

Classification of Kirkwood-Dirac positivity-preserving unitaries

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Kirkwood-Dirac (KD) quasiprobability distributions are increasingly used across quantum information science, yet their computational significance remains unclear. We classify unitary dynamics that preserve KD positivity and connect this structure to classical simulation. In contrast with the discrete Wigner setting, we show that KD positivity preservation, stochastic evolution of quasiprobabilities, and preservation of total nonpositivity do not coincide. We identify three classes of positivity-preserving unitaries: type I gates, which are exactly the KD-stochastic unitaries; type II gates, which are nonstochastic yet preserve total nonpositivity by permuting and conjugating KD entries; and, for Fourier-conjugate bases in dimension $d = pq$, type III gates, which preserve KD positivity but can change the total nonpositivity of nonreal distributions. The classification is complete for Haar-random bases and for Fourier-conjugate dimensions $d = p^k$ and $d = pq$, with p, q distinct primes. Adapting the sampling algorithm of Pashayan *et al.* [Phys. Rev. Lett. **115**, 070501 (2015)], we simulate all of these positivity-preserving circuits efficiently on KD-positive inputs; type III gates, however, create a sharp distinction between real inputs, which remain efficiently simulable, and nonreal inputs, whose sampling overhead can grow exponentially. Consequently, for $d = pq$ no resource theory can both treat the KD total nonpositivity as a monotone and admit every efficiently simulable positivity-preserving unitary as a free operation.

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I. INTRODUCTION

Demarcation between quantum and classical computational power is a central theme of quantum information science. Given the ability to implement a fixed set of quantum gates on an input state, whether the resulting circuit is powerful is typically understood in terms of its classical simulation complexity. The most famous example of this is the stabilizer formalism, which provides an efficient simulation scheme for Clifford circuits on stabilizer states that becomes inefficient upon introduction of additional nonstabilizer resources [1]. Concurrently, phase-space formulations of quantum mechanics have sought to identify nonclassical phenomena in terms of nonpositivity in quasiprobability distributions [2–4]. In his seminal paper, Gross [5] showed that stabilizer states form the only pure states with positive Wigner quasiprobability distributions, and that Clifford gates exhaust the set of positivity-preserving unitary evolutions. As a result, the discrete Wigner distribution gained a new operational interpretation and has become a popular tool for theorists seeking to understand when a quantum system achieves computational advantage [4,6–14]. As the Clifford gates rarely constitute natively implementable operations in quantum hardware, other

models of computation with sharp classical-quantum boundaries have been proposed [15–17]. A promising candidate for phase-space formulations of non-Clifford computation is the Kirkwood-Dirac (KD) distribution [18,19], which offers great flexibility for describing experimental state preparation and measurement in arbitrary reference bases [20]. The utility of the KD distribution for finite-dimensional systems has led to its revival, with successful applications to quantum metrology [21–26], thermodynamics [27–32], and the foundations of quantum mechanics [33–37] (see Ref. [38] for a comprehensive review). However, the KD distribution has received little attention in the context of quantum computation, where KD positivity lacks an operational meaning in terms of efficient classical simulability. A natural question is also whether this distribution can resolve issues faced by the Wigner distribution in even-dimensional systems [39]. In this work, we address these questions by classifying unitary evolutions that preserve KD positivity, and thus yield a natural candidate for free operations in resource theories built on Kirkwood-Dirac quasiprobabilities. As an application of our findings, we adapt the quasiprobabilistic Born rule probability estimation algorithm of Ref. [14] to KD distributions, which explicitly bounds simulation runtime with respect to the nonpositivity of the initial state and the nonpositivity induced by its unitary evolution. For our identified classes of positivity-preserving unitaries, we show that the algorithm proceeds efficiently on any KD-positive input. However, for a special class of positivity-preserving unitaries, the algorithm can blow up exponentially in runtime even if the input contains a very small amount of nonpositivity. Our insights lead us to identify a fundamental obstruction for resource theories defined on

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Fourier-conjugate KD distributions in squarefree semiprime dimensions.

This article is structured as follows: In Sec. II we review the Kirkwood-Dirac distribution, as well as its vectorized form. The latter gives a useful representation in which transformations of KD distributions induced by quantum channels take on the form of linear matrix multiplication. Section III contains our main results. We first classify unitaries which preserve KD positivity on pure states: up to phase, such unitaries always act as permutations on $\mathcal{A} \cup \mathcal{B} \cup \mathcal{C}$, where $\mathcal{A}, \mathcal{B}$ are the reference bases of the distribution, and $\mathcal{C}$ is the set of nonbasis KD-positive states. We identify three types of positivity-preserving unitaries: type I unitaries act as automorphisms on the sets $\mathcal{A}, \mathcal{B}, \mathcal{C}$, type II unitaries act as bijections between $\mathcal{A}$ and $\mathcal{B}$, and type III unitaries act as bijections among $\mathcal{A}, \mathcal{B}$ and subsets of $\mathcal{C}$. We then prove structural results: whenever $\mathcal{C} = \emptyset$, only type I or II unitaries can exist. Both types are covariant transformations which permute (and for type II additionally conjugate) the entries of the KD distribution, thus preserving the total nonpositivity of any input. Out of the three, only type I unitaries correspond to KD-stochastic unitaries, i.e., evolution which induces a stochastic superoperator in the vectorized picture. This stands in contrast with the discrete Wigner distribution, for which all positivity-preserving (Clifford) unitaries induce stochastic superoperators. The existence of positivity-preserving unitaries is predicated on symmetries between the reference bases of the distribution. By identifying necessary conditions for their existence, we show that for KD distributions defined on Haar-randomly sampled bases $\mathcal{A}, \mathcal{B}$, no nontrivial positivity-preserving unitaries exist with probability 1. We then focus on distributions defined on Fourier-conjugate bases. Recent work [40,41] has shown that for $V = \text{DFT}_d$ the Weyl-Heisenberg group is positivity preserving. In our classification, such unitaries fall into type I. Similarly, any product of type I unitaries with the discrete Fourier transform (DFT) matrix itself forms a type II unitary. We prove that for $d = p^k$ (with p prime), positivity-preserving unitaries can only be of type I or II. On the other hand, for any $d = pq$ (with p, q distinct primes) we prove the additional existence of type III unitaries: while such unitaries are shown to be positivity preserving on any KD-positive input, they can change the total nonpositivity of distributions containing complex entries. Furthermore, they do not form elements of the Weyl-Heisenberg group and their action is only guaranteed to be covariant on real-valued distributions. Section IV applies our findings to the quantum simulation algorithm of Ref. [14]: the original method relies on superoperator stochasticity (satisfied by type I) to be efficient; we show how to adapt it to also efficiently simulate type II unitaries. The existence of type III unitaries poses an additional problem for the algorithm, due to their general lack of covariance. We show that for circuits composed of type III unitaries, if an input distribution is real-valued, the simulation can proceed efficiently; however, if the input's distribution contains complex entries, then the simulation runtime can blow up exponentially in the worst case. Our insights lead to a no-go theorem for resource theories defined on $V = \text{DFT}_{pq}^{\otimes n}$ distributions: any such theory cannot simultaneously (i) include the efficiently simulable, positivity-preserving type III unitaries in its free operations, and (ii) treat

the total nonpositivity of the distribution as a monotone under the free operations. Our findings are summarized in Table I. The appendixes mostly contain additional standalone results: Appendix A shows how to apply the cycle test algorithm of Ref. [33] for experimental measurement of KD superoperator elements. Appendix B contains additional structural results on Fourier-conjugate KD distributions. Appendix C contains new bounds on the magnitudes of quasiprobabilities for any KD distribution. Finally, Appendix D presents an extended proof of Theorem 2 showing that our identified type III unitaries are positivity preserving beyond pure states, including for many-qudit systems where $V = \text{DFT}_{pq}^{\otimes n}$.

II. PRELIMINARIES

In this work, we consider informationally complete Kirkwood-Dirac (KD) quasiprobability distributions defined with respect to two orthonormal bases of a d -dimensional Hilbert space. Here, we state all the relevant properties. For a thorough review of KD distributions and their applications, we recommend [38].

Definition 1 (Kirkwood-Dirac distributions [38]). For a quantum state ρ , the Kirkwood-Dirac distribution is the set of complex numbers (quasiprobabilities) $Q(\rho)_{ij}$ given by

$$Q(\rho)_{ij} = \langle b_j | a_i \rangle \langle a_i | \rho | b_j \rangle, \quad (i, j) \in [[d]]^2, \quad (1)$$

where $\mathcal{A} = \{|a_i\rangle\}$ and $\mathcal{B} = \{|b_j\rangle\}$ are the reference bases of the distribution, related by a transition matrix V such that $|b_i\rangle = V|a_i\rangle$. If V is such that $m_{\mathcal{A},\mathcal{B}} = \min_{ij} |\langle a_i | b_j \rangle| > 0$, the KD distribution is said to be informationally complete.

The name “quasiprobability” arises from the fact that the quantities $Q(\rho)_{ij}$ satisfy some, but not all, of the Kolmogorov axioms. For instance, they sum to 1 and correctly reproduce Born rule probabilities upon marginalization:

$$\sum_j Q(\rho)_{ij} = \langle a_i | \rho | a_i \rangle, \quad \sum_i Q(\rho)_{ij} = \langle b_j | \rho | b_j \rangle.$$

As the KD distribution is invariant under a global change of basis (where $|a_i\rangle \rightarrow U|a_i\rangle$, $|b_j\rangle \rightarrow U|b_j\rangle$, $\rho \rightarrow U\rho U^\dagger$), it is often convenient to take $\{|a_i\rangle\}$ to be the computational basis and $|b_j\rangle = V|a_j\rangle$ for a unitary transition matrix V . For mutually unbiased bases (MUBs), $|\langle a_i | b_j \rangle| = m_{\mathcal{A},\mathcal{B}} = 1/\sqrt{d}$ for all (i, j) , and the corresponding V is a complex Hadamard matrix. One can also define the KD distribution in terms of frames Λ_{ij} , satisfying

$$\Lambda_{ij} = \frac{|a_i\rangle\langle b_j|}{\langle b_j | a_i \rangle}, \quad Q(\rho)_{ij} = \frac{\text{Tr}(\Lambda_{ij}^\dagger \rho)}{\text{Tr}(\Lambda_{ij} \Lambda_{ij}^\dagger)},$$

where the presence of complex-valued $Q(\rho)_{ij}$ can be directly seen as a consequence of the non-Hermiticity of Λ_{ij} . Finally, given a KD distribution one may reconstruct ρ via the weighted sum

$$\rho = \sum_{ij} \frac{|a_i\rangle\langle b_j|}{\langle b_j | a_i \rangle} Q(\rho)_{ij}, \quad (2)$$

which is only possible for informationally complete KD distributions, i.e., when $m_{\mathcal{A},\mathcal{B}} > 0$.

TABLE I. Summary of Results. This table summarizes the properties of type I, II, and III unitaries identified in this work. The first four rows follow from Lemmas 2, 3 and Theorems 2, 3 in Sec. III. The next two rows follow from Sec. IV, where γ is the induced permutation of indices in $Q(U\rho U^\dagger)_{ij} = Q(\rho)_{\gamma^{-1}(ij)}$ (types I, III) and $Q(U\rho U^\dagger)_{ij} = Q(\rho)^*_{\gamma^{-1}(ij)}$ (type II). For type III unitaries, “real inputs” refer to states ρ satisfying $Q(\rho)_{ij} \in \mathbb{R}$ for all i, j , directly prior to the action of U . The last three rows provide a complete classification of positivity-preserving unitaries for three types of KD distributions (see end of Sec. III), where the results for Haar-random V hold with probability 1.

