Characterizing quantum state-space with a single quantum measurement

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Can the state-space of d-dimensional quantum theory be derived from studying the behavior of a single "reference" measuring device? The answer is yes, if the measuring device corresponds to a complex-projective 3-design. In this privileged case, not only does each quantum state correspond to a probability distribution over the outcomes of a single measurement, but also the probability distributions which correspond to quantum states can be elegantly characterized as those which respect a generalized uncertainty principle. The latter takes the form of a lower-bound on the variance of a natural class of observables as measured by the reference. We also give simple equations which pure-state probability distributions must satisfy, and contextualize these results by showing how 3-designs allow the structure-coefficients of the Jordan algebra of observables to be extracted from the probabilities which characterize the reference measurement itself. This lends credence to the view that quantum theory ought to be primarily understood as a set of normative constraints on probability assignments which reflect nature's lack of hidden variables, and further cements the significance of 3-designs in quantum information science.

I. INTRODUCTION

In 1927, Niels Bohr introduced the notion of *complementarity*, that not all aspects of a physical system may be simultaneously definite, as the distinctive feature of the new quantum mechanics [1, 2]. For example, the Heisenberg uncertainty principle, $\sigma_x \sigma_p \geq \frac{1}{2}\hbar$, tells us that if we experiment upon an ensemble of identically prepared particles, then a small variance in the measured position of the particles implies a large variance in their momentum, and vice versa. In particular, regardless of the choice of ensemble, the variance of the two quantities cannot be made arbitrarily small together while remaining consistent with quantum theory. The uncertainty principle may be generalized e.g., to arbitrary pairs of observables, and even to collections of observables [3]. If Bohr was right that complementarity is the defining feature of quantum theory, then it ought to be possible to characterize "quantum states" as nothing other than probability-assignments which satisfy appropriate uncertainty relations for all possible observables.

From this point of view, what is essential is not the traditional Hilbert space formalism, but instead the constraints quantum theory urges on probability-assignments: indeed, the former can be seen as a convenient mathematical technique for imposing those very constraints. But from a contemporary vantage point, there are other techniques available. In particular, while Bohr and Heisenberg focused on relations between observables like position and momentum, contemporary quantum information theory contemplates a more general class of measurements, so-called *informationally-complete* measurements [4]. Remarkably, assigning appropriate probabilities to the outcomes of one single informationally-complete measurement is equivalent to assigning a quantum state. The caveat is that while all quantum states correspond to probability-assignments, not all probability-assignments correspond to quantum states [5]. On the Hilbert space side, such invalid assignments correspond to self-adjoint matrices which are not positive-semidefinite, and thus cannot be regarded as density matrices. In this letter, we demonstrate that for a privileged class of measurements, corresponding to *complex-projective 3-designs*, the set of valid probability-assignments, and so the shape of quantum state-space itself, may be elegantly characterized in terms of an uncertainty principle, precisely in the spirit of Bohr. Specifically, if one considers a natural subset of random variables, the latter defined by assigning numerical values to reference outcomes, the validity of a probability-assignment is equivalent to any such random variable satisfying a particular lower-bound on its variance. Thus probability-assignments to the outcomes of the reference measurement cannot be too sharp. This is so even as those same probability-assignments may imply a sharp distribution for the outcomes of some alternative measurement. This is a dramatic reversal of the situation classically, where any alternative measurement may be regarded as a coarse-graining of a reference measurement e.g., of the positions and momenta of a set of particles. In the classical case, on the one hand, certainty is achievable for the reference; on the other hand, one cannot achieve more certainty about alternative measurements than about the reference. Thus our result underscores in a novel and perspicacious way the degree to which quantum mechanics resists hidden variable interpretations.

We begin by reviewing the probability-first formalism for quantum mechanics furnished by an informationally-complete *reference device*, and then lay out the basic features of complex projective 3-designs. These mathematical preliminaries aside, we derive scalar constraints on probability-assignments corresponding to pure-states: pure-state probability-assignments turn out to live in the intersection of 2-norm and 3-norm spheres of specified

radii restricted to a natural subspace, and operationally these constraints can be interpreted as bounds on the agreement between several copies of the reference measurement when fed identically prepared systems. We then establish a vector constraint on pure-probability assignments, which draws our attention to a particular 3-index tensor built out of the probabilities which characterize the reference measurement itself. We then show more generally that the validity of mixed states is equivalent to the positive-semidefiniteness of a certain matrix, again constructed out of the probabilities which characterize the reference. This leads to the key insight that for a 3-design measurement, one can directly relate the variance of an observable as measured directly to the variance of the observable as measured by the reference, which allows quantum state-space to be characterized by an uncertainty principle. In closing, we observe that the reason 3-designs play such a privileged role is that for just these measurements, the structure-coefficients for the Jordan algebra of observables [6] can be expressed solely in terms of the probabilities which characterize the reference device. The essence of this observation was already made in [7, 8], but its significance for probabilistic representations of quantum mechanics was left unexplored. In fact, 3-designs are of great contemporary interest due to their special role in the theory of classical shadow estimation, where employing a 3-design allows one for example to achieve constant sample complexity in fidelity estimation independent of system size [9–12]. We hope the present work places these developments in a broader context.

II. THE REFERENCE DEVICE FORMALISM

In quantum mechanics, the most general form of a measurement with a finite number of outcomes consists in a set $\{E_i\}_{i=1}^n$ of positive-semidefinite matrices called *effects*, acting on a Hilbert space $\mathcal{H}_d$ satisfying $\sum_i E_i = I$. If the effects span the d^2-dimensional operator space, we call the measurement *informationally-complete*: the probabilities $P(E_i|\rho) = \text{tr}(E_i\rho)$ fully characterize the density matrix ρ representing a quantum state, which must itself be positive-semidefinite with $\text{tr}(\rho) = 1$. We call a measure-and-reprepare device which performs an informationally-complete measurement and conditional on the outcome, prepares one of a set $\{\sigma_i\}_{i=1}^n$ of informationally-complete reference states, a *reference device*. In what follows, we will always assume that our reference device prepares a reference state $\sigma_i = \text{tr}(E_i)^{-1}E_i$ proportional to the reference effect representing the outcome.

