:}\;\; |\langle X\rangle| \leq 1, |\langle Y\rangle| \leq 1, |\langle Z\rangle| \leq 1. \tag{44}$$

These are depicted in Fig. 2(b) of the main text alongside the quantum XYZ-uncertainty relation. Note that the relations for the gbit and simplicial theory again describe a lack of any nontrivial tradeoff, as X, Y and Z can all be made perfectly predictable by a single state.

Following logic analogous to that in the main text, we now study the consequences of noncontextuality for the tradeoff in predictabilities of these three measurements. We begin (as in the main text) by considering the quantum case, and noting that for each state of a qubit, one can find seven other states with the same X-predictability, Y-predictability and Z-predictability and where the eight states cover the 2^3 possible values of $\langle X\rangle$, $\langle Y\rangle$, and $\langle Z\rangle$. Denoting the real-valued vectors representing these eight states (i.e., their Bloch representations) by $\vec{s}_1, \ldots, \vec{s}_8$, this condition can be expressed as

$$\begin{aligned}
&\langle X\rangle_{\vec{s}_1} = \langle X\rangle_{\vec{s}_2} = \langle X\rangle_{\vec{s}_3} = \langle X\rangle_{\vec{s}_4} \\
&= -\langle X\rangle_{\vec{s}_5} = -\langle X\rangle_{\vec{s}_6} = -\langle X\rangle_{\vec{s}_7} = -\langle X\rangle_{\vec{s}_8}, \\
&\langle Y\rangle_{\vec{s}_1} = \langle Y\rangle_{\vec{s}_2} = \langle Y\rangle_{\vec{s}_5} = \langle Y\rangle_{\vec{s}_6} \\
&= -\langle Y\rangle_{\vec{s}_3} = -\langle Y\rangle_{\vec{s}_4} = -\langle Y\rangle_{\vec{s}_7} = -\langle Y\rangle_{\vec{s}_8}, \\
&\langle Z\rangle_{\vec{s}_1} = \langle Z\rangle_{\vec{s}_3} = \langle Z\rangle_{\vec{s}_5} = \langle Z\rangle_{\vec{s}_7} \\
&= -\langle Z\rangle_{\vec{s}_2} = -\langle Z\rangle_{\vec{s}_4} = -\langle Z\rangle_{\vec{s}_6} = -\langle Z\rangle_{\vec{s}_8}.
\end{aligned} \tag{45}$$

Such sets of eight states form a rectangular prism, as depicted in Fig. 3. As they can all be generated by the

orbit of the first state, $\vec{s}_1$, under the symmetry group of a rectangular prism, i.e., the Coxeter group A_1^3, we refer to this condition on the state as the A_1^3-*orbit-realizability condition*.

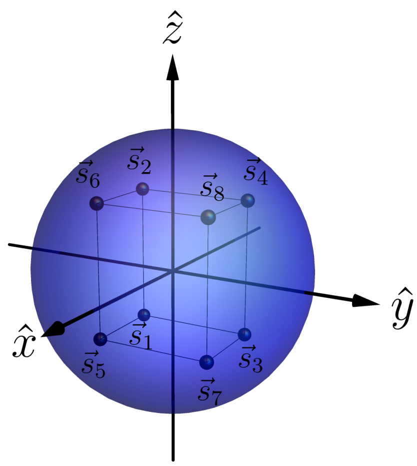

FIG. 3. Depiction of how an arbitrary state $\vec{s}_1$ in qubit quantum theory is part of an octuplet of states that satisfy the A_1^3-orbit-realizability condition.

Any eight such states necessarily satisfy the following operational equivalence relations:

$$\begin{aligned}
\frac{1}{2}\vec{s}_8 + \frac{1}{2}\vec{s}_1 &= \frac{1}{4}\vec{s}_1 + \frac{1}{4}\vec{s}_4 + \frac{1}{4}\vec{s}_6 + \frac{1}{4}\vec{s}_7 \\
\frac{1}{2}\vec{s}_5 + \frac{1}{2}\vec{s}_4 &= \frac{1}{4}\vec{s}_1 + \frac{1}{4}\vec{s}_4 + \frac{1}{4}\vec{s}_6 + \frac{1}{4}\vec{s}_7 \\
\frac{1}{2}\vec{s}_3 + \frac{1}{2}\vec{s}_6 &= \frac{1}{4}\vec{s}_1 + \frac{1}{4}\vec{s}_4 + \frac{1}{4}\vec{s}_6 + \frac{1}{4}\vec{s}_7 \\
\frac{1}{2}\vec{s}_2 + \frac{1}{2}\vec{s}_7 &= \frac{1}{4}\vec{s}_1 + \frac{1}{4}\vec{s}_4 + \frac{1}{4}\vec{s}_6 + \frac{1}{4}\vec{s}_7.
\end{aligned} \tag{46}$$

It is easy to verify geometrically that the four operational equivalence relations in Eq. (46) hold for these eight states, since each simply describes two different ensembles of states for which the ensemble-average is the completely mixed state. Furthermore, one can see that there are no further operational equivalences[2] that are logically independent of these. This is because four of the eight vectors under consideration are linearly independent (e.g., $\vec{s}_1$, $\vec{s}_4$, $\vec{s}_6$, and $\vec{s}_7$, which form the vertices of a regular tetrahedron), and the four operational equivalence relations above simply express the decomposition of the remaining four vectors in terms of these four.

Note that these operational equivalences hold for *any* eight states that are equal-predictability counterparts of one another in the sense of Eq. (45). This is a point of contrast with the situation for a pair of measurements considered in the main text, where the operational equivalence relation of Eq. (11) of the main text did not follow from the mere promise that four states were equal-predictability counterparts of one another (Eq. (10) of the main text), but needed to be imposed as an additional constraint. Thus, while A_1^2-orbit-realizability was defined as the conjunction of Eq. (10) and Eq. (11) of the main text, A_1^3-orbit-realizability is defined simply as the condition of Eq. (45).

As noted earlier, states can be represented by real-valued vectors not just in quantum theory, but in any operational theory. Consequently, the A_1^3-orbit-realizability condition of Eq. (45) can be articulated as a condition on a state in an arbitrary operational theory (relative to any triple of measurements therein).

We can now state the three-measurement analogue of our main result. In any operational theory, if one can find a triple of measurements (which we denote by X, Y, and Z) and a state that satisfies the A_1^3-orbit-realizability condition relative to this triple, then noncontextuality implies a nontrivial constraint on the predictabilities $|\langle X\rangle|$, $|\langle Y\rangle|$ and $|\langle Z\rangle|$ for that state, namely, that they satisfy:

$$|\langle X\rangle| + |\langle Y\rangle| + |\langle Z\rangle| \leq 1. \tag{47}$$

This noncontextuality inequality is the generalization (from two to three measurements) of the noncontextuality inequality of Eq. (12) from the main text. The proof is also exactly analogous, following the logic of Section I. As the quantifier elimination problem becomes much more difficult than in the case of two measurements, we do not provide an analytic proof here. It is straightforward to verify the result using computational algebra. One can also reduce the problem to a linear program in the manner described in Ref. [1] and solve the latter computationally.

Whether an operational theory has A_1^3-symmetry or not, Eq. (47) constrains the tradeoff between X-predictability, Y-predictability, and Z-predictability for any state within the theory that satisfies the A_1^3-orbit-realizability condition. Consequently, if the theory contains one or more such states that *violate* the inequality, this is a proof of the failure of that theory to admit of a noncontextual ontological model. For operational theories that *do* have A_1^3-symmetry, Eq. (47) has further significance. Because in such theories *all states* satisfy the A_1^3-orbit-realizability condition, our bound is a universal constraint on the predictability tradeoff within such theories, that is, it is a constraint on *the form of the* XYZ-*uncertainty relation* within such theories.