Property	Type I	Type II	Type III
Positivity preservation	✓	✓	✓
Total nonpositivity preservation	✓	✓	×
Induces stochastic superoperator	✓	×	×
Induces covariant transformation	✓	✓	✓ (real inputs only)
Efficient simulation in Ref. [14]	✓	✓	✓ (real inputs only)
Modification in Ref. [14]	None required	Set $I_k = \gamma(I_{k-1})$, conjugate phases.	Set $I_k = \gamma(I_{k-1})$ on real inputs; otherwise, none.
Existence for Haar-random V	✓ ($\{e^{i\theta}\mathbb{1}\}$ only)	×	×
Existence for $V = \text{DFT}_{p^k}$	✓	✓	×
Existence for $V = \text{DFT}_{pq}$	✓	✓	✓

Kirkwood-Dirac positivity. When a KD distribution takes on exclusively real non-negative values, it resembles a classical joint probability distribution. In those cases we say that it is KD-positive, or KD-classical.

Definition 2 (Total nonpositivity). The total nonpositivity of a KD distribution $Q(\rho)$ is defined as

$$\mathcal{N}(Q(\rho)) = \sum_{ij} |Q(\rho)_{ij}| \geq 1.$$

We call a KD distribution KD-positive if and only if $\mathcal{N}(Q(\rho)) = 1$, and nonpositive otherwise. Similarly, if $Q(\rho)_{ij} \in \mathbb{R}$ for all i, j we call the distribution KD-real, and nonreal otherwise.

KD nonpositivity has been linked to nonclassical phenomena in quantum noncontextuality, and advantages in quantum metrology. The bases $\mathcal{A}, \mathcal{B}$ are themselves pure KD-positive states, for which $Q_{ij}(a_k) = \delta_{ki} |\langle a_k | b_j \rangle|^2$ [and similarly for $Q_{ij}(b_m)$]. Recent work [42] has shown that for the vast majority of KD distributions (i.e., with probability 1, when V is sampled via the Haar measure on $U(d)$), the basis states from $\mathcal{A}, \mathcal{B}$ are the only KD-positive pure states. Nonetheless, for some choices of V pure, nonbasis KD-positive states exist, and there can also exist mixed KD-positive states lying outside of the convex set of pure KD-positive states [43].

Support uncertainties. For a pure state $|\psi\rangle$ described on a KD distribution, it is also useful to define the support uncertainties $n_{\mathcal{A}}, n_{\mathcal{B}}$, which count the number of nonzero inner products between $|\psi\rangle$ and the two reference bases:

$$\begin{aligned} n_{\mathcal{A}} &= |\mathcal{S}_{\mathcal{A}}| = |\{ |a_i\rangle \in \mathcal{A} : \langle a_i | \psi \rangle \neq 0 \}|, \\ n_{\mathcal{B}} &= |\mathcal{S}_{\mathcal{B}}| = |\{ |b_j\rangle \in \mathcal{B} : \langle b_j | \psi \rangle \neq 0 \}|. \end{aligned} \quad (3)$$

For informationally complete distributions, the product $n_{\mathcal{A}} n_{\mathcal{B}}$ gives the number of nonzero entries in the KD distribution $Q(\psi)_{ij}$, i.e., its support. In Ref. [44], it was shown that for all pure KD-positive states, the sum $n_{\mathcal{A}} + n_{\mathcal{B}}$ satisfies

$$n_{\mathcal{A}} + n_{\mathcal{B}} \leq d + 1,$$

and that for MUBs, all pure KD-positive states also satisfy [43,45]

$$n_{\mathcal{A}} n_{\mathcal{B}} = d.$$

KD-positive states. In Sec. III we classify unitaries which preserve KD positivity, i.e., unitaries which always map KD-positive states to other KD-positive states (Definition 3). A necessary condition for a unitary to satisfy this property is that, up to phase, it permutes elements of the set of pure KD-positive states, which we refer to as $\mathcal{E}_{\text{KD}+}^{\text{pure}}$. A large factor in our classification is whether the set $\mathcal{C} = \mathcal{E}_{\text{KD}+}^{\text{pure}} \setminus (\mathcal{A} \cup \mathcal{B})$ of pure, nonreference basis KD-positive states is empty. In general, we write $\mathcal{E}_{\text{KD}+}^{\text{pure}} = \mathcal{A} \cup \mathcal{B} \cup \mathcal{C}$ to cover both scenarios. Instances where $\mathcal{C} = \emptyset$ include Haar-random choices of V [43], as well as $V = \text{DFT}_d$ for d prime [45]. On the other hand, $\mathcal{C}$ is nonempty for $V = \text{DFT}_d$ when d is composite. In many KD distributions, the set of all KD-positive states $\mathcal{E}_{\text{KD}+}$ is known to be the convex hull of $\mathcal{E}_{\text{KD}+}^{\text{pure}}$. This is true for Haar-random V [42], as well as $V = \text{DFT}_d$ when $d = p^k$ is a prime power [40,43,46]. Whenever it holds true that $\mathcal{E}_{\text{KD}+} = \text{conv}(\mathcal{E}_{\text{KD}+}^{\text{pure}})$, positivity preservation for pure states is a sufficient condition for positivity preservation for all states. In other cases, whenever $\mathcal{E}_{\text{KD}+} \neq \text{conv}(\mathcal{E}_{\text{KD}+}^{\text{pure}})$ and “exotic” impure, KD-positive states exist (such as for $V = \text{DFT}_6$ or $V = H^{\otimes n}$ [40]), there remains a possibility that unitaries which permute elements of $\mathcal{E}_{\text{KD}+}^{\text{pure}}$ map impure, KD-positive states from $\mathcal{E}_{\text{KD}+} \setminus \text{conv}(\mathcal{E}_{\text{KD}+}^{\text{pure}})$ to nonpositive states. For all of our identified types of positivity-preserving unitaries (Lemma 2 and Theorem 2), we find that this is not the case.

KD distributions as vectors. We make use of vectorization, which is the process of representing quantum states $\rho \in \mathbb{C}^{d \times d}$ as vectors in $\mathbb{C}^{d^2}$, acted on by larger matrices in $\mathbb{C}^{d^2 \times d^2}$ known as superoperators. For KD distributions, this representation was explicitly studied in Ref. [34]. In practice, it allows us to represent any evolution of KD distributions as a linear transformation of the corresponding vectorized form. We proceed by stacking the rows of a KD distribution matrix $Q(\rho)$ into a single column vector:

$$|Q(\rho)\rangle\rangle = (Q_{11} \quad Q_{12} \quad \dots \quad Q_{1d} \quad Q_{21} \quad \dots \quad Q_{dd})^T.$$

It is also useful to define the dual row vector $\langle\langle \mathbf{1} | = (1, 1, \dots, 1)$, composed of all 1s. Clearly, all KD distribution vectors satisfy $\langle\langle \mathbf{1} | Q(\rho)\rangle\rangle = 1$. The total nonpositivity of a

KD distribution can then be written as the ℓ_1 norm of $|Q(\rho)\rangle\rangle$:

$$\mathcal{N}(Q(\rho)) = \| |Q(\rho)\rangle\rangle \|_1.$$

KD superoperators. In the context of classical simulation, we consider the evolution of a KD distribution $Q(\rho) \rightarrow Q(\mathcal{E}(\rho))$ under a quantum channel (a completely positive, trace-preserving map) $\mathcal{E}$ acting on ρ . In the larger space $\mathbb{C}^{d^2 \times d^2}$, this may be written as the multiplication of $|Q(\rho)\rangle\rangle$ by a $d^2 \times d^2$ matrix $\hat{\mathcal{E}}$:

$$|Q(\mathcal{E}(\rho))\rangle\rangle = \hat{\mathcal{E}}|Q(\rho)\rangle\rangle.$$

If $\mathcal{E}$ is composed of a set of Kraus operators $\{K_\mu\}$ (such that $\sum_\mu K_\mu^\dagger K_\mu = \mathbb{1}_d$), then the quasiprobabilities Q_{ij} evolve as follows:

$$\begin{aligned} Q_{ij} &\rightarrow \sum_\mu \langle b_j | a_i \rangle \langle a_i | K_\mu \rho K_\mu^\dagger | b_j \rangle \\ &= \sum_\mu \sum_{kl} \langle b_j | a_i \rangle \langle a_i | K_\mu | a_k \rangle \langle a_k | \rho | b_l \rangle \langle b_l | K_\mu^\dagger | b_j \rangle \\ &= \sum_{kl} \left(\sum_\mu \frac{\langle b_j | a_i \rangle}{\langle b_l | a_k \rangle} \langle a_i | K_\mu | a_k \rangle \langle b_l | K_\mu^\dagger | b_j \rangle \right) Q_{kl} \\ &= \sum_{kl} \hat{\mathcal{E}}_{ij,kl} Q_{kl}. \end{aligned}$$

This allows us to identify the matrix elements $\hat{\mathcal{E}}_{ij,kl}$:

$$\hat{\mathcal{E}}_{ij,kl} = \sum_\mu \frac{\langle b_j | a_i \rangle}{\langle b_l | a_k \rangle} \langle a_i | K_\mu | a_k \rangle \langle b_l | K_\mu^\dagger | b_j \rangle.$$

One may verify that $\hat{\mathcal{E}}$ preserves the element sum of KD quasiprobability vectors. This is because its columns sum to 1:

$$\begin{aligned} \sum_{ij} \hat{\mathcal{E}}_{ij,kl} &= \frac{1}{\langle b_l | a_k \rangle} \sum_{ij} \sum_\mu \langle b_l | K_\mu^\dagger | b_j \rangle \langle b_j | a_i \rangle \langle a_i | K_\mu | a_k \rangle \\ &= \frac{1}{\langle b_l | a_k \rangle} \sum_\mu \langle b_l | K_\mu^\dagger K_\mu | a_k \rangle = \langle b_l | a_k \rangle / \langle b_l | a_k \rangle = 1, \end{aligned}$$

from which it follows that $\langle \langle \mathbb{1} | \hat{\mathcal{E}} = \langle \langle \mathbb{1} |$, hence $\langle \langle \mathbb{1} | Q(\mathcal{E}(\rho)) \rangle \rangle = \langle \langle \mathbb{1} | \hat{\mathcal{E}} | Q(\rho) \rangle \rangle = 1$. In light of this, one may view the superoperators $\hat{\mathcal{E}}$ as left quasistochastic matrices acting on KD quasiprobability vectors (recall that a left stochastic matrix is a square matrix with non-negative entries whose columns sum to 1). In particular, when $\hat{\mathcal{E}}$ is stochastic, the triangle inequality implies it can only decrease the ℓ_1 norm of the KD distribution vector as $\| \hat{\mathcal{E}} | Q(\rho) \rangle \rangle \|_1 \leq \| |Q(\rho)\rangle\rangle \|_1$. For KD-positive inputs $|Q(\rho)\rangle\rangle$, it follows that the output distribution is also KD-positive, in full analogy to the evolution of a probability vector by a Markov chain.

