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Uniqueness of Noncontextual Models for Stabilizer Subtheories

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We give a complete characterization of the (non)classicality of all stabilizer subtheories. First, we prove that there is a *unique* nonnegative and diagram-preserving quasiprobability representation of the stabilizer subtheory in all odd dimensions, namely Gross's discrete Wigner function. This representation is equivalent to Spekkens' epistemically restricted toy theory, which is consequently singled out as the unique noncontextual ontological model for the stabilizer subtheory. Strikingly, the principle of noncontextuality is powerful enough (at least in this setting) to single out *one particular* classical realist interpretation. Our result explains the practical utility of Gross's representation by showing that (in the setting of the stabilizer subtheory) negativity in this particular representation implies generalized contextuality. Since negativity of this particular representation is a necessary resource for universal quantum computation in the state injection model, it follows that generalized contextuality is also a necessary resource for universal quantum computation in this model. In all even dimensions, we prove that there does not exist any nonnegative and diagram-preserving quasiprobability representation of the stabilizer subtheory, and, hence, that the stabilizer subtheory is contextual in all even dimensions.

Quantum computers have the potential to outperform classical computers at many tasks. One of the major outstanding problems in quantum computing is to understand what physical resources are necessary and sufficient for universal quantum computation. These resources may depend on one's model of computation [1–3], and in some cases it seems that neither entanglement nor even coherence is required in significant quantities [2].

The primary obstacle to building a quantum computer is that implementing low-noise gates is difficult in practice. While there are no gate sets which are easy to implement and also universal [4], the entire stabilizer subtheory [5, 6] can in fact be implemented in a fault-tolerant manner relatively easily. To promote the stabilizer subtheory to universal quantum computation, one must supplement it with additional nonstabilizer (or 'magic') processes. Because these nonstabilizer resources do not have a straightforward fault-tolerant implementation, they are typically noisy. To get around this problem, Bravyi and Kitaev [7] introduced the magic state distillation scheme, whereby fault-tolerant stabilizer operations are used to distill pure resource states out of the initially noisy resources. However, not every nonstabilizer resource can be distilled in this fashion to generate a state which promotes the stabilizer subtheory to universal quantum computation. It is a major open question to determine which states are in fact sufficient for this purpose.

Quasiprobability representations are a central tool for making progress on these and related problems. For finite-dimensional quantum systems, a number of quasiprobability representations have been studied. For example, Gibbons, Hoffman, and Wootters (GHW) identified a family of representations on a discrete phase space [8], and Gross then singled out one of these with a higher degree of symmetry [9], by virtue of satisfying a property known as "Clifford covariance". All of these have been used to study quantum computation [10–17].

Gross's representation in particular has been the most useful in understanding the resources required for computation. For instance, Ref. [12] extended the Gottesman-Knill theorem [6] by devising an explicit simulation protocol for quantum circuits composed of Clifford gates supplemented with arbitrary states and measurements that have nonnegative Gross's representation. Ref. [12] also proved that every state which is useful for magic state distillation necessarily has negativity in its Gross's representation. In Ref. [14], this result was leveraged to prove that every state that promotes the stabilizer subtheory to universal quantum computation via magic state distillation must also exhibit Kochen-Specker contextuality [18]. In recognition that negativity in Gross's representation is a resource for quantum computation in this sense, Ref. [13] introduced an entire resource theory [19] of Gross's negativity.

From a foundational perspective, it is surprising that any *particular* quasiprobability representation plays such a central role. As argued in Ref. [20], negativity of any one quasiprobability representation is not sufficient to establish nonclassicality in general scenarios. So how can it be that Gross's representation plays such an important role, e.g. that negativity in it is associated to a strong form of nonclassicality, namely computational speedups? Early clues were provided by Gross [9] and by Zhu [21], each of whom proved that Gross's representation was the unique representation with some natural symmetry properties. However, it has previously been unclear what these properties have to do with nonclassicality, and both Gross's and Zhu's arguments

relied on auxiliary mathematical assumptions that were not physically motivated (as we discuss below).

In this paper, we resolve this mystery by showing that the *only* nonnegative and diagram-preserving [22] quasiprobability representation of the stabilizer subtheory in any odd dimension is Gross's. We also prove that in all even dimensions (where Gross's representation is not defined), there is *no* nonnegative and diagram-preserving quasiprobability representation of the stabilizer subtheory. This implies that the stabilizer subtheory exhibits generalized contextuality in all even dimensions.