The minimal number of effects in an IC-measurement is d^2: moreover, at best an IC-measurement may furnish a linearly-independent, but not orthonormal basis [13], and more generally an informationally-*over*complete set. We must therefore take up the matter of its dual

representation—with a probabilistic twist. Let $|\sigma_i) = \text{vec}(\sigma_i) = (I \otimes \sigma_i)\sum_i |i,i\rangle$ be the vectorization of a reference state σ_i, and similarly let $(E_i| = \sum_i \langle i,i|(I \otimes E_i)$ be the vectorization of a reference effect. In general, $(A|B) = \text{tr}(A^\dagger B)$, and so arranging $(E_i|$ into the rows of a matrix $\mathbf{E}$, and $|\sigma_i)$ into the columns of a matrix $\mathbf{S}$, we can write the conditional-probability matrix with elements $P(E_i|\sigma_j)$, for the probability of a reference outcome given a reference state, $P \equiv \mathbf{ES}$. We call a *Born matrix* any matrix Φ which satifies $P\Phi P = P$, the defining equation of 1-inverse of P [14]. It follows from informational-completeness that $P\Phi P = P \iff \mathbf{S}\Phi\mathbf{E} = I$ [15], which provides a resolution of the identity, and thus a dual representation $|\rho) = \mathbf{S}\Phi\mathbf{E}|\rho)$ or,

$$\rho = \sum_{ij} \Phi_{ij} P(E_j|\rho)\sigma_i. \tag{2.1}$$

If the measurement operators (and states) are linearly independent, then P will be invertible, and thus $\Phi = P^{-1}$. Otherwise, there will be a variety of choices for the Born matrix[1], and different assignments of probabilities will lead to the same ascription of a density matrix.

Consider now some alternative measurement $\{A_i\}_{i=1}^m$. We can write the Born rule probability $P(A_i|\rho) = \text{tr}(A_i\rho)$ in terms of reference probabilities,

$$P(A_i|\rho) = \text{tr}(A_i\rho) = (A_i|\mathbf{S}\Phi\mathbf{E}|\rho) \tag{2.2}$$
$$= \sum_{jk} P(A_i|E_j)\Phi_{jk}P(E_k|\rho),$$

where we have taken $P(A_i|E_j) \equiv P(A_i|\sigma_j)$, using the outcomes of the reference device as a proxy for its state preparations. One may appreciate that the Born rule has become a simple *deformation* [16] of the law of total probability $P(A_i) = \sum_j P(A_i|E_j)P(E_j)$.

In particular, taking $\mathbf{A} = \mathbf{E}$, we have that $P(E_i|\rho) = \sum_{jk} P(E_i|\sigma_j)\Phi_{jk}P(E_k|\rho)$. This is a fundamental consistency-criterion in an overcomplete probability representation. It follows from the defining equation of a 1-inverse that $P\Phi$ is a projector, and in what follows we may take Φ to be invertible, so that $P\Phi$ projects onto $\text{col}(P)$: recall the column-space of P (or equivalently, its range) is the span of its columns. Now $P = \mathbf{ES}$ is in fact a full-rank factorization of P, and hence the columns of $\mathbf{E}$ form a basis for $\text{col}(P)$ [17]. Thus any vector with components $x_i = \text{tr}(E_i X)$, that is, $x = \mathbf{E}|X)$, must lie in $\text{col}(P)$. Conversely, if $x \in \text{col}(P)$, there must exist a vector $\tilde{x}$ such

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[1] The 1-inverses of a matrix $P = U\Sigma V^\dagger$ may all be calculated from its singular value decomposition by $\Phi = V \begin{pmatrix} \sigma^{-1} & A \\ B & C \end{pmatrix} U^\dagger$ where A, B, C are completely arbitrary matrices, and σ is the diagonal matrix of nonzero singular values. A typical example is the Moore-Penrose pseudo-inverse, for which $A = B = C = 0$ [14].

that $x_i = \sum_j P(E_i|\sigma_j)\tilde{x}_j = \text{tr}\left(E_i \sum_j \tilde{x}_j \sigma_j\right) = \text{tr}(E_i\tilde{X})$ for some operator $\tilde{X}$.

III. MAKING DESIGNS

It follows from the representation theory of the unitary and symmetric groups [18, 19] that the *t-th moment of quantum state-space*, that is, the t-th tensor power of a pure-state averaged over all pure-states is

$$\int |\psi\rangle\langle\psi|^{\otimes t} d\psi = \binom{d+t-1}{t}^{-1} \Pi_{\text{sym}^t}, \qquad (3.1)$$

where $d\psi$ denotes the Haar measure on pure-states, and Π_{sym^t} is the projector onto the permutation-symmetric subspace on t tensor-factors [20]. Note $\text{tr}(\Pi_{\text{sym}^t}) = \binom{d+t-1}{t}$ is just the dimension of that subspace. As Π_{sym^t} can be expressed as a sum over all permutation operators, we have in fact

$$\int |\psi\rangle\langle\psi|^{\otimes t} d\psi = \binom{d+t-1}{t}^{-1} \frac{1}{t!} \sum_{\pi \in S_t} T_\pi \qquad (3.2)$$

where $T_\pi = \sum_{a,b,c,\dots} |\pi(a), \pi(b), \pi(c), \dots\rangle\langle a, b, c, \dots|$.