Unitary channels. If $\mathcal{E}$ is an action of a unitary U , we write the corresponding superoperator as $\hat{\mathcal{E}}_U$. In this case, the matrix elements simplify to

$$(\hat{\mathcal{E}}_U)_{ij,kl} = \frac{\langle b_j | a_i \rangle}{\langle b_l | a_k \rangle} \langle a_i | U | a_k \rangle \langle b_l | U^\dagger | b_j \rangle. \quad (4)$$

Furthermore, each unitary-induced superoperator $\hat{\mathcal{E}}_U$ must have an inverse given by $\hat{\mathcal{E}}_U^{-1} = \hat{\mathcal{E}}_{U^\dagger}$, which follows from the

composition rule

$$\begin{aligned} \hat{\mathcal{E}}_{U^\dagger} \hat{\mathcal{E}}_U |Q(\rho)\rangle\rangle &= \hat{\mathcal{E}}_{U^\dagger} |Q(U \rho U^\dagger)\rangle\rangle = |Q(U^\dagger U \rho U U^\dagger)\rangle\rangle \\ &= |Q(\rho)\rangle\rangle. \end{aligned} \quad (5)$$

We may relate the elements of $\hat{\mathcal{E}}_U^{-1}$ to those of $\hat{\mathcal{E}}_U$:

$$\begin{aligned} (\hat{\mathcal{E}}_U^{-1})_{ij,kl} &= \frac{\langle b_j | a_i \rangle}{\langle b_l | a_k \rangle} \langle a_i | U^\dagger | a_k \rangle \langle b_l | U | b_j \rangle \\ &= \frac{\langle b_j | a_i \rangle}{\langle b_l | a_k \rangle} (\langle a_k | U | a_i \rangle \langle b_j | U^\dagger | b_l \rangle)^* \\ &= \frac{\langle b_j | a_i \rangle}{\langle b_l | a_k \rangle} \left(\frac{\langle b_j | a_i \rangle}{\langle b_l | a_k \rangle} (\hat{\mathcal{E}}_U)_{kl,ij} \right)^* \\ &= \left| \frac{\langle b_j | a_i \rangle}{\langle b_l | a_k \rangle} \right|^2 (\hat{\mathcal{E}}_U^*)_{kl,ij}. \end{aligned} \quad (6)$$

Thus, if $\mathcal{A}, \mathcal{B}$ are mutually unbiased, then $\hat{\mathcal{E}}_U$ is always a unitary matrix on $\mathbb{C}^{d^2 \times d^2}$. In this case, the rows of $\hat{\mathcal{E}}_U = \hat{\mathcal{E}}_{U^\dagger}^\dagger$ are the complex conjugated columns of $\hat{\mathcal{E}}_{U^\dagger}$ (which sum to 1), and therefore $\hat{\mathcal{E}}_U$ is a doubly quasistochastic matrix.

Positive-operator-valued measure (POVM) elements. Vectorization provides a recipe for representing and evolving KD quasiprobabilities through matrix multiplication in $\mathbb{C}^{d^2}$. To make this complete, we also need a way to calculate measurement probabilities, i.e., quantities $\text{Tr}(F U \rho U^\dagger)$, where F is some POVM element. This is very simple and involves dual vectors $\langle \langle F | \in (\mathbb{C}^{d^2})^*$ which map KD vectors to Born rule probabilities. The dual vectors $\langle \langle F |$ have elements

$$F_{ij} = \frac{\langle b_j | F | a_i \rangle}{\langle b_j | a_i \rangle},$$

so that measurement probabilities are given by

$$\text{Tr}(F U \rho U^\dagger) = \langle \langle F | \hat{\mathcal{E}}_U | Q(\rho) \rangle \rangle = \sum_{ij,kl} F_{ij} (\hat{\mathcal{E}}_U)_{ij,kl} Q_{kl}. \quad (7)$$

If F is a projective measurement in the basis $\mathcal{A}$ or $\mathcal{B}$ (for example $F = |a_k\rangle\langle a_k|$), then $\langle \langle F |$ has elements

$$F_{ij} = \frac{\langle b_j | a_k \rangle \langle a_k | a_i \rangle}{\langle b_j | a_i \rangle} = \delta_{ik},$$

and Eq. (7) reduces to the marginalization of the quasiprobability distribution:

$$\text{Tr}(F \rho) = \sum_{ij} \delta_{ik} Q_{ij} = \sum_j Q_{kj} = \langle a_k | \rho | a_k \rangle.$$

Experimental estimation of KD superoperator elements. In Appendix A, we offer a straightforward method for estimating the elements $(\hat{\mathcal{E}}_U)_{ij,kl}$ of a KD superoperator induced by a unitary U on any informationally complete choice of $\mathcal{A}, \mathcal{B}$. To do this, one can apply the cycle test algorithm [33,47], originally proposed for estimating Kirkwood-Dirac quasiprobabilities $Q(\rho)_{ij}$ of an unknown state.

III. CLASSIFICATION OF KD POSITIVITY-PRESERVING UNITARIES

We now classify unitaries which preserve KD positivity and total nonpositivity, as well as completely characterize

KD-stochastic unitaries. In Sec. IV we discuss the implications of these results for the classical simulability of KD-positive states. Our classification is complete for all distributions where $\mathcal{C} = \emptyset$, randomly sampled transition matrices, and Fourier-conjugate bases with $d = p^k, pq$ (with p, q distinct primes). Here and throughout, we assume informational completeness (i.e., $m_{\mathcal{A},\mathcal{B}} > 0$), stating otherwise where relevant. We leave other instances of KD distributions for future work.

Definition 3 (positivity preservation). A unitary $U \in \mathcal{U}_{\mathcal{N}+}$ is said to be positivity preserving if and only if for any density matrix ρ such that $\mathcal{N}(Q(\rho)) = 1$, it is true that $\mathcal{N}(Q(U\rho U^\dagger)) = 1$, i.e., $U \in \mathcal{U}_{\mathcal{N}+}$ maps KD-positive states to KD-positive states.

Definition 4 ($\mathcal{N}$ preservation). A unitary $U \in \mathcal{U}_{\mathcal{N}}$ is said to be $\mathcal{N}$ preserving if and only if for any density matrix ρ , $\mathcal{N}(Q(U\rho U^\dagger)) = \mathcal{N}(Q(\rho))$, i.e., $\mathcal{U}_{\mathcal{N}}$ preserves the KD total nonpositivity of ρ . If U is $\mathcal{N}$ preserving, then it is positivity preserving.

Definition 5 (Kirkwood-Dirac stochasticity). A unitary $U \in \mathcal{U}_{\text{stoch}}$ is said to be KD-stochastic if and only if its induced superoperator $\hat{\mathcal{E}}_U$ is a stochastic matrix. If U is KD-stochastic, then by Theorem 3 it is $\mathcal{N}$ preserving.

Depending on the geometry of $\mathcal{E}_{\text{KD}+}^{\text{pure}}$, the three notions may or may not be synonymous. Although an arbitrary stochastic superoperator cannot increase the ℓ_1 norm of a complex vector (and so is positivity preserving), Theorem 3 further implies that $\mathcal{U}_{\text{stoch}}$ can only contain superoperators which are permutations, and thus are $\mathcal{N}$ preserving. We identify examples where no such (nontrivial) unitaries exist, as well as examples where the sets are both nontrivial and distinct. In all cases, they satisfy $\mathcal{U}_{\text{stoch}} \subseteq \mathcal{U}_{\mathcal{N}} \subseteq \mathcal{U}_{\mathcal{N}+}$.

Methodology. A necessary condition for a unitary U to be positivity preserving for all states $\rho \in \mathcal{E}_{\text{KD}+}$ is that it is positivity preserving on pure states $|\psi\rangle \in \mathcal{E}_{\text{KD}+}^{\text{pure}}$. Therefore, our approach will be to identify all possible families of unitaries satisfying this necessary condition, and (where appropriate) verify that they are positivity preserving for $\rho \in \mathcal{E}_{\text{KD}+} \setminus \text{conv}(\mathcal{E}_{\text{KD}+}^{\text{pure}})$. We assume that the set of pure KD-positive states is finite—to the best of our knowledge, this is true for all informationally complete KD distributions. Then, any positivity-preserving unitary must form a generalized permutation of the set $\mathcal{A} \cup \mathcal{B} \cup \mathcal{C}$ of pure KD-positive states.

Definition 6 (generalized permutations). The set M_d of unitary generalized permutations (or monomial unitary matrices) is defined as

$$M_d = \{DP_\sigma : D = \text{diag}(e^{i\theta_1}, \dots, e^{i\theta_d}), \sigma \in S_d\}.$$

We begin with the simplest case where $\mathcal{C} = \emptyset$, and the only pure KD-positive states are the basis vectors from $\mathcal{A}$ and $\mathcal{B}$. For such distributions, we find that $\mathcal{U}_{\mathcal{N}}$ can only consist of two types of generalized permutations, which we call types I and II. Such unitaries are then shown to be $\mathcal{N}$ preserving, and so preserve positivity on any $\rho \in \mathcal{E}_{\text{KD}+}$ regardless of the existence of exotic, impure KD-positive states. Thus, for any distribution where $\mathcal{C} = \emptyset$ our classification of $\mathcal{U}_{\mathcal{N}} = \mathcal{U}_{\mathcal{N}+}$ into types I, II is exhaustive.

Lemma 1. If $\mathcal{C} = \emptyset$, i.e., $\mathcal{E}_{\text{KD}+}^{\text{pure}} = \mathcal{A} \cup \mathcal{B}$, then any positivity-preserving unitary U either satisfies $U(\mathcal{A}) = \mathcal{A}$ and $U(\mathcal{B}) = \mathcal{B}$ (type I), or $U(\mathcal{A}) = \mathcal{B}$ and $U(\mathcal{B}) = \mathcal{A}$ (type

II). The set of all such unitaries is given by

$$\mathcal{U}_{\mathcal{N}+} = \underbrace{(M_d \cap VM_d V^\dagger)}_{\text{Type I}} \cup \underbrace{(VM_d \cap M_d V^\dagger)}_{\text{Type II}}$$

Proof. Since the only pure KD-positive states are the basis states, any positivity-preserving map U must be a generalized permutation of the vectors in $\mathcal{A} \cup \mathcal{B}$ up to phase. Prima facie, there are three possibilities: type I, where U is a generalized permutation on $\mathcal{A}$ and $\mathcal{B}$, in which case $U \in M_d$ is a (possibly distinct) monomial unitary on both bases, hence $U \in M_d \cap VM_d V^\dagger$. For type II, U is a bijection between $\mathcal{A}$ and $\mathcal{B}$, in which case U can be written as $U = VDP_\sigma$ on the $\mathcal{A}$ basis, and as $U = D'P_{\sigma'}V^\dagger$ on the $\mathcal{B}$ basis, hence $U \in VM_d \cap M_d V^\dagger$. The third possibility is that U maps some vectors from $\mathcal{A}$ to $\mathcal{A}$, and some to $\mathcal{B}$ (and similarly for $\mathcal{B}$). This is not possible. Suppose $U|a_i\rangle = e^{i\theta_i}|a_{i'}\rangle$ and $U|a_j\rangle = e^{i\theta_j}|b_{j'}\rangle$ for some $i \neq j$. This would imply that

$$\langle a_i|U^\dagger U|a_j\rangle = e^{i(\theta_j - \theta_i)}\langle a_{i'}|b_{j'}\rangle = e^{i(\theta_j - \theta_i)}\langle a_{i'}|V|a_{j'}\rangle \neq 0,$$

which is a contradiction, since U is unitary and $\mathcal{A}$ is an orthonormal basis. Thus, positivity-preserving unitaries must be of type I or II. ■

Lemma 2. Positivity-preserving unitaries of type I or II are also $\mathcal{N}$ preserving. In other words, if $\mathcal{U}_{\mathcal{N}+} = (M_d \cap VM_d V^\dagger) \cup (VM_d \cap M_d V^\dagger)$, then $\mathcal{U}_{\mathcal{N}+} = \mathcal{U}_{\mathcal{N}}$.

