Quantum realization of arbitrary joint measurability structures

Ravi Kunjwal*
The Institute of Mathematical Sciences, C.I.T Campus, Tharamani, Chennai 600 113, India

Chris Heunen†
Department of Computer Science, University of Oxford, Oxford, United Kingdom

Tobias Fritz‡
Perimeter Institute for Theoretical Physics, Waterloo, Ontario, Canada

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In many a traditional physics textbook, a quantum measurement is defined as a projective measurement represented by a Hermitian operator. In quantum information theory, however, the concept of a measurement is dealt with in complete generality and we are therefore forced to confront the more general notion of positive-operator valued measures (POVMs), which suffice to describe all measurements that can be implemented in quantum experiments. We study the (in)compatibility of such POVMs and show that quantum theory realizes all possible (in)compatibility relations among sets of POVMs. This is in contrast to the restricted case of projective measurements for which commutativity is essentially equivalent to compatibility. Our result therefore points out a fundamental feature with respect to the (in)compatibility of quantum observables that has no analog in the case of projective measurements.

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I. INTRODUCTION

In the traditional textbook treatment of measurements in quantum theory one usually comes across projective measurements. For these measurements, commutativity of the associated Hermitian operators is necessary and sufficient for them to be compatible. That is, commuting Hermitian operators represent quantum observables that can be jointly measured in a single experimental setup. Furthermore, given a set of N projective measurements, commutativity means pairwise commutativity and we have the following equivalence: pairwise compatibility $\Leftrightarrow$ global compatibility. This equivalence is rather special since it reduces the problem of deciding whether a set of projective measurements is compatible to checking that every pair in the set commutes. Operationally, this also means that the measurement statistics obtained by performing these measurements sequentially on any preparation of a quantum system is independent of the sequence in which the measurements are performed, e.g., if A, B, C are Hermitian operators that commute pairwise, then the sequential measurements ABC, ACB, BAC, BCA, CAB, and CBA are all physically equivalent.

However, once the projective property is relaxed and the resulting positive-operator valued measures (POVMs) are considered, the implication "pairwise compatibility $\Rightarrow$ global compatibility" no longer holds. The converse implication is still true. Indeed, one can construct examples where a set of three POVMs is pairwise compatible but there is no global compatibility between them [1–4]. With this in mind, our purpose in this paper is to explore whether there really is any constraint on the (in)compatibility relations that one could realize between quantum measurements (POVMs). If, for example, certain sets of (in)compatibility relations were not allowed in quantum theory, then that would point out conceivable joint measurability structures that are nevertheless forbidden in nature. A basic understanding of what is allowed and what is forbidden in a physical theory is essential from a foundational point of view. Indeed, an example that readily comes to mind is the impossibility of faster-than-light signaling, a principle that has served as an invaluable guide to ruling out theories—and being highly skeptical of putative phenomena—that may suggest the contrary. Likewise, our larger endeavor in this work is to study the possibilities and limitations of quantum theory with respect to (in)compatibility relations.

It is a fact worth noting that the impossibility of jointly implementing arbitrary sets of measurements is a key ingredient that enables a demonstration of the nonclassicality of quantum theory in proofs of Bell's theorem [5] and the Kochen-Specker theorem [6]. A finite set of measurements is called *jointly measurable* or *compatible* if there exists a single measurement whose various coarse grainings recover the original measurements. The problem of characterizing the joint measurability of observables has been studied in the literature [7,8], and at least the joint measurability of binary qubit observables has been completely characterized [9,10]. The connection between Bell inequality violations and the joint measurability of observables has also been quantitatively studied [11,12].

A natural question that arises when thinking about the (in)compatibility of observables is the following: given a set of (in)compatibility relations on a set of vertices representing observables, do they admit a quantum realization? That is, can one write down a positive-operator valued measure (POVM) for each vertex such that the (in)compatibility relations among the vertices are realized by the assigned POVMs? After formally defining these notions, we answer this question in the affirmative by providing an explicit construction of

*rkunj@imsc.res.in
†heunen@cs.ox.ac.uk
‡tfritz@perimeterinstitute.ca

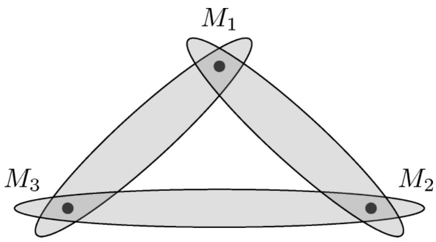

FIG. 1. Specker's scenario.