The noncontextual bound (Eq. (47)) is compared to the XYZ-uncertainty relation for a qubit (Eq. (2) of the main text) in Fig. 2(b) of the main text, where it is readily seen that there can be quantum violations of the bound. Indeed, only when $|\langle X\rangle| = 1$ or $|\langle Y\rangle| = 1$

[2] More precisely, there are no further operational equivalences in the case where the eight states are all distinct.

or $|\langle Z\rangle| = 1$ does the noncontextual bound intersect the quantum XYZ-uncertainty relation. The maximum quantum violation is achieved when $|\langle X\rangle| = |\langle Y\rangle| = |\langle Z\rangle| = \frac{1}{\sqrt{3}}$ and corresponds to $|\langle X\rangle| + |\langle Y\rangle| + |\langle Z\rangle| = \sqrt{3} \simeq 1.732$. Note that this is a larger relative violation than is possible for the inequality based on two Pauli observables, Eq. (12) of the main text, for which quantum theory achieves $|\langle X\rangle| + |\langle Z\rangle| = \sqrt{2} \simeq 1.414$.

We now compare this noncontextual bound with the XYZ-uncertainty relation of the three foil theories that are in the A_1^3-symmetry class. The XYZ-uncertainty relation for the η-depolarized qubit theory, Eq. (42), satisfies the noncontextual bound if $\eta \leq 1 - \frac{1}{\sqrt{3}} \simeq 0.423$. The uncertainty relation for the qubit stabilizer theory, Eq. (41), has exactly the same form as Eq. (47) and therefore precisely saturates the noncontextual bound. Finally, the uncertainty relation for the gbit theory, Eq. (43), yields the algebraic maximum possible violation of the noncontextual bound, namely, $|\langle X\rangle| + |\langle Y\rangle| + |\langle Z\rangle| = 3$.

By contrast, because the simplicial theory is *not* in the A_1^3-symmetry class, our result does not constrain the form of its XYZ-uncertainty relation. Therefore, although the relation for the simplicial theory (Eq. (44)) is equivalent to that of the gbit theory (Eq. (43)) and thus can violate the inequality of Eq. (13) of the main text, the only states in the theory that achieve this violation (for example, the vertices of the simplex) do not satisfy A_1^3-orbit realizability and therefore the bound is not applicable to them. Meanwhile, all of the states that *do* satisfy the A_1^3-orbit realizability—those inside of the embedded octahedron—satisfy the bound. In short, contextuality is not witnessed in the case of the simplicial theory, consistent with the fact that the latter admits of a noncontextual model.

Finally, note that, just as in the case of the two measurements, the single nonlinear noncontextuality inequality of Eq. (47) can also be expressed as a set of linear inequalities, namely,

$$
\begin{aligned}
\langle X\rangle + \langle Y\rangle + \langle Z\rangle &\leq 1, \\
\langle X\rangle + \langle Y\rangle - \langle Z\rangle &\leq 1, \\
\langle X\rangle - \langle Y\rangle + \langle Z\rangle &\leq 1, \\
\langle X\rangle - \langle Y\rangle - \langle Z\rangle &\leq 1, \\
-\langle X\rangle + \langle Y\rangle + \langle Z\rangle &\leq 1, \\
-\langle X\rangle + \langle Y\rangle - \langle Z\rangle &\leq 1, \\
-\langle X\rangle - \langle Y\rangle + \langle Z\rangle &\leq 1, \\
-\langle X\rangle - \langle Y\rangle - \langle Z\rangle &\leq 1.
\end{aligned}
$$

Again, these inequalities can be considered as bounds on fine-grained uncertainty relations. The space of values of $\langle X\rangle$, $\langle Y\rangle$, and $\langle Z\rangle$ consistent with these inequalities constitutes an octahedron, depicted in Fig. 4, with each inequality describing one of the facets.

It is worth noting that an operational theory with an octahedral state space has previously been derived axiomatically by starting from a classical theory and assuming an epistemic restriction [4, 5]. The results here demonstrate that if one starts with the landscape of possible operational theories for a system with a real-valued vector representation of dimension 4, and one takes as axioms that the state space has A_1^3-symmetry and that one can realize all states consistent with noncontextuality, then one can also derive the octahedral state space. This suggests that it might be worthwhile to try to better understand the starting point of epistemically restricted statistical theories [4–7]—specifically, what is assumed about the form of the ontic state space and the form of the epistemic restriction—from the perspective of what symmetry properties are encoded therein.