A *quantum t-design*, also called a *complex-projective t-design* [20], is an ensemble of pure-states $\{p_i, |\psi_i\rangle\}_{i=1}^n$ which satisfy

$$\sum_{i=1}^n p_i |\psi_i\rangle\langle\psi_i|^{\otimes t} = \int |\psi\rangle\langle\psi|^{\otimes t} d\psi : \qquad (3.3)$$

the average over the design-ensemble mimics the average over all pure-states up to the t-th moment. Here

$$n \geq \binom{d-1+\lfloor t/2 \rfloor}{\lfloor t/2 \rfloor} \binom{d-1+\lceil t/2 \rceil}{\lceil t/2 \rceil}.$$

We note that a t-design of any order always exists for sufficiently large n [21], and a t-design is also a $(t-1)$-design. For $t = 1$, we have $\sum_i p_i |\psi_i\rangle\langle\psi_i| = \frac{1}{d}I$ which shows that a 1-design furnishes a set of rank-1 projectors which, rescaled, sum to the identity: thus a 1-design is a quantum measurement. For a 2-design

$$\sum_i p_i |\psi_i\rangle\langle\psi_i|^{\otimes 2} = \frac{1}{d(d+1)}(I \otimes I + \mathcal{S}), \qquad (3.4)$$

where $\mathcal{S}$ is the swap operator: two typical examples are symmetric informationally-complete (SIC) states and states corresponding to a complete set of mutually unbiased bases (MUBs) [22]. In fact, it follows from Eq. 3.4 that for any unbiased 2-design reference device, we can take $\Phi = (d+1)I - \frac{d}{n}J$, where J is the Hadamard identity (Appendix A). Here unbiased means that $\forall i : p_i = \frac{1}{n}$. The Born rule then takes the profoundly elegant form

$$P(A|\rho) = \sum_i P(A|E_i)\left[(d+1)P(E_i|\rho) - \frac{d}{n}\right], \quad (3.5)$$

which was given an independent motivation in the case that $n = d^2$ in [23], and is related to the fact that 2-designs are optimal for linear quantum state tomography [24, 25]. The terrain of 3-designs is an area of active investigation: several examples were presented in [26], and more general constructions were given in [27, 28]. In particular, 3-designs have been studied for their use in the theory of classical shadows [9–11]. In $d = 2$, the complete set of MUBs forms a 3-design, as does the set of n-qubit stabilizer states [29]. When $t = 3$, $n \geq \frac{1}{2}d^2(d+1)$, a bound which is not tight [20].

IV. THE SHAPE OF QUANTUM STATE-SPACE

A. Bounding agreement

Suppose we prepare states $\rho_1, \dots, \rho_t$, and send each into its own copy of a reference device $\{E_i, \sigma_i\}_{i=1}^n$. What is the probability that all t reference devices give the same outcome? In other words, consider the agreement-probability

$$P(\text{agree}|\rho_1, \dots, \rho_t) \qquad (4.1)$$
$$= \sum_{i=1}^n \prod_{j=1}^t P(E_i|\rho_j) = \text{tr}\left(\sum_{i=1}^n E_i^{\otimes t} \otimes_{j=1}^t \rho_j\right).$$

Assuming the reference device is unbiased and that the reference states are proportional to effects ($E_i = \frac{d}{n}\sigma_i$), we have $P(\text{agree}|\rho_1, \dots, \rho_t) = \frac{d^t}{n^{t-1}}\text{tr}\left(\frac{1}{n}\sum_{i=1}^n \sigma_i^{\otimes t} \otimes_{j=1}^t \rho_j\right)$. For a t-design, $\frac{1}{n}\sum_i \sigma_i^{\otimes t} = \binom{d+t-1}{t}^{-1}\Pi_{\text{sym}^t}$, and so the agreement-probability can be written

$$P(\text{agree}|\rho_1, \dots, \rho_t) \qquad (4.2)$$
$$= \frac{d^t}{n^{t-1}} \binom{d+t-1}{t}^{-1} \frac{1}{t!} \sum_{\pi \in S_t} \text{tr}(T_\pi \otimes_{j=1}^t \rho_j).$$

To evaluate expressions like this, it suffices to consider traces with cyclic permutations. For $t = 2$, the swap operator $\mathcal{S} = \sum_{ab} |b, a\rangle\langle a, b|$ yields

$$\text{tr}\left((X \otimes Y) \sum_{ab} |b, a\rangle\langle a, b|\right) \qquad (4.3)$$
$$= \sum_{ab} \langle a|X|b\rangle\langle b|Y|a\rangle = \text{tr}(XY),$$

while similarly, for $t = 3$, a cyclic permutation of three elements delivers

$$\text{tr}\left((X \otimes Y \otimes Z) \sum_{abc} |b, c, a\rangle\langle a, b, c|\right) \qquad (4.4)$$
$$= \sum_{abc} \langle a|X|b\rangle\langle b|Y|c\rangle\langle c|Z|a\rangle = \text{tr}(XYZ).$$

In light of this, we have for the order-2 agreement-probability,

$$P(\text{agree}|\rho_1,\rho_2) = \frac{1}{d+1}\left(\frac{d}{n}\right)\left[\text{tr}(\rho_1)\text{tr}(\rho_2) + \text{tr}(\rho_1\rho_2)\right].$$
(4.5)

Now $\text{tr}(\rho_1\rho_2) \leq \sqrt{\text{tr}(\rho_1^2)\text{tr}(\rho_2^2)}$, while the purity satisfies $\text{tr}(\rho^2) \leq 1$. Thus when $\rho_1 = \rho_2 = \rho$ pure, we saturate the upper-bound of this quantity. For the lower-bound, we note $\text{tr}(\rho_1\rho_2) \geq 0$ with equality if and only if ρ_1, ρ_2 are orthogonal, which leads to bounds

$$\left(\frac{d}{n}\right)\frac{1}{d+1} \leq \sum_i P(E_i|\rho_1)P(E_i|\rho_2) \leq \left(\frac{d}{n}\right)\frac{2}{d+1}.$$
(4.6)