POVMs for any set of (in)compatibility relations. This is our main result. We will use the terms "(not) jointly measurable" and "(in)compatible" interchangeably in this paper. Part of our motivation in studying this question comes from the simplest example of joint measurability relations realizable with POVMs but not with projective measurements. This joint measurability scenario, referred to as Specker's scenario [1,2,13], involves three binary measurements that can be jointly measured pairwise but not triplewise: that is, for the set of binary measurements $\{M_1,M_2,M_3\}$, the (in)compatibility relations are given by the collection of compatible subsets $\{\{M_1,M_2\},\{M_2,M_3\},\{M_1,M_3\}\}$. The remaining nontrivial subset (with at least two observables), namely $\{M_1,M_2,M_3\}$, is incompatible. This can be pictured as a hypergraph (Fig. 1).

Specker's scenario has been exploited to violate a generalized noncontextuality inequality using a set of three qubit POVMs realizing this scenario [1,2,14]. This demonstration of contextuality in quantum theory raises the question whether there exist other contextuality scenarios—for example, in an observable-based hypergraph approach as in [15,16]—that do not admit a proof of quantum contextuality using projective measurements, but do admit such a proof using POVMs. A necessary first step towards answering this question is to figure out what compatibility scenarios are realizable in quantum theory. One can then ask whether these scenarios allow nontrivial correlations that rule out generalized noncontextuality [14]. We take this first step by proving that, in principle, all joint measurability hypergraphs are realizable in quantum theory. The realizability of all joint measurability graphs via projective measurements has been shown recently [3]. This prompted our question whether all joint measurability hypergraphs are realizable via POVMs. Our positive answer includes joint measurability hypergraphs that do not admit a realization using projective measurements. For our construction, it suffices to consider binary observables on finite-dimensional Hilbert spaces. We start with a more detailed discussion of the relevant concepts.

II. DEFINITIONS

POVMs. A positive-operator valued measure (POVM) on a Hilbert space $\mathcal{H}$ is a mapping $x \mapsto M(x)$ from an outcome set X to the set of positive semidefinite operators,

$$M(x) \in \mathcal{B}(\mathcal{H}), \quad M(x) \geqslant 0,$$

such that the POVM elements $M(x)$ sum to the identity operator,

$$\sum_{x\in X} M(x) = I.$$

If $M(x)^2 = M(x)$ for all $x \in X$, then the POVM becomes a "projection valued measure," or simply a projective measurement.

Joint measurability of POVMs. A finite set of POVMs,

$$\{M_1,\dots,M_N\},$$

where measurement M_i has outcome set X_i, is said to be *jointly measurable* or *compatible* if there exists a POVM M with outcome set $X_1 \times X_2 \times \cdots \times X_N$ that marginalizes to each M_i with outcome set X_i, meaning that

$$M_i(x_i) = \sum_{x_1,\dots,\not{x_i},\dots,x_N} M(x_1,\dots,x_N)$$

for all outcomes $x_i \in X_i$.

Joint measurability hypergraphs. A *hypergraph* consists of a set of vertices V, and a family $E \subseteq \{e \mid e \subseteq V\}$ of subsets of V called *edges*. We think of each vertex as representing a POVM, while an edge models joint measurability of the POVMs it links. Since every subset of a set of compatible measurements should also be compatible, a joint measurability hypergraph should have the property that any subset of an edge is also an edge,

$$e \in E, \quad e' \subseteq e \Rightarrow e' \in E.$$

Additionally, we focus on the case where each edge e is a finite subset of V. This makes a joint measurability hypergraph into an abstract simplicial complex.

Every set of POVMs on $\mathcal{H}$ has such an associated joint measurability hypergraph. Hence characterizing joint measurability of quantum observables comes down to figuring out their joint measurability hypergraph. Our main result solves the converse problem. Namely, every abstract simplicial complex arises from the joint measurability relations of a set of quantum observables.