In the setting of the full stabilizer subtheory, our result for odd dimensions proves that negativity *of this particular* quasiprobability representation is a rigorous signature of nonclassicality, i.e., the failure of generalized noncontextuality. *Generalized noncontextuality* is a principled [23–25], useful [26–38], and operational [39–44] notion of classicality. If one's process has negativity in Gross's representation, then our result establishes that there is no nonnegative representation of the full stabilizer subtheory together with that process. Since nonnegative quasiprobability representations are in one-to-one correspondence with generalized noncontextual ontological models [20, 22, 24], this means that there is no noncontextual representation for the scenario, and hence no classical explanation of it [45].

Our work also extends the body of known connections between contextuality, negativity, and computation [13–16, 46–51]. Using known links between resources for quantum computation and negativity in Gross's representation, together with our result connecting such negativity to the failure of generalized noncontextuality, one can derive connections between resources for quantum computation and generalized noncontextuality.

We illustrate this by giving an analogue of the celebrated result in Ref. [14]: namely, we prove that generalized contextuality is necessary for universal quantum computation in the state injection model.

Finally, we note that our main result demonstrates that the principle of generalized noncontextuality is a much stronger principle than was previously recognized, at least in some settings. This is exemplified by the fact that for stabilizer theories in odd dimensions, it does not merely provide constraints on ontological representations, it *completely fixes* the ontological representation. This offers some hope that if the notion of a generalized noncontextual model can be relaxed in such a way [52] that lifts the obstructions to modelling the entirety of quantum theory, such a model of the full theory might also be unique. In our view such a uniqueness result would offer a compelling reason to take the identified ontology seriously.

The stabilizer subtheory— The stabilizer subtheory is one of the most important subtheories of quantum theory in the field of quantum information, playing an important role in quantum computing [5–7, 14, 53, 54], quantum error correction [5, 6, 55–57], and quantum foundations [58–63]. We introduce it [64] briefly here, with more details in the Supplemental Material (which contains also Refs. [65–70]).

The stabilizer subtheory is built around the Clifford unitaries. To define these, we first introduce the *Weyl operators* (also called generalized Pauli operators). Consider a d-dimensional quantum system with computational basis $\{|0\rangle, \ldots, |d-1\rangle\}$. Writing $\omega = \exp(\frac{2\pi i}{d})$, we define the translation operator X and boost operator Z via

$$X|x\rangle = |x+1\rangle \qquad Z|x\rangle = \omega^x |x\rangle . \tag{1}$$

Note that here and throughout, all arithmetic is within $\mathbb{Z}_d$, the integers modulo d. The single-system Weyl operators are then defined as $W_{p,q} = Z^p X^q$, where $p, q \in \mathbb{Z}_d$. Note that these are often defined with an additional phase factor $\omega^{\gamma_{p,q}}$; however, the resulting operational theory is the same for any valid [49] phase choice, so we will set $\gamma_{p,q}$ to zero. The Clifford unitaries are defined as unitaries which—up to a phase—map Weyl operators to other Weyl operators under conjugation.

The stabilizer subtheory for a single system in dimension d is defined as the set of processes which can be generated by sequential composition of: i) pure states uniquely identified by being the simultaneous eigenstates of a given set of Weyl operators, ii) projective measurements in the spectral decomposition of the Weyl operators [71], and iii) Clifford unitary superoperators on the associated Hilbert space, as well as convex mixtures of such processes.

This construction is easily generalized to allow for parallel composition, that is, for systems made up of n qu*d*its [72], by defining the multiparticle Weyl operators as tensor products of those defined above, and defining the multiparticle Clifford operators as unitary superoperators that preserve the multiparticle Weyl operators under conjugation; see Ref. [9] for more details. An important feature is that in general the stabilizer subtheory defined by parallel composition of n qu*d*its is not the same as the stabilizer subtheory defined by a single d^n dimensional system—for instance, the latter generally has far fewer states [9]. Therefore, for a given dimension D there may be multiple different stabilizer theories which could be associated to it, depending on whether one views it as a single monolithic system of dimension D (which Gross calls the single-particle view), or views it as some tensor product of multiple qu*d*its (which Gross calls a multi-particle view).

Quasiprobability representations— A quasiprobability representation [22, 73, 74] is akin to a mathematical representation of quantum processes as stochastic processes on a sample space, except that the representation may take negative values. For the reasons laid out in Refs. [22, 52], we are only interested in quasiprobability representations that satisfy the

assumption of *diagram preservation* [22, 52]—namely, that the representation commutes with sequential and parallel composition of processes. This assumption is satisfied by most of the useful quasiprobability representations considered in the literature, including the standard (continuous-dimensional) Wigner function and Gross's representation.