Similarly, for $t = 3$, we have

$$P(\text{agree}|\rho_1,\rho_2,\rho_3)$$
(4.7)

$$= \frac{1}{(d+1)(d+2)}\left(\frac{d}{n}\right)^2\left[\text{tr}(\rho_1)\text{tr}(\rho_2)\text{tr}(\rho_3) + \text{tr}(\rho_1)\text{tr}(\rho_2\rho_3)\right.$$

$$\left. + \text{tr}(\rho_2)\text{tr}(\rho_1\rho_3) + \text{tr}(\rho_3)\text{tr}(\rho_1\rho_2) + \text{tr}(\rho_1\rho_2\rho_3) + \text{tr}(\rho_1\rho_3\rho_2)\right],$$

which is maximized when $\rho_1 = \rho_2 = \rho_3 = \rho$ pure, so that $\text{tr}(\rho^2) = \text{tr}(\rho^3) = 1$, and minimized when ρ_1, ρ_2, ρ_3 are mutually orthogonal, delivering bounds

$$\left(\frac{d}{n}\right)^2\frac{1}{(d+1)(d+2)} \leq \sum_i P(E_i|\rho_1)P(E_i|\rho_2)P(E_i|\rho_3)$$

$$\leq \left(\frac{d}{n}\right)^2\frac{6}{(d+1)(d+2)}.$$
(4.8)

Since the upper-bounds are saturated by pure-states, we conclude that pure-state probability assignments with respect to a 3-design lie in the nonnegative orthant, in the intersection of three kinds of spheres. From $\sum_i P(E_i|\rho)$, they live on a 1-norm sphere of radius 1; from $\sum_i P(E_i|\rho)^2$, they live on a 2-norm sphere of radius $\sqrt{\left(\frac{d}{n}\right)\frac{2}{d+1}}$; and from $\sum_i P(E_i|\rho)^3$, they live on a 3-norm sphere of radius $\sqrt[3]{\left(\frac{d}{n}\right)^2\frac{6}{(d+1)(d+2)}}$. Finally, since in our derivation we assumed that all probabilities could be obtained by taking the trace of a reference effect on a state, we must also restrict our probability assignments to those living in $\text{col}(P)$.

We could continue on, contemplating the t-fold agreement-probability for a t-design reference device for any t. Since a pure-state satisfies $\forall t: \text{tr}(\rho^t) = 1$, we'd find that pure probability vectors live on t-norm spheres with fixed radii determined by the agreement-probability

$$P(\text{agree}|\rho^{\otimes t}) = \sum_i P(E_i|\rho)^t = \frac{d^t}{n^{t-1}}\binom{d+t-1}{t}^{-1}.$$
(4.9)

But the following lemma [30, 31] assures us that a 3-design is all we need.

Lemma IV.1. *A Hermitian operator A is a rank-1 projector if and only if $\text{tr}(A^2) = \text{tr}(A^3) = 1$.*

Proof. Let $\{\lambda_i\}$ be the eigenvalues of A. $\text{tr}(A^2) = \text{tr}(A^3) = 1$ means that $\sum_i \lambda_i^2 = \sum_i \lambda_i^3 = 1$. On the one hand, $\sum_i \lambda_i^2 = 1$ implies that $\forall i: -1 \leq \lambda_i \leq 1$. On the other hand, $\sum_i \lambda_i^3 \leq \sum_i \lambda_i^2$ with equality if and only if $\forall i: \lambda_i \in \{0, 1\}$. But since the whole sum must be 1, we must have exactly one $\lambda_i = 1$ and the rest 0. Thus A is a rank-1 projector, or equivalently a pure-state ρ. $\square$

In light of this, as long $t \geq 3$, we can fully characterize the pure-states of quantum theory with respect to an (unbiased) t-design reference device by $\forall i: P(E_i|\rho) \geq 0$ and

$$\sum_i P(E_i|\rho) = 1$$
(4.10)

$$\sum_i P(E_i|\rho)^2 = \left(\frac{d}{n}\right)\frac{2}{d+1}$$
(4.11)

$$\sum_i P(E_i|\rho)^3 = \left(\frac{d}{n}\right)^2\frac{6}{(d+1)(d+2)},$$
(4.12)

along with the consistency-condition required by over-completeness $P(E_i|\rho) = \sum_{jk} P(E_i|\sigma_j)\Phi_{jk}P(E_k|\rho)$. Again, the latter is crucial since in our derivation we have appealed only to probabilities obtained from $P(E_i|\rho) = \text{tr}(E_i\rho)$ (Appendix B). Quantum state-space is then the convex hull of such pure-state probability-assignments.

B. The contour of idempotents

Alternatively, we can derive a single equation picking out pure-state probability-assignments using the fact for a normalized state $\rho = \rho^2$ if and only if ρ is pure. Substiting the resolution of the identity $\rho = \sum_{ij} \Phi_{ij}P(E_j|\rho)\sigma_i$ into $P(E_i|\rho^2) = \text{tr}(E_i\rho^2)$, we find that

$$P(E_i|\rho)$$
(4.13)

$$= \sum_{lm} P(E_l|\rho)P(E_m|\rho)\sum_{jm}\Phi_{jl}\Phi_{km}\Re\left[\text{tr}(E_i\sigma_j\sigma_k)\right].$$

We need only consider the real-part since $\text{tr}(E_i\sigma_k\sigma_j) = \text{tr}(E_i(\sigma_j\sigma_k)^\dagger) = \text{tr}(E_i(\sigma_j^*\sigma_k^*)^T) = \text{tr}(E_i^T\sigma_j^*\sigma_k^*) = \text{tr}(E_i^*\sigma_j^*\sigma_k^*) = \text{tr}(E_i\sigma_j\sigma_k)^*$ as E_i, σ_j, σ_k are all positive-semidefinite: thus every term in Eq. 4.13 is added to its complex conjugate.