Proof. Clearly, by definition $\mathcal{U}_{\mathcal{N}} \subseteq \mathcal{U}_{\mathcal{N}+}$. We show that $\mathcal{U}_{\mathcal{N}+} \subseteq \mathcal{U}_{\mathcal{N}}$. Suppose $U \in \mathcal{U}_{\mathcal{N}+}$. We can consider types I and II separately. In the first case, U acts as

$$U|a_i\rangle = e^{i\theta_i}|a_{\sigma(i)}\rangle, \quad U|b_j\rangle = e^{i\phi_j}|b_{\tau(j)}\rangle.$$

Hence,

$$U^\dagger|a_i\rangle\langle a_i|U = |a_{\sigma^{-1}(i)}\rangle\langle a_{\sigma^{-1}(i)}|,$$

$$U^\dagger|b_j\rangle\langle b_j|U = |b_{\tau^{-1}(j)}\rangle\langle b_{\tau^{-1}(j)}|.$$

Hence, $\rho \rightarrow U\rho U^\dagger$ induces the following transformation on the KD distribution:

$$\begin{aligned} Q_{ij}(U\rho U^\dagger) &= \langle b_j|U U^\dagger|a_i\rangle\langle a_i|U\rho U^\dagger|b_j\rangle \\ &= \langle b_{\tau^{-1}(j)}|a_{\sigma^{-1}(i)}\rangle\langle a_{\sigma^{-1}(i)}|\rho|b_{\tau^{-1}(j)}\rangle \\ &= Q_{\sigma^{-1}(i), \tau^{-1}(j)}(\rho). \end{aligned}$$

This implies that $\mathcal{N}(Q(U\rho U^\dagger)) = \mathcal{N}(Q(\rho))$ for all ρ . For unitaries of type II, we may write

$$U|a_i\rangle = e^{i\theta_i}|b_{\sigma(i)}\rangle, \quad U|b_j\rangle = e^{i\phi_j}|a_{\tau(j)}\rangle.$$

Hence,

$$U^\dagger|a_i\rangle\langle a_i|U = |b_{\tau^{-1}(i)}\rangle\langle b_{\tau^{-1}(i)}|,$$

$$U^\dagger|b_j\rangle\langle b_j|U = |a_{\sigma^{-1}(j)}\rangle\langle a_{\sigma^{-1}(j)}|,$$

and so

$$\begin{aligned} Q_{ij}(U\rho U^\dagger) &= \langle b_j|U U^\dagger|a_i\rangle\langle a_i|U\rho U^\dagger|b_j\rangle \\ &= \langle a_{\sigma^{-1}(j)}|b_{\tau^{-1}(i)}\rangle\langle b_{\tau^{-1}(i)}|\rho|a_{\sigma^{-1}(j)}\rangle \\ &= Q_{\sigma^{-1}(j), \tau^{-1}(i)}^*(\rho). \end{aligned}$$

This again implies that the total nonpositivity is preserved for any state. Thus, if $U \in \mathcal{U}_{\mathcal{N}+}$ is of type I or II, it also preserves the total nonpositivity of any KD distribution. If these are the

only types of unitaries in $\mathcal{U}_{\mathcal{N}_+}$, then any $\mathcal{N}$ preserving unitary must also be positivity preserving, and so $\mathcal{U}_{\mathcal{N}_+} = \mathcal{U}_{\mathcal{N}}$. ■

Remark 1. If $U \in \mathcal{U}_{\mathcal{N}_+}$ is a type I or II unitary, then it must also form a generalized permutation on $\mathcal{C}$, and be $\mathcal{N}$ preserving for all $\rho \in \mathcal{E}_{\text{KD}+}$.

Proof. We know from Lemma 2 that if U is of type I or II, then $U \in \mathcal{U}_{\mathcal{N}}$ and thus maps all KD-positive states to KD-positive states. The only way for this to be true is if U also forms a generalized permutation on $\mathcal{C}$. Since type I and II unitaries always permute entries of the KD distribution, they also preserve the total nonpositivity of any impure state. ■

When $\mathcal{C} = \emptyset$, any positivity preserving unitary is also $\mathcal{N}$ preserving. Furthermore, the action of any type I or II unitary on KD distributions is said to be covariant, meaning that it corresponds to a relabelling and conjugation of the matrix elements Q_{ij} . In particular, in Sec. IV we show this implies that the evolution of positive KD distributions under any quantum circuit composed of such unitaries can be classically efficiently simulated.

Fourier-conjugate bases. For a variety of interesting choices of transition matrices it holds that $\mathcal{C} \neq \emptyset$, including in the case of the discrete Fourier transform. We now prove that when $V = \text{DFT}_d$ in dimension $d = p^k$ with p prime, the structure of the set $\mathcal{C}$ of nonbasis pure KD-positive states still forces positivity-preserving unitaries to only be of type I or II. As such unitaries act covariantly, this will imply that any positivity-preserving unitary can be efficiently simulated.

Theorem 1. For $V = \text{DFT}_d$ in dimension $d = p^k$ with p prime, $\mathcal{U}_{\mathcal{N}_+}$ consists of type I and II unitaries only. Consequently, $\mathcal{U}_{\mathcal{N}_+} = \mathcal{U}_{\mathcal{N}}$.

Proof. If $k = 1$, then $\mathcal{C} = \emptyset$ and the result is immediate from Lemma 1. For $k > 1$, it has been shown that the set $\mathcal{C}$ of nonbasis pure KD-positive states decomposes as follows [44,45]:

$$\mathcal{C} = \bigcup_{uv=d} \mathcal{C}_{u,v},$$

where each $\mathcal{C}_{u,v} = \{|m, s\rangle_{u,v}\}$ is an orthonormal basis on $\mathbb{C}^d$ defined as

$$|m, s\rangle_{u,v} = \frac{1}{\sqrt{v}} \sum_{k=0}^{v-1} e^{\frac{2\pi i}{v} sk} |a_{ku+m}\rangle, \quad m \in \mathbb{Z}_u, s \in \mathbb{Z}_v.$$

We show that despite $\mathcal{C}$ being nonempty for $d = p^k$, any generalized permutation on the set of KD-positive states $\mathcal{A} \cup \mathcal{B} \cup \mathcal{C}$ must be of either type I or II. First, we calculate all possible inner products between $|m, s\rangle_{u,v}$ and $|x, y\rangle_{a,b}$:

$$\langle m, s | x, y \rangle = \frac{1}{\sqrt{vb}} \sum_{k=0}^{v-1} \sum_{l=0}^{b-1} e^{\frac{-2\pi i}{v} sk} e^{\frac{2\pi i}{b} yl} \delta_{ku+m, la+x}.$$

From the delta function, the double sum only receives contributions from pairs (k, l) satisfying $ku - la = x - m$. This is a linear Diophantine equation, whose solutions exist if and only if $g | (x - m)$, where $g = \gcd(u, a)$. We therefore assume $x = m \bmod g$. We pick a solution (k_0, l_0) . Then, $(k, l) = (k_0 + ra/g, l_0 + ru/g)$ also form solutions. Since u/g and a/g are coprime, we have $uv/g = ab/g$, which implies that $v = ha/g$ and $b = hu/g$ where $h = \gcd(v, b)$. Since $a/g = v/h$ and $u/g = b/h$, there are $h = \gcd(v, b)$ unique solutions in the

allowed ranges. Hence, the inner product can be rewritten as

$$\begin{aligned} \langle m, s | x, y \rangle &= \frac{1}{\sqrt{vb}} \sum_{r=0}^{h-1} e^{\frac{-2\pi i}{v} s(k_0 + r \frac{a}{g})} e^{\frac{2\pi i}{b} y(l_0 + r \frac{u}{g})} \\ &= \frac{e^{2\pi i \left(\frac{y l_0}{b} - \frac{s k_0}{v} \right)}}{\sqrt{vb}} \sum_{r=0}^{h-1} e^{2\pi i r \left(\frac{yu}{gb} - \frac{sa}{gv} \right)}. \end{aligned}$$

From $uv = ab$, we have $\frac{yu}{gb} - \frac{sa}{gv} = \frac{a}{gv} (y - s)$, where $a/gv = 1/h$. Hence, the inner product is given by

$$\begin{aligned} \langle m, s | x, y \rangle &= \frac{e^{2\pi i \left(\frac{y l_0}{b} - \frac{s k_0}{v} \right)}}{\sqrt{vb}} \sum_{r=0}^{h-1} e^{\frac{2\pi i}{h} r(y-s)} \\ &= \begin{cases} \frac{h}{\sqrt{vb}} e^{2\pi i \left(\frac{y l_0}{b} - \frac{s k_0}{v} \right)}, & x = m \bmod g \\ & y = s \bmod h \\ 0, & \text{otherwise.} \end{cases} \quad (8) \end{aligned}$$

Now, suppose that $d = p^k$. For two KD-positive bases $\mathcal{C}_{u,v}$ and $\mathcal{C}_{a,b}$ with $ab = uv = d$, the nonzero overlaps satisfy $|\langle m, s | x, y \rangle|^2 = \gcd(b, v)^2 / bv$. Since every divisor of d is now a power of p , we may write $b = p^r$ and $v = p^s$, where $r, s \in \{0, \dots, k\}$. Then, $|\langle m, s | x, y \rangle|^2 = 1/p^{|r-s|}$. For mutually unbiased bases, we require $|r - s| = k$, which can only occur when $(r, s) = (k, 0)$ or $(r, s) = (0, k)$. This implies that $\mathcal{A}, \mathcal{B}$ are the only mutually unbiased pair of KD-positive bases and that for any state $|c_i\rangle \in \mathcal{C}$ and any other KD-positive state $|\phi\rangle \in \mathcal{E}_{\text{KD}+}^{\text{pure}}$, $|\langle c_i | \phi \rangle|^2 \neq 1/d$. Since U preserves inner products, its images $U(\mathcal{A})$ and $U(\mathcal{B})$ must also form an MUB pair. Thus, if U were to map any element of $\mathcal{A}$ to an element of $\mathcal{C}$, then $|\langle b_j | U^\dagger U | a_i \rangle|^2 = |\langle \phi | c_i \rangle|^2 \neq 1/d$, violating the unitarity of U . This narrows down U to be of type I or II only. From Lemma 2, it follows that $\mathcal{U}_{\mathcal{N}_+} = \mathcal{U}_{\mathcal{N}}$. ■

Interestingly, Theorem 1 does not apply for composite dimensions d , where additional mutually unbiased pairs $\mathcal{C}_{u,v}$ and $\mathcal{C}_{a,b}$ can exist. Consequently, we can identify unitaries which permute $\mathcal{A} \cup \mathcal{B} \cup \mathcal{C}$ but are not of type I or II. One class of such unitaries turns out to belong in $\mathcal{U}_{\mathcal{N}_+} \setminus \mathcal{U}_{\mathcal{N}}$, meaning they are positivity preserving but not $\mathcal{N}$ preserving on pure states. To demonstrate this, take $d = 6$. From the above decomposition of $\mathcal{C}$, the full set of pure, KD-positive states is given by $\mathcal{E}_{\text{KD}+}^{\text{pure}} = \mathcal{A} \cup \mathcal{B} \cup \mathcal{C}_{2,3} \cup \mathcal{C}_{3,2}$. The transition matrix is $V = \text{DFT}_6$, with elements $V_{ij} = \omega^{ij} / \sqrt{6}$, where $\omega = e^{\pi i/3}$. Consider the unitary $U_\star$ defined by

$$U_\star = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & \omega^2 & 0 & 1 & 0 & \omega^4 \\ 1 & 0 & \omega^2 & 0 & \omega^4 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & \omega^4 & 0 & \omega^2 & 0 \\ 0 & \omega^4 & 0 & 1 & 0 & \omega^2 \end{pmatrix}.$$

When applied to $\mathcal{B}$, its image (in the $\mathcal{A}$ basis) is given by the rows of $U_\star V$:

$$U_\star V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 \end{pmatrix}.$$

Direct calculation thus shows that $U_\star(\mathcal{A}) = \mathcal{C}_{2,3}$, $U_\star(\mathcal{B}) = \mathcal{C}_{3,2}$, $U_\star(\mathcal{C}_{2,3}) = \mathcal{A}$, and $U_\star(\mathcal{C}_{3,2}) = \mathcal{B}$. Hence, $U_\star$ is a generalized permutation on the set of pure KD-positive states. However, it is not of type I or II. In addition, its action on the KD distribution does not preserve the total nonpositivity. To see this, consider the state $|\psi\rangle = (|a_1\rangle + |a_2\rangle + |a_3\rangle)/\sqrt{3}$, which is nonpositive with $\mathcal{N}(Q(|\psi\rangle)) = 4/3$. The state $U_\star|\psi\rangle$ is also nonpositive, but with $\mathcal{N}(Q(U_\star|\psi\rangle)) = 7/3$. Hence, $U_\star$ does not preserve the total nonpositivity of the KD distribution, and so $U_\star \notin \mathcal{U}_\mathcal{N}$.