III. QUANTUM REALIZATION OF ANY JOINT MEASURABILITY STRUCTURE

Theorem. Every joint measurability hypergraph admits a quantum realization with POVMs.

Proof. We begin by proving a necessary and sufficient criterion for the joint measurability of N binary POVMs $M_k := \{E^k_+,E^k_-\}$ of the form

$$E^k_\pm := \tfrac{1}{2}(I \pm \eta\Gamma_k), \tag{1}$$

where the Γ_k are generators of a Clifford algebra as in the Appendix. The variable $\eta \in [0,1]$ is a purity parameter. Since $\Gamma_k^2 = I$, the eigenvalues of Γ_k are ± 1, so that $E^k_\pm$ is indeed positive. The following derivation of a joint measurability criterion is adapted from a proof first obtained in [1], and subsequently revised in [2], for the joint measurability of a set of noisy qubit POVMs. Because Γ_k is traceless by (A3), we can recover the purity parameter η as

$$\mathrm{Tr}(\Gamma_k E^k_\pm) = \pm\frac{\eta}{2}d,$$

so that

$$\eta = \frac{1}{Nd}\sum_{k=1}^{N}\sum_{x_k\in X_k}\mathrm{Tr}\big(x_k\Gamma_k E^k_{x_k}\big), \tag{2}$$

where we have introduced one separate outcome $x_k \in X_k := \{+1, -1\}$ for each measurement M_k.

If all $M_k = \{E_+^k, E_-^k\}$ together are jointly measurable, then there exists a joint POVM $M = \{E_{x_1 \ldots x_N}\}$ satisfying

$$E_{x_k}^k = \sum_{x_1, \ldots, \not{x_k}, \ldots x_N} E_{x_1 \ldots x_N}.$$

Writing $\vec{x} := (x_1, \ldots, x_N)$ and $\vec{\Gamma} := (\Gamma_1, \ldots, \Gamma_N)$, this assumption together with (2) implies that

$$\begin{aligned} \eta &= \frac{1}{Nd} \sum_{\vec{x}} \mathrm{Tr}\left[\left(\sum_{k=1}^{N} x_k \Gamma_k\right) E_{x_1 \ldots x_N}\right], \\ &\leqslant \frac{1}{Nd} \sum_{\vec{x}} \|\vec{x} \cdot \vec{\Gamma}\| \, \mathrm{Tr}[E_{\vec{x}}], \\ &= \frac{1}{N} \|\vec{x} \cdot \vec{\Gamma}\|, \end{aligned}$$

where the last step used the normalization $\sum_{\vec{x}} E_{\vec{x}} = I$. Since $(\vec{x} \cdot \vec{\Gamma})^2 = \sum_k X_k^2 = N \cdot I$ by (A4), we have $\|\vec{x} \cdot \vec{\Gamma}\| = \sqrt{N}$, and therefore

$$\eta \leqslant \frac{1}{\sqrt{N}},$$

a necessary condition for joint measurability of M_k. To show that this condition is also sufficient, we consider the joint POVM $M = \{E_{\vec{x}}\}$ given by

$$E_{x_1 \ldots x_N} := \frac{1}{2^N}(I + \eta \, \vec{x} \cdot \vec{\Gamma}). \tag{3}$$

We start by showing that this indeed defines a POVM,

$$E_{x_1 \ldots x_N} \geqslant 0, \quad \sum_{x_1, \ldots, x_N} E_{x_1 \ldots x_N} = I.$$

Positivity follows again from noting that the eigenvalues of $\vec{x} \cdot \vec{\Gamma}$ are $\pm\sqrt{N}$ by (A4), and normalization from $\sum_{\vec{x}} \vec{x} \cdot \vec{\Gamma} = 0$. Since

$$\sum_{x_1, \ldots, \not{x_k}, \ldots, x_N} E_{x_1 \ldots x_N} = \frac{1}{2}(I + \eta x_k \Gamma_k)$$

coincides with (1), we have indeed found a joint POVM marginalizing to the given M_k.

Thus $\eta \leqslant \frac{1}{\sqrt{N}}$ is a necessary and sufficient condition for the joint measurability of $M_1, \ldots, M_N$.