Let $\mathcal{M}_t = \int |\psi\rangle\langle\psi|^{\otimes t}d\psi$ be the t-th moment of quantum state-space. This is itself a valid state, and so we can consider its probability distribution $P(E_i, E_j, E_k, \ldots|\mathcal{M}_t)$ with respect to t copies of the reference measurement. If we assume an unbiased set of effects, by the same argument as in Section IV A, it fol-

lows that

$$P(E_i|\mathcal{M}_1) = \frac{1}{n} \tag{4.14}$$

$$P(E_i, E_j|\mathcal{M}_2) = \frac{1}{d+1}\left(\frac{1}{n}\right)\left[\frac{d}{n} + P(E_i|\sigma_j)\right] \tag{4.15}$$

$$P(E_i, E_j, E_k|\mathcal{M}_3) = \frac{1}{(d+1)(d+2)}\left(\frac{d}{n^2}\right) \times \tag{4.16}$$

$$\left[\frac{d}{n} + P(E_j|\sigma_k) + P(E_i|\sigma_j) + P(E_i|\sigma_k) + 2\Re\big[\mathrm{tr}(E_i\sigma_j\sigma_k)\big]\right].$$

If we further assume that the reference states form a 3-design then $\mathcal{M}_3 = \frac{1}{n}\sum_i \sigma_i^{\otimes 3}$ and so $P(E_i, E_j, E_k|\mathcal{M}_3) = \frac{1}{n}\sum_m P(E_i|\sigma_m)P(E_j|\sigma_m)P(E_k|\sigma_m)$, allowing us to calculate $\Re\big[\mathrm{tr}(E_i\sigma_j\sigma_k)\big]$ directly from the conditional probability matrix $P(E_i|\sigma_j)$ for the reference outcomes given the reference states (Appendix C). Then Eq. 4.13, which expresses $\rho = \rho^2$ in terms of probability-assignments, simplifies to

$$P(E_i|\rho) \tag{4.17}$$

$$= \frac{1}{2}\left[\frac{1}{2}(d+1)(d+2)\left(\frac{n}{d}\right)\sum_m P(E_i|\sigma_m)P(E_m|\rho)^2 - \frac{d}{n}\right],$$

which depends only upon $P(E_i|\sigma_j)$ and $P(E_i|\rho)$. Supposing $P(E_i|\rho)$ satisfies Eq. 4.17, it is straightforward to check that $P(E|\rho) \in \mathrm{col}(P)$, and substituting the same into the expressions for $\mathrm{tr}(\rho^2) = \mathrm{tr}(\rho^3) = 1$ shows that the scalar constraints must be satisfied.

C. An uncertainty principle

Finally, we give a condition for the validity of *any* probability-assignment, pure or mixed. We first note that ρ is positive-semidefinite if and only if its second-moment with respect to all Hermitian observables X is nonnegative:

$$\forall X : \mathrm{tr}(X^2\rho) \geq 0 \iff \rho \geq 0. \tag{4.18}$$

Substituting in $X = \sum x_i E_i$ and $\rho = \sum_{ij} \Phi_{ij}P(E_j|\rho)\sigma_i$, we find that

$$\forall x : \mathrm{tr}(X^2\rho) = \tag{4.19}$$

$$\left(\frac{d}{n}\right)\sum_{ijkl} x_i x_j \Re[\mathrm{tr}(E_i\sigma_j\sigma_k)]\Phi_{kl}P(E_l|\rho) \geq 0.$$

This implies that probability-assignments $P(E_i|\rho)$ are valid if and only if the operator $\mathcal{L}[\rho]_{ij} = \sum_{kl}\Re[\mathrm{tr}(E_i\sigma_j\sigma_k)]\Phi_{kl}P(E_l|\rho)$ is positive-semidefinite. The form of this expression assures that this result is insensitive to any redundancy in the $P(E_i|\rho)$'s allowed by overcompleteness. For an unbiased 3-design reference device the expression for $\mathcal{L}[\rho]_{ij}$ simplifies to

$$\mathcal{L}[\rho]_{ij} \tag{4.20}$$

$$= \frac{1}{2}\left[(d+1)(d+2)\left(\frac{n}{d}\right)\sum_m P(E_m|\sigma_i)P(E_m|\sigma_j)P(E_m|\rho)\right.$$

$$\left. - P(E_i|\sigma_j) - P(E_i|\rho) - P(E_j|\rho) - \frac{d}{n}\right],$$

which again depends only upon reference device probabilities. Let us now assume that, in fact, $x \in \mathrm{col}(P)$. In Appendix D, we show that $\mathrm{tr}(X^2\rho)$ then reduces to

$$\mathrm{tr}(X^2\rho) \tag{4.21}$$

$$= \frac{1}{2}\left(\frac{d+2}{d+1}\right)\left[\langle X^2|\rho\rangle - \frac{d}{d+2}\Big(\langle X^2|\mu\rangle - 2\langle X|\mu\rangle\langle X|\rho\rangle\Big)\right],$$

where e.g. $\langle X^2|\rho\rangle = \sum_i x_i^2 P(E_i|\rho)$ and $\forall i : P(E_i|\mu) = \frac{1}{n}$ are the probabilities for the maximally mixed state. Remarkably, this expression relates the second-moment of X with respect to a standard von Neumann measurement to the second-moment of X *with respect to the reference device*, where now the x_i's are interpreted as numerical values assigned to reference measurement outcomes. The restriction that $x \in \mathrm{col}(P)$ (for real x) is equivalent to the assumption that $x_i = \mathrm{tr}(E_i\tilde{X})$ for some Hermitian $\tilde{X}$. Therefore if the RHS of Eq. 4.21 is nonnegative for all real $x \in \mathrm{col}(P)$, it is nonnegative for all Hermitian X. We conclude that probability-assignments $P(E_i|\rho)$ are valid if and only if

$$\forall x \in \mathrm{col}(P) : \tag{4.22}$$

$$\mathrm{Var}[X] \geq \frac{d}{d+2}\Big(\langle X^2|\mu\rangle - 2\langle X|\mu\rangle\langle X|\rho\rangle\Big) - \langle X|\rho\rangle^2,$$

where $\mathrm{Var}[X] = \sum_i x_i^2 P(E_i|\rho) - \left(\sum_i x_i P(E_i|\rho)\right)^2$. Thus the shape of quantum state-space can be understood in terms of an uncertainty principle: valid probability-assignments on reference outcomes cannot be too sharp lest they violate a lower-bound on the variance for any observable in $\mathrm{col}(P)$. We note that a related inequality was derived recently in [12] in the context of bounding the variance of expectation values in shadow estimation.