The arguments of Ref. [22] imply that every diagram-preserving quasiprobability representation of a full dimensional subtheory [75] of quantum theory can be written as a minimal frame representation [73], i.e. one whose frame elements form a basis, as follows. One first associates to each system a basis $\{F_\lambda\}_\lambda$ for the real vector space of Hermitian operators, where

$$\mathsf{tr}[F_\lambda] = 1. \tag{2}$$

Every basis has a unique dual basis, $\{D_\lambda\}_\lambda$, as proved in the Supplemental Material, where

$$\sum_\lambda D_\lambda = \mathbb{1}, \qquad \mathsf{tr}[D_{\lambda'} F_\lambda] = \delta_{\lambda\lambda'}. \tag{3}$$

In this representation, a completely-positive trace-preserving map [76, 77] $\mathcal{E}$ is represented by a quasistochastic map defined by

$$\xi_{\mathcal{E}}(\lambda'|\lambda) = \mathsf{tr}[D_{\lambda'} \mathcal{E}(F_\lambda)]. \tag{4}$$

As special cases, the representations of a state ρ and an effect E are given by

$$\xi_\rho(\lambda) = \mathsf{tr}[D_\lambda \rho], \qquad \xi_E(\lambda) = \mathsf{tr}[F_\lambda E], \tag{5}$$

and the quantum probabilities are recovered as

$$\mathsf{tr}[E\mathcal{E}(\rho)] = \sum_{\lambda',\lambda} \xi_E(\lambda') \xi_{\mathcal{E}}(\lambda'|\lambda) \xi_\rho(\lambda). \tag{6}$$

A quasiprobability representation is said to be *nonnegative* if for every process $\mathcal{E}$, $0 \leq \xi_{\mathcal{E}}(\lambda'|\lambda) \leq 1$ for every λ, λ'. In this case, the representation is in one-to-one correspondence with a noncontextual ontological model [23, 52].

Gross's representation— The particular quasiprobability representation introduced by Gross [9] is for odd dimensional quantum systems and takes the sample space to be a phase space $V = \mathbb{Z}_d \times \mathbb{Z}_d$, and so its elements will be labelled by $a := (p, q)$, rather than λ. Hence, the basis operators in Gross's representation are indexed by $a \in V$, and we will denote them by A_a.

The basis operators in Gross's representation can be written in terms of the Weyl operators as follows:

$$\{A_a\}_a := \left\{ \frac{1}{d} \sum_b \omega^{-[a,b]} W_b^{G\dagger} \right\}_a, \tag{7}$$

where Gross's Weyl operators $W^G_{p,q}$ are related to ours via $W^G_{p,q} := \omega^{2^{-1}pq} W_{p,q}$. These operators form an orthogonal basis, and so the basis is essentially self-dual, so that both $\{F_\lambda\}$ and $\{D_\lambda\}$ are proportional to $\{A_a\}$, with $D_\lambda = \frac{1}{d} F_\lambda$. They moreover satisfy a number of useful properties (see, e.g., Lemma 29 of Ref. [9]) including a key feature of *translational covariance* [9] where:

$$W_{p',q'} A_{p,q} W^\dagger_{p',q'} = A_{p+p',q+q'} \quad \forall p, q, p', q'. \tag{8}$$

Main result— Our main result is a complete characterization of the (non)classicality of the stabilizer subtheory in every finite dimension.

Theorem 1.

(a) For any stabilizer subtheory (single- or multi-particle) in **odd** *dimensions, the* unique *nonnegative and diagram-preserving quasiprobability representation for it is Gross's representation.*

(b) For any stabilizer subtheory (single- or multi-particle) in **even** *dimensions, there is no nonnegative and diagram-preserving quasiprobability representation.*

The proof is given in the Supplemental Material.

As shown in Ref. [58, 60], Gross's representation is identical to Spekkens' epistemically restricted toy theory [78] for odd dimensions [58]. Through the equivalences between various notions of classicality [22], our result can be stated in a number of ways. Perhaps the most natural equivalent statement of Theorem 1 is the following: For odd dimensions, the unique noncontextual representation of the stabilizer subtheory is Spekkens' epistemically restricted toy theory. For even dimensions, the stabilizer subtheory is contextual.

There are several senses in which our uniqueness result, Theorem 1(a), is stronger than that proven by Gross [9] or that proven by Zhu [21]. Most importantly, the principle of generalized noncontextuality is a well-established notion of classicality, while Gross's notion of Clifford covariance and Zhu's (weaker) notion of Clifford covariance are not. Additionally, our result starts from the very weak assumption of classical realism [52]—that is, the ontological models framework—while Gross's and Zhu's results rely on additional assumptions which have not been given physical motivation. In particular, both Gross's and Zhu's arguments only single out Gross's representation if one assumes that one's representation is on a $d \times d$ phase space, and that it gives the correct marginal probabilities [79]. In our approach, both of these are derived. Finally, our uniqueness result holds in all odd dimensions, while Gross's uniqueness result was proven only for odd prime dimensions, and Zhu's only for prime power dimensions.