For this choice of KD distribution, it has been shown that positive, mixed states outside $\text{conv}(\mathcal{E}_{\text{KD}+}^{\text{pure}})$ exist [40]. We now show that $U_\star$ preserves positivity for all states in $\mathcal{E}_{\text{KD}+}$, including ones outside the convex hull of $\mathcal{E}_{\text{KD}+}^{\text{pure}}$, and so $U_\star \in \mathcal{U}_{\mathcal{N}+}$.

Theorem 2. For $V = \text{DFT}_{pq}$, the type III unitary $U_\star$ maps all KD-positive states to KD-positive states.

Proof. Here we prove the $d = 6$ case for our given example of $U_\star$ explicitly. For any $d = pq$, the unitary $U_\star$ can be shown to always exist (we show this next, in Lemma 3), and the proof that this choice of $U_\star$ is $\mathcal{N}$ preserving for all KD-real states is given in Appendix D. We label states from $\mathcal{C}_{2,3}$ as $|c_i\rangle = V_c|a_i\rangle$

and states from $\mathcal{C}_{3,2}$ as $|d_i\rangle = V_d|a_i\rangle$, where

$$V_c = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & \omega^2 & \omega^4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & \omega^2 & \omega^4 \\ 1 & \omega^4 & \omega^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & \omega^4 & \omega^2 \end{pmatrix},$$

$$V_d = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{pmatrix}.$$

We make use of a recent result of Ref. [48], which shows that any KD-real state ρ (including $\rho \in \mathcal{E}_{\text{KD}+}$) can be decomposed as a linear combination of pure states from $\mathcal{E}_{\text{KD}+}^{\text{pure}}$, with real coefficients:

$$\rho = \sum_{i=1}^6 (\alpha_i |a_i\rangle\langle a_i| + \beta_i |b_i\rangle\langle b_i| + \gamma_i |c_i\rangle\langle c_i| + \varepsilon_i |d_i\rangle\langle d_i|), \quad (9)$$

where the (real) coefficients sum as

$$\sum_{i=1}^6 (\alpha_i + \beta_i + \gamma_i + \varepsilon_i) = 1.$$

By linearity [cf. Eq. (1)], we may write any $Q(\rho)$ as a linear combination of KD distributions of pure states. Explicitly, we get $Q(\rho) = \sum_i [\alpha_i Q(|a_i\rangle) + \beta_i Q(|b_i\rangle) + \gamma_i Q(|c_i\rangle) + \varepsilon_i Q(|d_i\rangle)]$. Even more explicitly, we may write $Q(\rho)$ as a sum of four matrices:

$$\frac{1}{6} \begin{pmatrix} \alpha_1 & \alpha_1 & \alpha_1 & \alpha_1 & \alpha_1 & \alpha_1 \\ \alpha_2 & \alpha_2 & \alpha_2 & \alpha_2 & \alpha_2 & \alpha_2 \\ \alpha_3 & \alpha_3 & \alpha_3 & \alpha_3 & \alpha_3 & \alpha_3 \\ \alpha_4 & \alpha_4 & \alpha_4 & \alpha_4 & \alpha_4 & \alpha_4 \\ \alpha_5 & \alpha_5 & \alpha_5 & \alpha_5 & \alpha_5 & \alpha_5 \\ \alpha_6 & \alpha_6 & \alpha_6 & \alpha_6 & \alpha_6 & \alpha_6 \end{pmatrix} + \frac{1}{6} \begin{pmatrix} \beta_1 & \beta_2 & \beta_3 & \beta_4 & \beta_5 & \beta_6 \\ \beta_1 & \beta_2 & \beta_3 & \beta_4 & \beta_5 & \beta_6 \\ \beta_1 & \beta_2 & \beta_3 & \beta_4 & \beta_5 & \beta_6 \\ \beta_1 & \beta_2 & \beta_3 & \beta_4 & \beta_5 & \beta_6 \\ \beta_1 & \beta_2 & \beta_3 & \beta_4 & \beta_5 & \beta_6 \\ \beta_1 & \beta_2 & \beta_3 & \beta_4 & \beta_5 & \beta_6 \end{pmatrix} + \frac{1}{6} \begin{pmatrix} \gamma_1 & \gamma_2 & \gamma_3 & \gamma_1 & \gamma_2 & \gamma_3 \\ \gamma_4 & \gamma_5 & \gamma_6 & \gamma_4 & \gamma_5 & \gamma_6 \\ \gamma_1 & \gamma_2 & \gamma_3 & \gamma_1 & \gamma_2 & \gamma_3 \\ \gamma_4 & \gamma_5 & \gamma_6 & \gamma_4 & \gamma_5 & \gamma_6 \\ \gamma_1 & \gamma_2 & \gamma_3 & \gamma_1 & \gamma_2 & \gamma_3 \\ \gamma_4 & \gamma_5 & \gamma_6 & \gamma_4 & \gamma_5 & \gamma_6 \end{pmatrix}$$

$$+ \frac{1}{6} \begin{pmatrix} \varepsilon_1 & \varepsilon_2 & \varepsilon_1 & \varepsilon_2 & \varepsilon_1 & \varepsilon_2 \\ \varepsilon_3 & \varepsilon_4 & \varepsilon_3 & \varepsilon_4 & \varepsilon_3 & \varepsilon_4 \\ \varepsilon_5 & \varepsilon_6 & \varepsilon_5 & \varepsilon_6 & \varepsilon_5 & \varepsilon_6 \\ \varepsilon_1 & \varepsilon_2 & \varepsilon_1 & \varepsilon_2 & \varepsilon_1 & \varepsilon_2 \\ \varepsilon_3 & \varepsilon_4 & \varepsilon_3 & \varepsilon_4 & \varepsilon_3 & \varepsilon_4 \\ \varepsilon_5 & \varepsilon_6 & \varepsilon_5 & \varepsilon_6 & \varepsilon_5 & \varepsilon_6 \end{pmatrix}.$$

Each entry $Q(\rho)_{ij}$ is one of 36 linear combinations of the coefficients $\alpha_x, \beta_y, \gamma_z, \varepsilon_w$ for some $x, y, z, w \in [6]$. Assume that ρ is an impure, KD-positive state not in $\text{conv}(\mathcal{E}_{\text{KD}+}^{\text{pure}})$. Although the individual coefficients in Eq. (9) are not necessarily positive, from the KD positivity of ρ it follows that each entry combination corresponding to a quasiprobability satisfies

$Q(\rho)_{ij} \geq 0$. Now, recall that $U_\star$ is a generalized permutation on the set of pure KD-positive states. We can directly compute $U_\star \rho U_\star^\dagger$ by conjugating each pure state in the decomposition of (9), and then taking the sum. This gives us a new linear combination of pure state KD distributions. Thus, $Q(U_\star \rho U_\star^\dagger)$ is given by

$$\begin{aligned}
& \frac{1}{6} \begin{pmatrix} \alpha_1 & \alpha_3 & \alpha_5 & \alpha_1 & \alpha_3 & \alpha_5 \\ \alpha_4 & \alpha_6 & \alpha_2 & \alpha_4 & \alpha_6 & \alpha_2 \\ \alpha_1 & \alpha_3 & \alpha_5 & \alpha_1 & \alpha_3 & \alpha_5 \\ \alpha_4 & \alpha_6 & \alpha_2 & \alpha_4 & \alpha_6 & \alpha_2 \\ \alpha_1 & \alpha_3 & \alpha_5 & \alpha_1 & \alpha_3 & \alpha_5 \\ \alpha_4 & \alpha_6 & \alpha_2 & \alpha_4 & \alpha_6 & \alpha_2 \end{pmatrix} + \frac{1}{6} \begin{pmatrix} \beta_1 & \beta_4 & \beta_1 & \beta_4 & \beta_1 & \beta_4 \\ \beta_5 & \beta_2 & \beta_5 & \beta_2 & \beta_5 & \beta_2 \\ \beta_3 & \beta_6 & \beta_3 & \beta_6 & \beta_3 & \beta_6 \\ \beta_1 & \beta_4 & \beta_1 & \beta_4 & \beta_1 & \beta_4 \\ \beta_5 & \beta_2 & \beta_5 & \beta_2 & \beta_5 & \beta_2 \\ \beta_3 & \beta_6 & \beta_3 & \beta_6 & \beta_3 & \beta_6 \end{pmatrix} + \frac{1}{6} \begin{pmatrix} \gamma_1 & \gamma_1 & \gamma_1 & \gamma_1 & \gamma_1 & \gamma_1 \\ \gamma_5 & \gamma_5 & \gamma_5 & \gamma_5 & \gamma_5 & \gamma_5 \\ \gamma_3 & \gamma_3 & \gamma_3 & \gamma_3 & \gamma_3 & \gamma_3 \\ \gamma_4 & \gamma_4 & \gamma_4 & \gamma_4 & \gamma_4 & \gamma_4 \\ \gamma_2 & \gamma_2 & \gamma_2 & \gamma_2 & \gamma_2 & \gamma_2 \\ \gamma_6 & \gamma_6 & \gamma_6 & \gamma_6 & \gamma_6 & \gamma_6 \end{pmatrix} \\
& + \frac{1}{6} \begin{pmatrix} \varepsilon_1 & \varepsilon_6 & \varepsilon_3 & \varepsilon_2 & \varepsilon_5 & \varepsilon_4 \\ \varepsilon_1 & \varepsilon_6 & \varepsilon_3 & \varepsilon_2 & \varepsilon_5 & \varepsilon_4 \\ \varepsilon_1 & \varepsilon_6 & \varepsilon_3 & \varepsilon_2 & \varepsilon_5 & \varepsilon_4 \\ \varepsilon_1 & \varepsilon_6 & \varepsilon_3 & \varepsilon_2 & \varepsilon_5 & \varepsilon_4 \\ \varepsilon_1 & \varepsilon_6 & \varepsilon_3 & \varepsilon_2 & \varepsilon_5 & \varepsilon_4 \\ \varepsilon_1 & \varepsilon_6 & \varepsilon_3 & \varepsilon_2 & \varepsilon_5 & \varepsilon_4 \end{pmatrix}.
\end{aligned}$$

Direct observation shows that of the 36 possible combinations of coefficients $\alpha_x, \beta_y, \gamma_z, \varepsilon_w$ that appear in the entries of $Q(\rho)$, each appears exactly once in $Q(U_\star \rho U_\star^\dagger)$. Hence, each entry of $Q(U_\star \rho U_\star^\dagger)$ is a permuted entry of $Q(\rho)$. Therefore, $U_\star$ maps ρ to a KD-positive state. Since ρ was an arbitrary KD-positive state, we conclude that $U_\star$ maps all KD-positive states to KD-positive states. We additionally conclude that $U_\star$ is covariant on all KD-real states, satisfying $Q(U_\star \rho U_\star^\dagger)_{ij} = Q(\rho)_{\gamma^{-1}(ij)}$ for some permutation γ^{-1} of the indices. This permutation can be explicitly read off by comparing the above expressions for $Q(\rho)$ and $Q(U_\star \rho U_\star^\dagger)$. Notably, it is not a product of row and column permutations. A *Mathematica* notebook containing our calculations is provided in the Supplemental Material [49]. ■

Next, we prove that $U_\star$ always exists for $V = \text{DFT}_{pq}$ with p, q being distinct primes:

Lemma 3. For $V = \text{DFT}_d$ in dimension $d = pq$ with p, q distinct primes, there always exist type III unitaries $U_\star \in \mathcal{U}_{\mathcal{N}_+}$, such that $U_\star(\mathcal{A}) = \mathcal{C}_{p,q}$, $U_\star(\mathcal{C}_{p,q}) = \mathcal{A}$, $U_\star(\mathcal{B}) = \mathcal{C}_{q,p}$, and $U_\star(\mathcal{C}_{q,p}) = \mathcal{B}$. Furthermore, action by $U_\star$ is not covariant on the KD distribution in general, and types I, II, and III exhaust the set $\mathcal{U}_{\mathcal{N}_+}$.