V. THE JORDAN PRODUCT

To further contextualize our result, we note there is another interpretation of the operator $\mathcal{L}[\rho]$. Recall that under the Jordan product $A \circ B = \frac{1}{2}(AB + BA)$, Hermitian matrices over $\mathbb{C}$ form a *Euclidean Jordan algebra* [6, 32, 33]. A *Jordan algebra* is a nonassociative algebra which satisfies the commutative law and the Jordan identity,

$$A \circ B = B \circ A$$

$$A^2 \circ (B \circ A) = A \circ (B \circ A^2).$$

If we define $L[A]$ to be the linear operator which takes the Jordan product with A, that is, $L[A]B = A \circ B$, the Jordan identity is equivalent to $\big[L[A], L[A^2]\big] = 0$. A *Euclidean* Jordan algebra enjoys the additional property that there exists an inner-product on the underlying vector space $\mathcal{V}$ such that $\forall A, B, C \in \mathcal{V} : \langle L[A]B, C \rangle = \langle B, L[A]C \rangle$.

By introducing an informationally-complete reference device, we identify quantum states with probability distributions. We may then ask: how can we represent the Jordan product in terms of probabilities? If $|\rho \circ \tau) = L[\rho]|\tau)$, using the resolution of the identity $\mathbf{S}\Phi\mathbf{E} = I$, we have

$$\mathbf{E}L[\rho]|\tau) = \mathbf{E}L[\rho]\mathbf{S}\Phi\mathbf{E}|\tau) = \mathcal{L}[\rho]\Phi P(E|\tau), \quad (5.1)$$

where $\mathcal{L}[\rho] = \mathbf{E}L[\rho]\mathbf{S}$, whose matrix-elements are

$$\mathcal{L}[\rho]_{ij} = \text{tr}(E_i L[\rho](\sigma_j)) = \frac{1}{2}\big(\text{tr}(E_i \rho \sigma_j) + \text{tr}(E_i \sigma_j \rho)\big)$$
$$= \sum_{kl} \Re[\text{tr}(E_i \sigma_j \sigma_k)]\Phi_{kl} P(E_l|\rho). \quad (5.2)$$

Indeed, this is precisely the matrix we constructed earlier whose positive-semidefiniteness diagnoses the validity of probability-assignments $P(E_i|\rho)$.

On the one hand, the three-index tensor $\Re[\text{tr}(E_i \sigma_j \sigma_k)]$ encodes the structure-coefficients for the Jordan product, and thus implies the entire shape of quantum state-space. On the other hand, we have shown that the components of this tensor can be extracted from the joint probability distribution $P(E_i, E_j, E_k|\mathcal{M}_3)$. In this way, a state-assignment $\mathcal{M}_3$ is as much a judgement of the Jordan structure-coefficients, and through them the third moment of quantum state-space implies all its higher moments. Finally, taking our reference device to be an unbiased 3-design means that $P(E_i, E_j, E_k|\mathcal{M}_3) = \frac{1}{n}\sum_m P(E_i|\sigma_m)P(E_j|\sigma_m)P(E_k|\sigma_m)$ so that $P(E_i|\sigma_j)$ *alone* is sufficient to characterize the theory.

VI. CONCLUSION

We have thus shown that the shape of quantum state-space can be understood in terms of an uncertainty principle which constrains the probabilities one ought to assign to the outcomes of a 3-design reference device. Practically speaking, the validity of one's probability-assignments can be diagnosed through the positive-semidefiniteness of the matrix $\mathcal{L}[\rho]$; moreover we have provided two alternative, simple characterizations of the pure-states of the theory. Crucially, each term that appears in our equations is grounded in a probability-assignment, and even better, these probabilities refer to the behavior of a single measure-and-reprepare reference device. The possibility of achieving this rests on the delicate interplay between unitary symmetry and the Jordan algebra of observables. The algebraic structure of

quantum theory implies that the 3rd moment of quantum state-space determines them all, and so does a reference measurement furnished by a 3-design. This further vindicates the centrality of 3-designs already suggested by their optimality in classical shadow estimation tasks.

In closing, we observe that our result holds particular significance for the QBist research program in the foundations of quantum mechanics. QBism argues that quantum theory is best understood not as a description of physical reality, but rather as a set of normative guidelines for gambling on the consequences of one's actions in a world undergoing ceaseless creation [4, 34, 35]. Consequently, QBist "reconstructions" of quantum mechanics proceed [36, 37] by motivating the constraints on probability-assignments implied by quantum theory in the same spirit in which de Finetti derived the usual rules of probability theory by contemplating what constraints a gambler ought to place on their different bets in order to prevent a sure loss. The simplicity of our result is very much in the spirit of [32], which suggests that the constraints implied by quantum theory are in some sense the "most symmetrical" compatible with what the author calls "vitality," i.e. the non-existence of a hidden-variable model. Indeed, our result shows that these constraints may be understood as a fundamental expression of complementarity. That said, our derivation presumes a prior knowledge of traditional quantum theory: the significance of our work here is that it exposes the structure that must be aimed for in any future reconstructive effort.