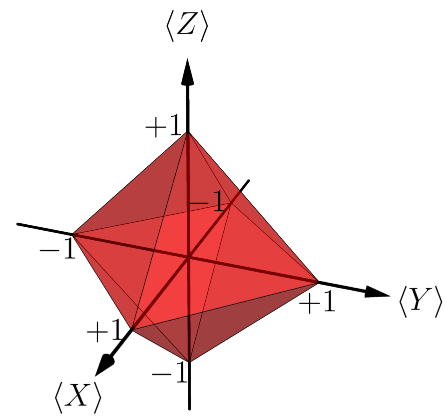

FIG. 4. The noncontextually realizable expectation values of X, Y, and Z for states that satisfy the A_1^3-orbit realizability condition.

IV. UNCERTAINTY RELATIONS FOR A QUBIT

We here describe the strongest uncertainty relation for a qubit and we demonstrate various forms in which it can be expressed.

We denote the ± 1 eigenstates of Pauli observables X, Y and Z as $|\pm x\rangle, |\pm y\rangle, |\pm z\rangle$, respectively. Letting $p_x = \mathrm{Tr}\,(\rho\,|x\rangle\langle x|)$, $p_y = \mathrm{Tr}\,(\rho\,|y\rangle\langle y|)$, $p_z = \mathrm{Tr}\,(\rho\,|z\rangle\langle z|)$, the set of valid quantum states lie inside the Bloch ball, corresponding to the constraint

$$\left(p_x - \frac{1}{2}\right)^2 + \left(p_y - \frac{1}{2}\right)^2 + \left(p_z - \frac{1}{2}\right)^2 \leq \frac{1}{4}. \tag{49}$$

One can also express the constraint defining the Bloch ball in terms of the predictabilities defined in the text, that is, the absolute values of the expectation values of

X, Y and Z. Recalling that

$$\begin{aligned}\langle X\rangle &= \mathrm{Tr}\left[\rho(|{+x}\rangle\langle{+x}| - |{-x}\rangle\langle{-x}|)\right] \\ &= 2p_x - 1,\end{aligned}$$

so that the X-predictability is

$$|\langle X\rangle| = |2p_x - 1|,$$

and similarly for Y and Z, Eq. (49) can be also expressed as

$$\langle X\rangle^2 + \langle Y\rangle^2 + \langle Z\rangle^2 \leq 1, \tag{50}$$

where we do not bother to write the absolute value explicitly when the quantity is squared.

We can also rewrite this in terms of standard deviations or, more precisely, variances. The variance of X, ΔX^2, is related to the expectation value by

$$\begin{aligned}\Delta X^2 &= \langle X^2\rangle - \langle X\rangle^2 \\ &= \langle \mathbb{I}\rangle - \langle X\rangle^2 \\ &= 1 - \langle X\rangle^2,\end{aligned}$$

where we have made use of the identity $X^2 = \mathbb{I}$. The analogous relations hold for Y and Z. Therefore, Eqs. (49) and (50) can also be written as

$$\Delta X^2 + \Delta Y^2 + \Delta Z^2 \geq 2. \tag{51}$$

To our knowledge, this form of the uncertainty relation first appears in Ref. [8], which builds the work of Ref. [9].

We mention one final form of this uncertainty relation. Ref. [8] defines the *certainty* for X, denoted C_x, to be

$$C_x^2 \equiv p_x^2 + (1 - p_x)^2,$$

so that

$$\left(p_x - \frac{1}{2}\right)^2 = \frac{1}{2}C_x^2 - \frac{1}{4}$$

and similarly for Y and Z. It follows that Eqs. (49),(50),(51) can also be expressed as

$$C_x^2 + C_y^2 + C_z^2 \leq 2. \tag{52}$$

The terminology introduced for C_x, C_y and C_z stems from the fact that they measure the degree of certainty about the outcomes of the Pauli measurements, rather than the degree of uncertainty about these. Eq. (52) is termed a "certainty relation" in Ref. [8].

In this article, we have preferred to use the absolute values of the expectation values of Pauli observables, which are related to the certainties by

$$|\langle X\rangle| = \frac{1}{\sqrt{2}}C_x, \tag{53}$$

and similarly for Y and Z, and to refer to these as measures of *predictability*. (Both the certainty and the predictability measures vary inversely to the standard deviations ΔX, ΔY, and ΔZ, which are measures of uncertainty.) Since $\langle X\rangle^2 = |\langle X\rangle|^2$, and similarly for Y and Z, Eq. (50) can be understood as a tradeoff relation between the predictabilities.