Proof. In this case, $\mathcal{E}_{\text{KD}+}^{\text{pure}} = \mathcal{A} \cup \mathcal{B} \cup \mathcal{C}_{p,q} \cup \mathcal{C}_{q,p}$. Taking $(a, b) = (q, p)$ and $(u, v) = (p, q)$ in Eq. (8), we have that $|\langle m, s|x, y \rangle|^2 = \gcd(q, p)^2 / qp = 1/d$. Hence, the bases $\mathcal{C}_{p,q}$ and $\mathcal{C}_{q,p}$ are mutually unbiased. Since p and q are coprime, we can associate each index $i \in \mathbb{Z}_d$ with a pair of indices $(i_p, i_q) \in \mathbb{Z}_p \times \mathbb{Z}_q$ as follows:

$$\begin{aligned}
(i_p, i_q) &= (i \bmod p, i \bmod q), \\
i &= i_p q \bar{q} + i_q p \bar{p} \bmod pq,
\end{aligned} \tag{10}$$

where $\bar{p} = p^{-1} \bmod q$ and $\bar{q} = q^{-1} \bmod p$. This mapping is bijective by the Chinese remainder theorem. We can therefore define a unitary permutation P , which decomposes $\mathbb{C}^d$ into a tensor product $\mathbb{C}^p \otimes \mathbb{C}^q$:

$$P|a_i\rangle = |i_p\rangle \otimes |i_q\rangle, \quad P^\dagger(|i_p\rangle \otimes |i_q\rangle) = |a_{i_p q \bar{q} + i_q p \bar{p}}\rangle,$$

where $|i_p\rangle \in \mathbb{C}^p$ and $|i_q\rangle \in \mathbb{C}^q$. We can define $U_\star$ as follows:

$$U_\star = P^\dagger(\mathbb{1}_p \otimes \text{DFT}_q)P. \tag{11}$$

Its action on the $\mathcal{A}$ basis is

$$\begin{aligned}
U_\star|a_i\rangle &= P^\dagger(|i_p\rangle \otimes \text{DFT}_q|i_q\rangle) \\
&= P^\dagger\left(|i_p\rangle \otimes \frac{1}{\sqrt{q}} \sum_{s_q=0}^{q-1} e^{\frac{2\pi i}{q} s_q i_q} |s_q\rangle\right) \\
&= \frac{1}{\sqrt{q}} \sum_{s_q=0}^{q-1} e^{\frac{2\pi i}{q} s_q i_q} |a_{i_p q \bar{q} + s_q p \bar{p}}\rangle.
\end{aligned}$$

Now, write $n = i_p q \bar{q} + s_q p \bar{p} \in \mathcal{I}$ as the indices of the $\mathcal{A}$ basis states entering the sum. For all $n \in \mathcal{I}$, we have that $n \bmod p = i_p$ is fixed, so as s_q runs over all of $\mathbb{Z}_q$ it always contributes a multiple of p . Therefore, we may write $\mathcal{I} = \{i_p, i_p + p, \dots, i_p + (q-1)p\}$. We therefore reindex the sum by writing $n = i_p + kp$, where $s_q = n \bmod q = (i_p + kp) \bmod q$ enters the exponent:

$$\begin{aligned}
U_\star|a_i\rangle &= \frac{1}{\sqrt{q}} \sum_{k=0}^{q-1} e^{\frac{2\pi i}{q} i_q (i_p + kp)} |a_{kp+i_p}\rangle \\
&= e^{\frac{2\pi i}{q} i_q i_p} \frac{1}{\sqrt{q}} \sum_{k=0}^{q-1} e^{\frac{2\pi i}{q} p i_q k} |a_{kp+i_p}\rangle \\
&= e^{\frac{2\pi i}{q} i_q i_p} |i_p, p i_q\rangle_{p,q}.
\end{aligned}$$

Therefore, $U_\star(\mathcal{A}) = \mathcal{C}_{p,q}$. Similarly, we can show that $U_\star(\mathcal{B}) = \mathcal{C}_{q,p}$. First we calculate the action of P on the $\mathcal{B}$ states:

$$\begin{aligned}
P|b_j\rangle &= \frac{1}{\sqrt{pq}} \sum_{l=0}^{pq-1} e^{\frac{2\pi i}{pq} jl} P|a_l\rangle = \frac{1}{\sqrt{pq}} \sum_{l=0}^{pq-1} e^{\frac{2\pi i}{pq} jl} |l_p\rangle \otimes |l_q\rangle \\
&= \frac{1}{\sqrt{pq}} \sum_{l_p=0}^{p-1} \sum_{l_q=0}^{q-1} e^{\frac{2\pi i}{pq} (j_p q \bar{q} + j_q p \bar{p})(l_p q \bar{q} + l_q p \bar{p})} |l_p\rangle \otimes |l_q\rangle \\
&= \frac{1}{\sqrt{pq}} \sum_{l_p=0}^{p-1} \sum_{l_q=0}^{q-1} e^{\frac{2\pi i}{p} \bar{q} j_p l_p} e^{\frac{2\pi i}{q} \bar{p} j_q l_q} |l_p\rangle \otimes |l_q\rangle \\
&= \text{DFT}_p[\bar{q} j_p] \otimes \text{DFT}_q[\bar{p} j_q].
\end{aligned} \tag{12}$$

Here, between the third and fourth lines, the cross terms in the exponent are integers. Hence,

$$\begin{aligned} U_\star |b_j\rangle &= P^\dagger (\text{DFT}_p |\bar{q} j_p\rangle \otimes \text{DFT}_q^2 |\bar{p} j_q\rangle) \\ &= P^\dagger (\text{DFT}_p |\bar{q} j_p\rangle \otimes |-\bar{p} j_q\rangle) \\ &= P^\dagger \left(\frac{1}{\sqrt{p}} \sum_{s_p=0}^{p-1} e^{\frac{2\pi i}{p} s_p \bar{q} j_p} |s_p\rangle \otimes |-\bar{p} j_q\rangle \right) \\ &= \frac{1}{\sqrt{p}} \sum_{s_p=0}^{p-1} e^{\frac{2\pi i}{p} s_p \bar{q} j_p} |a_{s_p q \bar{q} - \bar{p} j_q p \bar{p}}\rangle, \end{aligned}$$

where we used $\text{DFT}_d^2 |i\rangle = |-i \bmod d\rangle$ for all $i \in \mathbb{Z}_d$. Again, we reindex the sum, which runs over a set $\mathcal{J}$ consisting of integers $n = s_p q \bar{q} - \bar{p} j_q p \bar{p}$ with $n \bmod q = -\bar{p} j_q \bmod q$ fixed. Thus, we take $n = kq + (-\bar{p} j_q \bmod q)$ and substitute $s_p = [kq + (-\bar{p} j_q \bmod q)] \bmod p$:

$$\begin{aligned} U_\star |b_j\rangle &= \frac{1}{\sqrt{p}} \sum_{k=0}^{p-1} e^{\frac{2\pi i}{p} \bar{q} j_p [kq + (-\bar{p} j_q \bmod q)]} |a_{kq + (-\bar{p} j_q \bmod q)}\rangle \\ &= e^{\frac{2\pi i}{p} \bar{q} j_p (-\bar{p} j_q \bmod q)} \frac{1}{\sqrt{p}} \sum_{k=0}^{p-1} e^{\frac{2\pi i}{p} j_p k} |a_{kq + (-\bar{p} j_q \bmod q)}\rangle \\ &= e^{\frac{2\pi i}{p} \bar{q} j_p (-\bar{p} j_q \bmod q)} |-\bar{p} j_q, j_p\rangle_{q,p}. \end{aligned}$$

It follows that $U_\star(\mathcal{B}) = \mathcal{C}_{q,p}$. Moreover, $U_\star^2 = P^\dagger (\mathbb{1}_p \otimes \text{DFT}_q^2) P$, so $U_\star^2$ is a permutation on $\mathcal{A}$ and $\mathcal{B}$. Hence, $U_\star(\mathcal{C}_{p,q}) = U_\star^2(\mathcal{A}) = \mathcal{A}$ and $U_\star(\mathcal{C}_{q,p}) = U_\star^2(\mathcal{B}) = \mathcal{B}$. Therefore, $U_\star$ is a positivity-preserving generalized permutation on the set of all pure KD-positive states. Appendix D additionally shows it is positivity preserving on any KD-positive state under $V = \text{DFT}_{pq}^{\otimes n}$.

Next, we show that the action of $U_\star$ is not covariant with respect to nonreal KD distributions. Instead, the resulting KD distribution $Q(U_\star \rho U_\star^\dagger)$ can be expressed as a complex linear combination over elements of $Q(\rho)$. First, we perform a global change of basis. We change into the $P(\mathcal{A})$ basis $|i_p, i_q\rangle = |i_p\rangle \otimes |i_q\rangle$, and the $P(\mathcal{B})$ basis $|j_p, j_q\rangle = \text{DFT}_p |\bar{q} j_p\rangle \otimes \text{DFT}_q |\bar{p} j_q\rangle$. The quantum state becomes $\tilde{\rho} = P \rho P^\dagger$. This gives an identical KD distribution, with entries indexed by pairs of indices (i_p, i_q) and (j_p, j_q) instead:

$$\begin{aligned} Q_{i_p, i_q; j_p, j_q} &= \langle b_j | P^\dagger P | a_i \rangle \langle a_i | P^\dagger P \rho P^\dagger P | b_j \rangle \\ &= \langle j_p, j_q | i_p, i_q \rangle \langle i_p, i_q | \tilde{\rho} | j_p, j_q \rangle. \end{aligned}$$

Following the global change of basis, $U_\star$ is given by $PU_\star P^\dagger = \mathbb{1}_p \otimes \text{DFT}_q$. Hence $Q_{i_p, i_q; j_p, j_q}$ transforms as

$$\begin{aligned} Q_{i_p, i_q; j_p, j_q} &\rightarrow \langle j_p, j_q | i_p, i_q \rangle \langle i_p, i_q | (\mathbb{1}_p \otimes \text{DFT}_q) \\ &\quad \times \tilde{\rho} (\mathbb{1}_p \otimes \text{DFT}_q^\dagger) | j_p, j_q \rangle. \end{aligned}$$

The second term may be expanded as

$$\begin{aligned} \langle i_p, i_q | (\mathbb{1}_p \otimes \text{DFT}_q) \tilde{\rho} (\mathbb{1}_p \otimes \text{DFT}_q^\dagger) | j_p, j_q \rangle \\ = \frac{1}{q} \sum_{s_q, t_q=0}^{q-1} e^{\frac{2\pi i}{q} (i_q s_q - \bar{p} j_q \bar{p} t_q)} \langle i_p, s_q | \tilde{\rho} | j_p, t_q \rangle, \end{aligned}$$

where we used the fact that $\langle j_p, t_q | \mathbb{1}_p \otimes \text{DFT}_q^\dagger | j_p, j_q \rangle = \langle \bar{p} t_q | \text{DFT}_q^\dagger | \bar{p} j_q \rangle$. From substituting this in along with $\langle i_p, s_q | \tilde{\rho} | j_p, t_q \rangle = Q_{i_p, s_q; j_p, t_q} / \langle j_p, t_q | i_p, s_q \rangle$, expanding out the ratio $\langle j_p, j_q | i_p, i_q \rangle / \langle j_p, t_q | i_p, s_q \rangle$ and factorizing, we obtain

$$Q_{i_p, i_q; j_p, j_q} \rightarrow \frac{1}{q} \sum_{s_q, t_q=0}^{q-1} e^{\frac{2\pi i}{q} (i_q + \bar{p} t_q)(s_q - \bar{p} j_q)} Q_{i_p, s_q; j_p, t_q} \quad (13)$$

which, in general, is not a covariant transformation. Furthermore, for a generic choice of $Q(\rho)$ there is no reason to expect that $\mathcal{N}(Q(U_\star \rho U_\star^\dagger)) = \mathcal{N}(Q(\rho))$, and indeed we have found examples where this is not the case. Hence, $U_\star \notin \mathcal{U}_\mathcal{N}$.