[1] N. Bohr, The quantum postulate and the recent development of atomic theory, Nature **121**, 580 (1928).
[2] J. Baggott, *The Quantum Story: A history in 40 moments* (OUP Oxford, 2011).
[3] J. Hou and K. He, Uncertainty relations for any multi observables, (2016), arXiv:1601.06338 [quant-ph].
[4] C. A. Fuchs and B. C. Stacey, QBism: Quantum Theory as a Hero's Handbook, Proceedings of the International

School of Physics "Enrico Fermi" **197**, 133–202 (2019), arXiv:1612.07308 [quant-ph].

[5] D. M. Appleby, A. Ericsson, and C. A. Fuchs, Properties of QBist State Spaces, Foundations of Physics **41**, 564–579 (2010), arXiv:0910.2750 [quant-ph].

[6] J. Faraut and A. Korányi, *Analysis on Symmetric Cones* (Oxford University Press, 1994).

[7] V. Obst, A. Heimendahl, T. Singal, and D. Gross, Wigner's Theorem for stabilizer states and quantum designs, Journal of Mathematical Physics **65**, 10.1063/5.0222546 (2024), arXiv:2405.17565 [quant-ph].

[8] M. Heinrich and D. Gross, Robustness of Magic and Symmetries of the Stabiliser Polytope, Quantum **3**, 132 (2019).

[9] H.-Y. Huang, R. Kueng, and J. Preskill, Predicting many properties of a quantum system from very few measurements, Nature Physics **16**, 1050–1057 (2020).

[10] C. Mao, C. Yi, and H. Zhu, The Magic in Qudit Shadow Estimation based on the Clifford Group (2024), arXiv:2410.13572 [quant-ph].

[11] M. Kliesch and I. Roth, Theory of Quantum System Certification, PRX Quantum **2**, 10.1103/prxquantum.2.010201 (2021).

[12] D. Chen and H. Zhu, Nonstabilizerness enhances thrifty shadow estimation (2024), arXiv:2410.23977 [quant-ph].

[13] J. B. DeBrota, C. A. Fuchs, and B. C. Stacey, The Varieties of Minimal Tomographically Complete Measurements, International Journal of Quantum Information **19**, 2040005 (2021), arXiv:1812.08762 [quant-ph].

[14] A. Ben-Israel and T. N. E. Greville, *Generalized Inverses*, 2nd ed., CMS Books in Mathematics (Springer, New York, NY, 2003).

[15] M. B. Weiss, Depolarizing reference devices in generalized probabilistic theories (2024), arXiv:2312.12790 [quant-ph].

[16] C. Ferrie, Quasi-probability representations of quantum theory with applications to quantum information science, Reports on Progress in Physics **74**, 116001 (2011).

[17] R. Piziak and P. L. Odell, Full rank factorization of matrices, Mathematics Magazine **72**, 193 (1999).

[18] A. W. Harrow, The Church of the Symmetric Subspace (2013), arXiv:1308.6595 [quant-ph].

[19] D. Bacon, I. L. Chuang, and A. W. Harrow, The Quantum Schur transform: I. Efficient Qudit Circuits (2005), arXiv:quant-ph/0601001 [quant-ph].

[20] S. F. D. Waldron, *An Introduction to Finite Tight Frames* (Springer New York, 2018).

[21] P. Seymour and T. Zaslavsky, Averaging sets: A generalization of mean values and spherical designs, Advances in Mathematics **52**, 213 (1984).

[22] I. Bengtsson and K. Zyczkowski, On discrete structures in finite Hilbert spaces (2017), arXiv:1701.07902 [quant-ph].

[23] J. B. DeBrota, C. A. Fuchs, and B. C. Stacey, Symmetric informationally complete measurements identify the irreducible difference between classical and quantum systems, Physical Review Research **2**, 10.1103/physrevresearch.2.013074 (2020).

[24] A. J. Scott, Tight informationally complete quantum measurements, Journal of Physics A: Mathematical and General **39**, 13507–13530 (2006).

[25] H. Zhu and B.-G. Englert, Quantum state tomography with fully symmetric measurements and product measurements, Physical Review A **84**, 10.1103/physreva.84.022327 (2011).

[26] W. Słomczyński and A. Szymusiak, Morphophoric POVMs, generalised qplexes, and 2-designs, Quantum **4**, 338 (2020).

[27] D. Gross, S. Nezami, and M. Walter, Schur–Weyl Duality for the Clifford Group with Applications: Property Testing, a Robust Hudson Theorem, and de Finetti Representations, Communications in Mathematical Physics **385**, 1325–1393 (2021).

[28] H. Zhu, C. Mao, and C. Yi, Third moments of qudit Clifford orbits and 3-designs based on magic orbits (2024), arXiv:2410.13575 [quant-ph].

[29] H. Zhu, Multiqubit Clifford groups are unitary 3-designs, Physical Review A **96**, 10.1103/physreva.96.062336 (2017).

[30] N. S. Jones and N. Linden, Parts of quantum states, Physical Review A **71**, 10.1103/physreva.71.012324 (2005).

[31] C. A. Fuchs, M. Schlosshauer, and B. C. Stacey, My Struggles with the Block Universe (2015), arXiv:1405.2390 [quant-ph].

[32] B. C. Stacey, Quantum Theory as Symmetry Broken by Vitality (2023), arXiv:1907.02432 [quant-ph].

[33] A. Wilce, A Royal Road to Quantum Theory (or Thereabouts), Entropy **20**, 227 (2018), arXiv:1606.09306 [quant-ph].

[34] C. A. Fuchs, QBism, Where Next?, in *Phenomenology and QBism* (Routledge, 2023) p. 78–143, arXiv:2303.01446 [quant-ph].

[35] J. B. DeBrota, C. A. Fuchs, and R. Schack, Quantum Dynamics Happens Only on Paper: QBism's Account of Decoherence, Phys. Rev. A **110**, 052205 (2024), arXiv:2312.14112 [quant-ph].