For arbitrary N, then, we can construct N POVMs on a Hilbert space of appropriate dimension such that any $N-1$ of them are compatible, whereas all N together are incompatible: simply take $M_1, \ldots, M_N$ from (1) for any purity parameter η satisfying

$$\frac{1}{\sqrt{N}} < \eta \leqslant \frac{1}{\sqrt{N-1}}.$$

For example, $\eta = 1/\sqrt{N-1}$ will work. The above reasoning guarantees that all N of them together are not compatible, and also that the $M_1, \ldots, M_{N-1}$ are compatible. By permuting the labels and observing that the above reasoning did not rely on any specific ordering of the Γ_k, we conclude that *any* $N-1$ measurements among the $M_1, \ldots, M_N$ are compatible.

What we have established so far is that, if we are given any N-vertex joint measurability hypergraph where every subset of $N-1$ vertices is compatible (i.e., belongs to a common edge), but the N-vertex set is incompatible, then the above construction provides us with a quantum realization of it. These "Specker-like" hypergraphs are crucial to our construction. For example, for $N=3$, we obtain a simple realization of Specker's scenario (Fig. 1). For $N=2$, we simply obtain a pair of incompatible observables. Given an arbitrary joint measurability hypergraph, the procedure to construct a quantum realization is now the following.

(1) Identify the minimal incompatible sets of vertices in the hypergraph. A minimal incompatible set is an incompatible set of vertices such that any of its proper subsets *is* compatible. In other words, it is a Specker-like hypergraph embedded in the given joint measurability hypergraph.

(2) For each minimal incompatible set, construct a quantum realization as above. Vertices that are outside this minimal incompatible set can be assigned a trivial POVM in which one outcome is deterministic, represented by the identity operator I. Let $\mathcal{H}_i$ denote the Hilbert space on which the minimal incompatible set is realized, where i indexes the minimal incompatible sets.

(3) Having thus obtained a quantum representation of each minimal incompatible set, we simply "stack" these together in a direct sum over the Hilbert spaces on which each of the minimal incompatible sets are realized. On this larger direct sum Hilbert space $\mathcal{H} = \oplus_i \mathcal{H}_i$, we then have a quantum realization of the joint measurability hypergraph we started with.

For any edge $e \in E$, the associated measurements are compatible on every $\mathcal{H}_i$, and therefore also on $\mathcal{H}$. On the other hand, every $e' \subseteq V$ that is not an edge is contained in some minimal incompatible set (or is itself already minimal), and therefore the associated POVMs are incompatible on some $\mathcal{H}_i$, and hence also on $\mathcal{H}$. ■

IV. SIMPLE EXAMPLE

To illustrate these ideas, we construct a POVM realization of a simple joint measurability hypergraph that does not admit a representation with projective measurements (Fig. 2). This hypergraph can be decomposed into three minimal

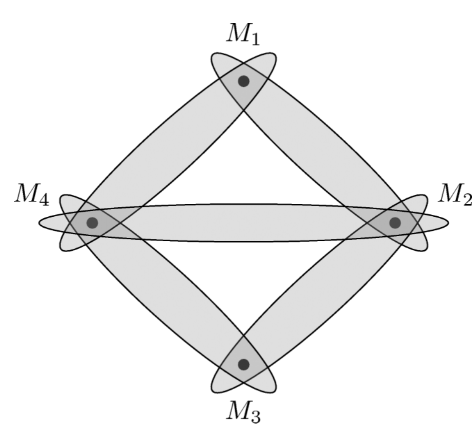

FIG. 2. Joint measurability hypergraph for $N = 4$.