Finally, we show that no positivity-preserving unitaries can exist beyond types I, II, and III. Inner product preservation under U is again the key constraint. Each set $\mathcal{A}, \mathcal{B}, \mathcal{C}_{p,q}, \mathcal{C}_{q,p}$ forms an orthonormal basis. The inner products between states across different sets are as follows:

Basis pair	Possible overlap magnitudes
$(\mathcal{A}, \mathcal{B}), (\mathcal{C}_{p,q}, \mathcal{C}_{q,p})$	$1/\sqrt{pq}$
$(\mathcal{A}, \mathcal{C}_{p,q}), (\mathcal{B}, \mathcal{C}_{q,p})$	$0, 1/\sqrt{q}$
$(\mathcal{A}, \mathcal{C}_{q,p}), (\mathcal{B}, \mathcal{C}_{p,q})$	$0, 1/\sqrt{p}$

Without loss of generality, suppose that the image $U(\mathcal{A})$ is “split,” so that U maps $|a_1\rangle$ and $|a_2\rangle$ to two different basis sets. If these two sets are mutually unbiased—i.e., $\mathcal{A}$ and $\mathcal{B}$, or $\mathcal{C}_{q,p}$ and $\mathcal{C}_{p,q}$, then this implies $|\langle a_1 | U^\dagger U | a_2 \rangle| \neq 0$. On the other hand, if these sets are not mutually unbiased, then no matter which set U maps $|b_i\rangle \in \mathcal{B}$ to, either $|\langle a_1 | U^\dagger U | b_i \rangle| \neq 1/\sqrt{d}$ or $|\langle a_2 | U^\dagger U | b_i \rangle| \neq 1/\sqrt{d}$. In all cases, this implies that U does not preserve the inner product, so (by the same reasoning as for $\mathcal{A}$) the image of each basis set cannot be split across distinct basis sets. In effect, only types I, II, and III unitaries are possible. We also note that by symmetry, the above lemma straightforwardly applies to the case of $U_\star = P^\dagger (\text{DFT}_p \otimes \mathbb{1}_q) P$, which is another instance of a type III unitary. ■

Although in general the action of $U_\star$ on nonreal KD distributions is not covariant, it is still more straightforward to describe over generic unitaries—for which a full construction of the superoperator $\hat{\mathcal{E}}_U$ is typically required. Regardless of this fact, the presence of such unitaries in any KD-based classical simulation algorithm poses an additional difficulty. We discuss the implications of this result in Sec. IV.

KD-stochastic unitaries. We now turn to the question of identifying unitaries U which induce stochastic superoperators $\hat{\mathcal{E}}_U$ in the vectorized picture. Stochastic matrices have the property of preserving the ℓ_1 norm of KD-positive inputs. However, we have seen that positivity-preserving unitaries do not need to induce a stochastic $\hat{\mathcal{E}}_U$ to preserve positivity. For example, if the transition matrix V is Hermitian, then the unitary $U = V$ has a nonstochastic KD superoperator, but maps the KD matrix $Q(\rho)$ to its Hermitian conjugate:

$$Q(\rho)_{ij} \rightarrow \langle b_j | U^\dagger U | a_i \rangle \langle a_i | U \rho U^\dagger | b_j \rangle = Q_{ji}^*(\rho).$$

This corresponds to a $\mathcal{N}$ -preserving unitary of type II. In contrast, for the odd-dimensional discrete Wigner distribution such a situation does not occur, as all positivity-preserving

gates induce stochastic superoperators [5,14]. We now show that KD-stochastic unitaries are precisely of type I.

Theorem 3. For a KD distribution defined on the bases $\mathcal{A} = \{|a_i\rangle\}$ and $\mathcal{B} = \{|b_j\rangle\}$, a unitary $U \in \mathcal{U}_{\text{stoch}}$ if and only if $U \in M_d \cap VM_d V^\dagger$. In other words, U satisfies

$$U|a_i\rangle = e^{i\theta_i}|a_{\sigma(i)}\rangle, \quad U|b_j\rangle = e^{i\phi_j}|b_{\tau(j)}\rangle,$$

where $\sigma, \tau \in S_d$. It follows that $\mathcal{U}_{\text{stoch}}$ consists of $\mathcal{N}$ -preserving type I unitaries.

Proof. Suppose $U \in M_d \cap VM_d V^\dagger$, i.e., U satisfies $U|a_i\rangle = e^{i\theta_i}|a_{\sigma(i)}\rangle$ and $U|b_j\rangle = e^{i\phi_j}|b_{\tau(j)}\rangle$. Then,

$$\begin{aligned} (\hat{\mathcal{E}}_U)_{ij,kl} &= \frac{\langle b_j|a_i\rangle}{\langle b_l|U^\dagger U|a_k\rangle} e^{i\theta_k} \langle a_i|a_{\sigma(k)}\rangle e^{-i\phi_l} \langle b_{\tau(l)}|b_j\rangle \\ &= \delta_{i,\sigma(k)} \delta_{j,\tau(l)} \frac{\langle b_j|a_i\rangle}{\langle b_{\tau(l)}|a_{\sigma(k)}\rangle} \frac{e^{i(\theta_k - \phi_l)}}{e^{i(\theta_k - \phi_l)}} \\ &= \delta_{i,\sigma(k)} \delta_{j,\tau(l)}, \end{aligned}$$

so $\hat{\mathcal{E}}_U \in S_d \times S_d$ is the Kronecker product of two permutation matrices.

For the other direction, suppose the induced superoperator $\hat{\mathcal{E}}_U$ is stochastic. Then, all of its entries are non-negative. By Eq. (5), it will always have a quasistochastic inverse $\hat{\mathcal{E}}_U^{-1}$. By Eq. (6), this inverse will only contain non-negative entries and thus also be stochastic. A basic fact of linear algebra [50] is that if a matrix and its inverse are both stochastic, then that matrix must be a permutation. Therefore, $\hat{\mathcal{E}}_U$ must be a permutation. Hence, for each pair of indices i, j there is a unique pair of indices i^*, j^* such that $(\hat{\mathcal{E}}_U)_{ij,i^*j^*} \neq 0$. By Eq. (4), $\langle a_i|U|a_{i^*}\rangle \langle b_j|U^\dagger|b_{j^*}\rangle \neq 0$, therefore $\langle a_i|U|a_{i^*}\rangle \neq 0$ and $\langle b_j|U^\dagger|b_{j^*}\rangle \neq 0$. Holding i, j, j^* fixed, we deduce that $\langle a_i|U|a_k\rangle = 0$ for $k \neq i^*$, and holding i, j, i^* fixed we deduce that $\langle b_j|U^\dagger|b_l\rangle = 0$ for $l \neq j^*$. Hence, U is a generalized permutation on the bases $\mathcal{A}$ and $\mathcal{B}$. ■

Randomly sampled bases. Given the stringent conditions for their existence, whether $\mathcal{U}_{\mathcal{N}}$, $\mathcal{U}_{\mathcal{N}+}$, and $\mathcal{U}_{\text{stoch}}$ contain nontrivial unitaries is highly sensitive to the symmetries of the transition matrix V . Consequently, for most KD distributions this is not the case.

Remark 2. The vast majority of Kirkwood-Dirac distributions do not admit nontrivial positivity-preserving, $\mathcal{N}$ -preserving, or KD-stochastic unitaries.

Proof. (sketch) We already know from Ref. [42] that for a generic choice of V [with probability one, under the Haar measure on $U(d)$], $\mathcal{E}_{\text{KD}+} = \text{conv}(\mathcal{A} \cup \mathcal{B})$, and $\mathcal{C} = \emptyset$. Therefore, only type I and II can exist. In the first case, $U \in M_d \cap VM_d V^\dagger$. Elements of this set are those which satisfy $U \in M_d$ and $V^\dagger UV \in M_d$. Hence, for some $U = D_\alpha P_\sigma$ there must exist some $D_\beta P_\tau$ such that $V^\dagger D_\alpha P_\sigma V = D_\beta P_\tau$. Therefore,

$$D_\alpha P_\sigma V = V D_\beta P_\tau \rightarrow V_{\sigma(i)\tau(j)} = \alpha_{\sigma(i)} \beta_{\tau(j)}^* V_{ij},$$

where P_σ and P_τ are permutation matrices, and the above holds for all i, j . Hence, $|V_{\sigma(i)\tau(j)}| = |V_{ij}|$, implying that the modulus matrix $|V|$ must be invariant under some row and column permutation σ, τ . Excluding the identity permutations, we therefore require at least one pair of distinct entries of V to have the same modulus (this is a necessary, although not sufficient condition). Under the Haar measure on $U(d)$ the probability of this occurring is zero. Hence, for a generic

choice of V , no nontrivial type I unitaries exist. Similarly, for nontrivial type II unitaries in $VM_d \cap M_d V^\dagger$ to exist, the necessary condition is that $|V_{i,\tau(j)}| = |V_{j,\sigma^{-1}(i)}|$ under some nonidentity pair σ, τ . Again, under the Haar measure this happens with probability zero. Therefore, for a randomly sampled V , with probability one we have $\mathcal{U}_{\mathcal{N}} = \mathcal{U}_{\mathcal{N}+} = \mathcal{U}_{\text{stoch}} = \{e^{i\theta} \mathbb{1}\}$. ■

Examples of type I and II unitaries. Although type I and II unitaries are rare, they do exist for symmetric choices of V . For example, in the Fourier-conjugate distribution in any dimension, type I unitaries are given by the Weyl-Heisenberg group [40,41] (see Appendix B for a definition), whereas type II unitaries are given by a product of the Weyl-Heisenberg unitaries and the DFT matrix. In multiqubit systems (where $\mathcal{A}$ and $\mathcal{B}$ are the computational and Hadamard-transformed bases), the positivity-preserving group is generated by single-qubit Pauli gates and CNOT for type I, and $U = H^{\otimes n}$ for type II [51]. Notably, single-qubit Hadamard gates are of neither type and can be shown to not preserve positivity. For non-Fourier distributions, in the spin-1 distribution presented in Ref. [43] with an involutory transition matrix (referred to as U^*), one can identify type I unitaries with any 3×3 permutation matrix on the $\mathcal{A}$ basis, and type II unitaries with the product of any permutation and U^* . As the states in the set $\mathcal{C}$ for the spin-1 system are not pairwise orthogonal, by a similar argument to Theorem 1 we can show that no other types of positivity-preserving unitaries can exist. Finally, we remark that our classification is not exhaustive, since there may be other positivity-preserving generalized permutations on $\mathcal{A} \cup \mathcal{B} \cup \mathcal{C}$ not of the three types we have identified. For example, it is in principle possible that such unitaries map some subset of $\mathcal{A}$ to a subset of $\mathcal{B}$, and some other subset of $\mathcal{A}$ to a subset of $\mathcal{C}$. In our search we have not found any such examples—whether they could exist for an arbitrary choice of V can usually be ruled out by symmetry arguments (namely the preservation of inner products between all the positive pure states under U , as we have argued in Theorem 1). These could be used to fully characterize $\mathcal{U}_{\mathcal{N}+}$ for DFT_d in the general case, which we leave for future work.