[36] J. B. DeBrota, C. A. Fuchs, J. L. Pienaar, and B. C. Stacey, Born's rule as a quantum extension of Bayesian coherence, Physical Review A **104**, 10.1103/physreva.104.022207 (2021).

[37] M. Appleby, C. A. Fuchs, B. C. Stacey, and H. Zhu, Introducing the qplex: a novel arena for quantum theory, The European Physical Journal D **71**, 10.1140/epjd/e2017-80024-y (2017).

Appendix A: Φ for an unweighted 2-design

For a 2-design $\{\sigma_i\}_{i=1}^n$, $\frac{1}{n}\sum_i \sigma_i^{\otimes 2} = \frac{1}{d(d+1)}(I \otimes I + \mathcal{S})$. Taking the partial transpose yields

$$\frac{1}{n}\sum_i \sigma_i \otimes \sigma_i^T = \frac{1}{d(d+1)}\left(I \otimes I + |I)(I|\right). \qquad (A1)$$

For a pure-state σ, $|\sigma)(\sigma| = \sigma \otimes \sigma^T$ where $|\sigma) = \text{vec}(\sigma)$. Letting $E_i = \frac{d}{n}\sigma_i$, we arrive at the resolution of the identity $I = (d+1)\sum_i |\sigma_i)(E_i| - |I)(I|$. Comparing this to $\mathbf{S}\Phi\mathbf{E} = I = \sum_{ij} \Phi_{ij}|\sigma_i)(E_j|$, it follows that we may take $\Phi = (d+1)I - \frac{d}{n}J$, where J is the matrix of all 1's.

Appendix B: Scalar conditions and overcompleteness

Let $\rho = \sum_{ij} \Phi_{ij}P(E_j|\rho)\sigma_i$. Then $\text{tr}(\rho^2) = \frac{n}{d}\sum_{ij} \Phi_{ij}P(E_j|\rho)\sum_{kl} P(E_i|\sigma_k)\Phi_{kl}P(E_l|\rho)$. Decompos-

ing $P(E|\rho) = x + y$, for $x \in \text{col}(P)$ and $y \in \text{col}(P)^\perp$, and using the form of Φ for an unbiased 2-design, we find $\text{tr}(\rho^2) = \frac{n}{d}\left[(d+1)\sum_i x_i^2 - \frac{d}{n}\right]$. Thus if and only if $\sum_i x_i^2 = \left(\frac{d}{n}\right)\frac{2}{d+1}$ does $\text{tr}(\rho^2) = 1$. The result is analogous for $\text{tr}(\rho^3) = 1$

Appendix C: The real-part of the triple-products

$$\Re\big[\text{tr}(E_i\sigma_j\sigma_k)\big] \tag{C1}$$

$$= \frac{1}{2}\Bigg[(d+1)(d+2)\left(\frac{n}{d}\right)\sum_m P(E_i|\sigma_m)P(E_j|\sigma_m)P(E_k|\sigma_m)$$

$$- P(E_j|\sigma_k) - P(E_i|\sigma_j) - P(E_i|\sigma_k) - \frac{d}{n}\Bigg]$$

Appendix D: Simplifying the variance

Let x be an assignment of real numerical values to the outcomes of the reference device. This is equivalent to the assignment of a self-adjoint operator X since $\langle X \rangle = \sum_i x_i P(E_i|\rho) = \text{tr}\left(\sum_i x_i E_i \rho\right) = \text{tr}(X\rho)$, although in an overcomplete representation different choices of x will yield the same operator X. The variance with respect to a standard von Neumann measurement of X

is $\text{Var}[X]_{\text{vn}} = \text{tr}(X^2\rho) - \text{tr}(X\rho)^2$, where $\text{tr}(X^2\rho) = \left(\frac{d}{n}\right)\sum_{ijkl} x_i x_j \Re[\text{tr}(E_i\sigma_j\sigma_k)]\Phi_{kl}P(E_l|\rho)$. Substituting in the expression for $\Re[\text{tr}(E_i\sigma_j\sigma_k)]$ yields

$$\text{tr}(X^2\rho) \tag{D1}$$

$$= \frac{1}{2}\Bigg[(d+1)(d+2)\sum_k\left(\sum_i P(E_k|\sigma_i)x_i\right)^2 P(E_k|\rho)$$

$$- \left(\frac{d}{n}\right)\sum_{ij} x_i P(E_i|\sigma_j)x_j - 2d\langle X|\mu\rangle\langle X|\rho\rangle - d^2\langle X|\mu\rangle^2\Bigg],$$

Let us assume that $x \in \text{col}(P)$ so that $x_i = \text{tr}(E_i\tilde{X})$ for some Hermitian $\tilde{X}$. By the 2-design property, $\sum_j P(E_i|\sigma_j)\text{tr}(\tilde{X}\sigma_j) = n\text{tr}\left(\frac{1}{n}\sum_j \sigma_j^{\otimes 2}(E_i \otimes \tilde{X})\right) = \frac{n}{d(d+1)}\text{tr}\big((I+\mathcal{S})(E_i \otimes \tilde{X})\big) = \frac{1}{d+1}\big(\text{tr}(\tilde{X}) + \text{tr}(\tilde{X}\sigma_i)\big)$, so that in particular,

$$\sum_j P(E_i|\sigma_j)x_j = \frac{d\langle X|\mu\rangle + x_i}{d+1} \tag{D2}$$

$$\left(\sum_j P(E_i|\sigma_j)x_j\right)^2 = \frac{d^2\langle X|\mu\rangle^2 + 2d\langle X|\mu\rangle x_i + x_i^2}{(d+1)^2} \tag{D3}$$

$$\sum_{ij} x_i P(E_i|\sigma_j)x_j = \frac{n\big(d\langle X|\mu\rangle^2 + \langle X^2|\mu\rangle\big)}{d+1}. \tag{D4}$$

Substituting these expressions into Eq. D1 yields Eq. 4.21.