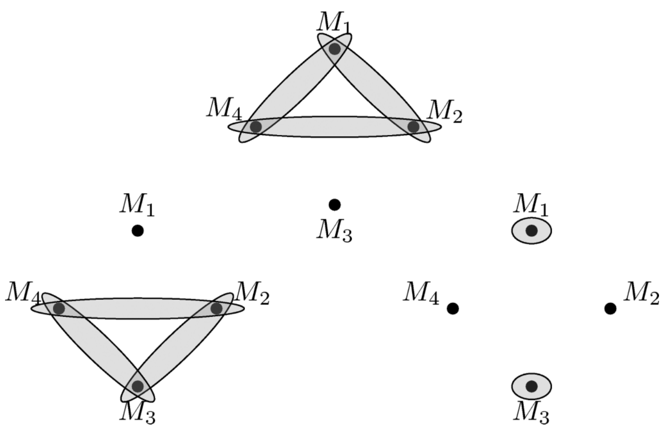

FIG. 3. Minimal incompatible sets for the joint measurability hypergraph in Fig. 2.

incompatible sets of vertices (Fig. 3). Two of these are Specker scenarios for $\{M_1,M_2,M_4\}$ and $\{M_2,M_3,M_4\}$, and the third one is a pair of incompatible vertices $\{M_1,M_3\}$. For the minimal incompatible set $\{M_1,M_2,M_4\}$, we construct a set of three binary POVMs, $A_k \equiv \{A^k_+,A^k_-\}$ with $k \in \{1,2,4\}$ on a qubit Hilbert space $\mathcal{H}_1$ given by

$$A^k_\pm := \frac{1}{2}\left(I \pm \frac{1}{\sqrt{2}}\Gamma_k\right), \tag{4}$$

where the matrices $\{\Gamma_1,\Gamma_2,\Gamma_4\}$ can be taken to be the Pauli matrices,

$$\Gamma_1 = \sigma_z, \quad \Gamma_2 = \sigma_x, \quad \Gamma_4 = \sigma_y,$$

similar to (A2). The remaining vertex M_3 can be taken to be the trivial POVM $A_3 = \{0,I\}$ on $\mathcal{H}_1$. A similar construction works for the second Specker scenario $\{M_2,M_3,M_4\}$ by setting $B_k := \{B^k_+,B^k_-\}$ with $k \in \{2,3,4\}$ to be

$$B^k_\pm := \frac{1}{2}\left(I \pm \frac{1}{\sqrt{2}}\Gamma_k\right), \tag{5}$$

where

$$\Gamma_2 = \sigma_z, \quad \Gamma_3 = \sigma_x, \quad \Gamma_4 = \sigma_y$$

act on another qubit Hilbert space $\mathcal{H}_2$. The remaining vertex M_1 can be assigned the trivial POVM, $B_1 = \{0,I\}$. The third minimal incompatible set $\{M_1,M_3\}$ can similarly be obtained on another qubit Hilbert space $\mathcal{H}_3$ as $C_k := \{C^k_+,C^k_-\}$, with $k \in \{1,3\}$, given by

$$C^k_\pm := \tfrac{1}{2}(I \pm \Gamma_k), \tag{6}$$

where now, e.g., $\Gamma_1 = \sigma_z$ and $\Gamma_3 = \sigma_x$. The remaining vertices M_2 and M_4 can both be assigned the trivial POVM $C_2 = C_4 := \{0,I\}$ on $\mathcal{H}_3$.

In the direct sum Hilbert space $\mathcal{H} := \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3$, we then have a POVM realization of the joint measurability hypergraph of Fig. 2, given by

$$M^k_\pm := A^k_\pm \oplus B^k_\pm \oplus C^k_\pm.$$

V. DISCUSSION

We have shown, by construction, that any conceivable set of (in)compatibility relations for any number of quantum measurements can be realized using a set of binary POVMs. Our result thus demonstrates that quantum theory is not constrained to admit only a restricted set of (in)compatibility relations, such as those where pairwise compatibility ⇔ global compatibility, which is the case with projective measurements. Indeed, quantum theory admits all possible (in)compatibility relations. With respect to (in)compatibility relations, therefore, quantum theory is as far away from classical theories (where there are no incompatibilities) as possible. By "classical theories" we mean those where all measurements commute.