Insofar as Eqs. (49)-(52) all describe the Bloch ball, they are the strongest possible uncertainty relation for a qubit. To our knowledge, this uncertainty relation was first presented in Ref. [9]. We refer to it here as the XYZ-uncertainty relation.

Notice that the uncertainty relations above involve the three observables X, Y, Z. However, they imply the uncertainty relations for two observables only, like in the case of the uncertainty relation Eq. (1) that we consider in the main text.

Starting from Eq. (49), the positivity of $\left(p_y - \frac{1}{2}\right)^2$ implies that

$$\left(p_x - \frac{1}{2}\right)^2 + \left(p_z - \frac{1}{2}\right)^2 \leq \frac{1}{4}.$$

This relation is easily shown to be equivalent to

$$\langle X\rangle^2 + \langle Z\rangle^2 \leq 1,$$

and to

$$\Delta X^2 + \Delta Z^2 \geq 1,$$

and to

$$C_x^2 + C_z^2 \leq \frac{3}{2}.$$

The second and third forms are the ones appearing in the main text of the article (see the discussion around Eq. (1) in the main text). To our knowledge, this uncertainty relation for X and Z first appeared in Ref. [8], in the fourth form just described, where it was derived in much the same way as we have done here, starting from the uncertainty relation for three Pauli observables.

Note that the XYZ-uncertainty relation can also be conceptualized as a *state-dependent* ZX-uncertainty relation, namely,

$$\Delta X^2 + \Delta Z^2 \geq 2 - \Delta Y^2. \tag{54}$$

To get back to the state-*independent* ZX-uncertainty relation $\Delta X^2 + \Delta Z^2 \geq 1$, it suffices to minimize the right-hand side under a variation over the state. This occurs when the state is in the plane of the Bloch sphere wherein $\langle Y\rangle = 0$, so that $\Delta Y^2 = 1$. Only in the $\langle Y\rangle = 0$ plane can one saturate the state-independent ZX-uncertainty relation. Outside this plane, one has a tighter bound. Indeed, in the extreme case of an eigenstate of Y, we have $\langle Y\rangle^2 = 1$ and hence $\Delta Y^2 = 0$, so that $\langle X\rangle^2 + \langle Z\rangle^2 \geq 2$. Because each of the terms on the left-hand side are

bounded above by 1, saturating this inequality requires that they both be equal to 1. This simply captures the fact that for an eigenstate of Y, it is indeed the case that $\langle X\rangle = 0$ and $\langle Z\rangle = 0$, and hence that $\Delta X^2 = 1$ and $\Delta Z^2 = 1$.

Suppose one starts with the usual state-dependent uncertainty relation for X and Z, which is of the form

$$\Delta X^2 \Delta Z^2 \geq \langle Y\rangle^2. \tag{55}$$

(This is the form one generally encounters in the textbooks.) To get to an uncertainty relation that is state-independent, it suffices to minimize the right-hand side under a variation over the state. Doing so, we obtain $\Delta X^2 \Delta Z^2 \geq 0$. However, given that ΔX^2 and ΔZ^2 are bounded below by 0, this inequality is trivial. This problem has been pointed out by many authors [10, 11]. By contrast, the state-dependent uncertainty relation of Eq. (54), which involves a *sum* rather than a *product* of the standard deviations *does* yield a nontrivial state-independent uncertainty relation.

Using the *product* of standard deviations was no doubt inspired by the original formulation of uncertainty relations for position and momentum observables by Heisenberg, Kennard, and Robertson [12–14]. Many other ways of expressing the predictability tradeoffs that quantum theory implies have been studied in the literature on the subject [3, 10, 15–22], and many of these have been proposed specifically to solve the problem of the triviality of the implications of the usual form. Note, however, that because the XYZ-uncertainty relation we have described above (Eqs. (49)-(52) are the different forms of it) characterizes the Bloch ball completely, no other uncertainty relation for a qubit can express a more stringent constraint on the probability distributions over outcomes of X, Y and Z measurements.

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