Theorem 1(b) establishes that every stabilizer subtheory of even dimension exhibits contextuality. While this result has previously been claimed to be true, it had not in fact been proven (to our knowledge). For

$d = 2$, there are well-known proofs of contextuality, e.g. in Ref. [62]. It follows that every subtheory which contains all the processes in the qubit stabilizer subtheory is also contextual. However, it is not known whether every even-dimensional stabilizer subtheory contains the qubit stabilizer as a subtheory (see Ref. [9]), and so the claim of Theorem 1(b) does not trivially follow in this manner.

Generalized contextuality as a resource for quantum computation— The stabilizer subtheory is efficiently simulable [6]. However, if one supplements it with appropriate nonstabilizer states, one can achieve universal quantum computation through magic state distillation [7].

Any state which promotes the stabilizer subtheory to universal quantum computation must have negativity in its Gross's representation [12]. Ref. [14] further showed that Kochen-Specker contextuality is necessary for universality in this model of quantum computation.

The key argument of Ref. [14] was a graph-theoretic proof that if a state is negative in Gross's representation, then it admits a (state-dependent) proof of Kochen-Specker contextuality using only stabilizer measurements. Our main theorem, Theorem 1, is analogous, establishing that if a state is negative in Gross's representation, then it admits a proof of *generalized* contextuality.

Hence, we immediately arrive at a result akin to that of Ref. [14]: generalized contextuality is necessary for universality in the state injection model of quantum computation.

Theorem 2. *Consider any state ρ which promotes the stabilizer subtheory to universal quantum computation. There is no generalized noncontextual model for the stabilizer subtheory together with ρ.*

We comment in the Supplemental Material on two other routes to proving this theorem.

On the sufficiency of generalized contextuality for universal quantum computation— Thus far we have focused on the necessity of contextuality for quantum computation. However, the fact that Gross's representation provides the unique noncontextual representation of the stabilizer subtheory may also be useful for discovering in what sense (if any) generalized contextuality is *sufficient* for quantum computation.

Without any caveats, generalized contextuality is clearly not sufficient for universal quantum computation. This can be seen by the example of the stabilizer subtheory in dimension 2, which admits proofs of contextuality [62] and yet is efficiently simulable [6].

Still, it is conceivable that there is a more nuanced sufficiency result relating contextuality and computation, e.g. by leveraging quantitative measures of generalized contextuality [80] or by focusing on particular dimensions and models of quantum computation. We now prove a related result (without explicit reliance on Theorem 1).

From Ref. [12, 81], we know that access to enough copies of any nonstabilizer pure state promotes the stabilizer subtheory to universal quantum computation. Similarly, access to enough copies of any nonstabilizer unitary promotes the stabilizer subtheory to universal quantum computation, since the Clifford unitaries together with any other unitary gate forms a universal gate set [82, 83].

It is well known that every pure nonstabilizer state is negatively represented in Gross's representation [9]. Additionally, it is not hard to see that every nonstabilizer unitary gate is negatively represented in Gross's representation. By the universal gate set property [82, 83], combining the positively represented Clifford gates with any given nonstabilizer unitary allows the approximation of any other unitary—including one that maps some pure stabilizer state to some pure nonstabilizer state. Since the stabilizer state is represented positively and the nonstabilizer state must be represented negatively in Gross's representation, the unitary mapping between them must have negativity in its Gross's representation, and hence so must the given nonstabilizer unitary used to construct it. Hence we obtain the following theorem:

Theorem 3. *A (necessary and) sufficient condition for any unitary or pure state to promote the stabilizer subtheory to universal quantum computation is that it be negatively represented in Gross's representation.*

For the case of pure states, this result was pointed out in Refs. [12, 81]. Perhaps the most important open question that remains is whether an analogous sufficiency result holds for mixed states and generic quantum channels.

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[79] Zhu does not actually make the latter assumption, but as a consequence he does not uniquely single out Gross's representation; rather, he single out a family of representations in terms of the so-called Wigner-Wootters bases. But Gross's paper (the last paragraph in the proof of Theorem 23) shows explicitly that this assumption regarding marginal probabilities is exactly what is required to single out Gross's representation from among the Wigner-Wootters representations.

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