Although our simple construction works for all joint measurability hypergraphs, it is probably not the most efficient one for a given joint measurability hypergraph: for Fig. 2, our representation lives on a six-dimensional Hilbert space. For a joint measurability hypergraph with a fixed number of vertices, the dimension of the Hilbert space $\mathcal{H}$ on which our construction is realized depends on the number of minimal incompatible sets in the hypergraph: that is, $\dim \mathcal{H} = \sum_i \dim \mathcal{H}_i$, where $\mathcal{H}_i$ is the Hilbert space on which the ith minimal incompatible set is realized. It remains open what the most efficient construction—requiring the smallest Hilbert space dimension—for a given joint measurability hypergraph is. Concerning quantum contextuality, in future work we intend to study whether our sets of POVMs can lead to nonclassical correlations in the scenarios associated with the underlying joint measurability hypergraphs. This will open up new avenues for exploiting the nonclassicality of quantum correlations in potential information-theoretic tasks. On the theoretical side, our result also opens the door to the use in quantum contextuality of homology theory, matroid theory, and other powerful combinatorial machinery that relies on hypergraphs, and vice versa. Another potential application of our result could be in situations where the (in)compatibility of observables is a resource for some task: for example, in such scenarios one could require a set of measurements to satisfy a specific set of (in)compatibility relations to be useful for the task at hand and our construction may then offer a way to realize those (in)compatibility relations.

Quite independent of potential applications, our result is of foundational significance for physics since it captures all conceivable (in)compatibility relations within the framework of quantum theory. We have shown that POVMs allow joint measurability structures that have no analog when thinking of projective measurements alone, and in doing so our contribution sheds light on the structure of quantum theory and what it really allows us to do.

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APPENDIX: CLIFFORD ALGEBRAS

A *Clifford algebra* consists of a finite set of Hermitian matrices $\Gamma_1, \ldots, \Gamma_N$ satisfying the relations[1]

$$\Gamma_j \Gamma_k + \Gamma_k \Gamma_j = 2\delta_{jk} I. \tag{A1}$$

Clifford algebras are the mathematical structure behind the definition of spinors and the Dirac equation [17]. They can be constructed recursively as follows [[17], Sec. 16.3]. Given $\Gamma_1, \ldots, \Gamma_N$ living on a Hilbert space $\mathcal{H}_N$, one obtains $\Gamma_1, \ldots, \Gamma_{N+2}$ on $\mathcal{H}_N \otimes \mathbb{C}^2$ by the following rules.

(1) For each $i = 1, \ldots, N$, substitute

$$\Gamma_i \to \Gamma_i \otimes \sigma_z.$$

(2) Further, define

$$\Gamma_{N+1} := I \otimes \sigma_x, \quad \Gamma_{N+2} := I \otimes \sigma_y.$$

It is easy to show that if the original Γ_i satisfy (A1), then so do the new ones. One can simply start the recursion with $\Gamma_1 = 1$ on the one-dimensional Hilbert space $\mathcal{H}_1 := \mathbb{C}$, and then apply the construction as often as necessary to obtain any finite number of matrices satisfying (A1). For example, a single iteration gives the Pauli matrices

$$\Gamma_1 = \sigma_z, \quad \Gamma_2 = \sigma_x, \quad \Gamma_3 = \sigma_y, \tag{A2}$$

while after two iterations one has

$$\Gamma_1 = \sigma_z \otimes \sigma_z, \quad \Gamma_2 = \sigma_x \otimes \sigma_z,$$
$$\Gamma_3 = \sigma_y \otimes \sigma_z, \quad \Gamma_4 = I \otimes \sigma_x, \quad \Gamma_5 = I \otimes \sigma_y.$$

The Clifford algebra relations (A1) have many interesting consequences. For example for $N \geqslant 2$, one has for any k and $j \neq k$,

$$\begin{aligned}\mathrm{Tr}(\Gamma_k) &= \mathrm{Tr}(\Gamma_k \Gamma_j \Gamma_j) = -\mathrm{Tr}(\Gamma_j \Gamma_k \Gamma_j)\\ &= -\mathrm{Tr}(\Gamma_k \Gamma_j \Gamma_j) = -\mathrm{Tr}(\Gamma_k),\end{aligned}$$

so that

$$\mathrm{Tr}(\Gamma_k) = 0. \tag{A3}$$

Another consequence is that

$$\left(\sum_k X_k \Gamma_k\right)^2 = \left(\sum_k X_k^2\right) \cdot I \tag{A4}$$

for arbitrary real coefficients X_k.

[1] Strictly speaking, this is a *representation* of a Clifford algebra, but the difference between algebras and their representations is not relevant here.

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