Completeness of our classification. Collecting the results of this section, we formulate a general method for classifying positivity-preserving unitaries for arbitrary distributions: if $\mathcal{C} = \emptyset$, then only types I, II can exist (Lemma 1). As they are always $\mathcal{N}$ preserving (Lemma 2), this concludes the classification. If $\mathcal{C} \neq \emptyset$, one must check whether generalized permutations on $\mathcal{E}_{\text{KD}+}^{\text{pure}}$ beyond types I, II exist. Typically, they can be ruled out using symmetry arguments. If they are found, and $\mathcal{E}_{\text{KD}+} = \text{conv}(\mathcal{E}_{\text{KD}+}^{\text{pure}})$, then this concludes the classification. Otherwise, one must also check if they preserve positivity of $\rho \in \mathcal{E}_{\text{KD}+} \setminus \text{conv}(\mathcal{E}_{\text{KD}+}^{\text{pure}})$. Overall, our classification is complete for three cases: for the Haar-random choice of V , our method terminates at the first step. For $V = \text{DFT}_{p^k}$, it terminates at the second. Finally, for $V = \text{DFT}_{pq}$, it terminates at the third.

IV. ESTIMATING BORN RULE PROBABILITIES VIA KD DISTRIBUTIONS

We now apply the results of Sec. III to the problem of estimating Born rule outcome probabilities via KD

distributions. Throughout this section, “efficient simulation” means additive-error estimation of Born outcome probabilities, with sample complexity polynomial in $(1/\epsilon, \log(1/\delta))$, and the circuit size, assuming efficient access to the relevant KD quasiprobabilities and superoperator elements. To do this, we modify the algorithm of Ref. [14], which makes use of a Monte Carlo-style method to estimate the outcome probability via Eq. (7). Consider an n -qudit input state ρ , a quantum circuit U , and a measurement operator F . We first decompose U into a product of one- and two-qudit gates $U = U_N \cdots U_1$, and write pairs of indices [summed over in (7)] as $(i_0 j_0) = I_0, \dots, (i_N j_N) = I_N$. The probability of the measurement outcome is given by

$$\text{Tr}(FU\rho U^\dagger) = \sum_{I_0, \dots, I_N} F_{I_N} (\hat{\mathcal{E}}_{U_N})_{I_N, I_{N-1}} \cdots (\hat{\mathcal{E}}_{U_2})_{I_2, I_1} (\hat{\mathcal{E}}_{U_1})_{I_1, I_0} Q(\rho)_{I_0}. \quad (14)$$

Assumptions. We assume that the objects $|Q\rangle\rangle$, $\langle\langle F|$, and $\hat{\mathcal{E}}_{U_m}$ are efficiently describable (for example, when the state preparation and measurement is conducted in a product state basis and each U_m acts on at most two qudits), and that individual elements from their rows and columns can be sampled efficiently under some probability distribution. We can use this decomposition to classically estimate Born rule outcome

probabilities. We make use of several norms:

$$\begin{aligned} \| |Q\rangle\rangle \|_1 &= \sum_I |Q(\rho)_I| = \mathcal{N}(Q(\rho)) \\ \|\langle\langle F| \|_1 &= \sum_I |F_I| = \mathcal{N}(F) \quad \|\langle\langle F| \|_\infty = \max_I |F_I| \\ \|(\hat{\mathcal{E}}_U)_{\cdot, I} \|_1 &= \sum_J |(\hat{\mathcal{E}}_U)_{J, I}| \\ \|\hat{\mathcal{E}}_U \|_1 &= \max_I \sum_J |(\hat{\mathcal{E}}_U)_{J, I}| = \max_I \|(\hat{\mathcal{E}}_U)_{\cdot, I} \|_1, \end{aligned}$$

where the first two are KD total nonpositivities, the third is the largest absolute element of the POVM dual vector $\langle\langle F|$, the fourth is the ℓ_1 norm of the column I of $\hat{\mathcal{E}}_U$, and the last is the induced ℓ_1 norm on $\hat{\mathcal{E}}_U$.

The probability estimation protocol. We proceed as follows: first, take the absolute values of the quasiprobabilities in $|Q\rangle\rangle$, and randomly sample an index pair $(i_0, j_0) = I_0$ with probability $\text{Pr}(I_0) = |Q(\rho)_{I_0}|/\mathcal{N}(Q(\rho))$. Then, randomly sample the index pair I_1 with probability $\text{Pr}(I_1) = |(\hat{\mathcal{E}}_{U_1})_{I_1, I_0}|/\|(\hat{\mathcal{E}}_{U_1})_{\cdot, I_0}\|_1$. Repeat this up to I_{N-1} , and then sample I_N with probability $\text{Pr}(I_N) = |(\hat{\mathcal{E}}_{U_N})_{I_N, I_{N-1}}|/\|(\hat{\mathcal{E}}_{U_N})_{\cdot, I_{N-1}}\|_1$. After sampling $I_0, I_1, \dots, I_N$, also compute the complex phases $\text{Ph}(Q_{I_0}) = Q(\rho)_{I_0}/|Q_{I_0}|$, and $\text{Ph}((\hat{\mathcal{E}}_{U_k})_{I_k, I_{k-1}}) = (\hat{\mathcal{E}}_{U_k})_{I_k, I_{k-1}}/|(\hat{\mathcal{E}}_{U_k})_{I_k, I_{k-1}}|$ for $k \in [N]$. Finally, calculate the complex random variable $Z(I_0, \dots, I_N)$ and its real part:

$$X(I_0, \dots, I_N) = \text{Re}(Z(I_0, \dots, I_N)) = \text{Re}\left(F_{I_N} \left[\prod_{k=1}^N \|(\hat{\mathcal{E}}_{U_k})_{\cdot, I_{k-1}}\|_1 \text{Ph}((\hat{\mathcal{E}}_{U_k})_{I_k, I_{k-1}}) \right] \mathcal{N}(Q(\rho)) \text{Ph}(Q_{I_0}) \right).$$

This is then repeated many times, with the average $\bar{X}$ forming an estimate of $\text{Tr}(FU\rho U^\dagger)$. In expectation (over the choices of random index pairs),

$$\begin{aligned} \mathbb{E}(Z(I_0, \dots, I_N)) &= \text{Tr}(FU\rho U^\dagger), \\ \mathbb{E}(X(I_0, \dots, I_N)) &= \text{Tr}(FU\rho U^\dagger). \end{aligned}$$

Now, define the total induced nonpositivity as the product of induced ℓ_1 norms of the intermediate superoperators $\hat{\mathcal{E}}_{U_k}$ and the largest absolute element of $\langle\langle F|$:

$$\mathcal{N}_I = \left[\prod_{k=1}^N \|\hat{\mathcal{E}}_{U_k}\|_1 \right] \|\langle\langle F| \|_\infty$$

Each $Z(I_0, \dots, I_N)$ is then bounded to have magnitude:

$$|Z(I_0, \dots, I_N)| \leq \mathcal{N}(Q(\rho)) \mathcal{N}_I.$$

As $Z(I_0, \dots, I_N)$ is a complex random variable, in order to bound the number of samples required we can consider its real part, also bounded as $|X(I_0, \dots, I_N)| \leq \mathcal{N}(Q(\rho)) \mathcal{N}_I$, and use the Hoeffding inequality (in the same way as was done in Ref. [14]) to show that estimating the Born rule probabilities up to precision ϵ (and success probability $1 - \delta$) requires $s(\epsilon, \delta)$

samples, where

$$s(\epsilon, \delta) = \frac{2}{\epsilon^2} \mathcal{N}(Q(\rho))^2 \mathcal{N}_I^2 \ln(2/\delta).$$

Clearly, the runtime of the estimation algorithm is bounded by $O(\mathcal{N}(Q(\rho))^2 \mathcal{N}_I^2)$, and thus the efficiency of the estimation procedure is determined by the total nonpositivity $\mathcal{N}(Q(\rho))$ of the input state, multiplied by the total induced nonpositivity $\mathcal{N}_I$. In the case of the Wigner distribution, the input and induced nonpositivities are independent. For example, when a Clifford circuit satisfies $\mathcal{N}_I = O(1)$ the additional sample complexity of estimation on a nonpositive input is multiplicative in $\mathcal{N}(Q(\rho))^2$. We show that, for the KD distribution, this happens by default with type I unitaries. For type II unitaries, the same holds once their covariance is accounted for. For type III unitaries, the induced nonpositivity implicitly depends on whether the input distribution contains complex entries.

Incorporating type I, II unitaries. We now show how to accommodate KD positivity preserving unitaries in the algorithm. For type I unitaries, we have already established via Theorem 3 that the induced superoperator $\hat{\mathcal{E}}_U$ is a permutation matrix. Hence, for such unitaries the induced nonpositivity is $\|\hat{\mathcal{E}}_U\|_1 = 1$, and no modification is necessary. For type II unitaries, in general $\|\hat{\mathcal{E}}_U\|_1 > 1$. However, Lemma 2 asserts that for any state ρ , $Q(U\rho U^\dagger)_{ij} = Q_{\sigma^{-1}(j), \tau^{-1}(i)}^*(\rho)$ for

some $\sigma, \tau \in S_d$. Suppose that the circuit U contains a type II unitary U_k at step k . We may write $V = U_N \cdots U_{k+1}$ and $W = U_{k-1} \cdots U_1$, so that $U = VU_kW$. Also, writing $(\sigma^{-1}(j), \tau^{-1}(i)) = \gamma^{-1}(I)$ and $Q(U\rho U^\dagger)_I = Q(\rho)_{\gamma^{-1}(I)}$ as a shorthand, Eq. (14) becomes

$$\begin{aligned}
& \text{Tr}(F(VU_kW)\rho(VU_kW)^\dagger) \\
&= \sum_{H,I_k,J,L} F_H(\hat{\mathcal{E}}_V)_{H,I_k}(\hat{\mathcal{E}}_{U_k})_{I_k,J}(\hat{\mathcal{E}}_W)_{J,L}Q(\rho)_L \\
&= \sum_{H,I_k,J} F_H(\hat{\mathcal{E}}_V)_{H,I_k}(\hat{\mathcal{E}}_{U_k})_{I_k,J}Q(W\rho W^\dagger)_J \\
&= \sum_{H,I_k} F_H(\hat{\mathcal{E}}_V)_{H,I_k}Q(U_kW\rho W^\dagger U_k^\dagger)_{I_k} \\
&= \sum_{H,I_k} F_H(\hat{\mathcal{E}}_V)_{H,I_k}Q(W\rho W^\dagger)_{\gamma^{-1}(I_k)}^* \\
&= \sum_{H,I_k,L} F_H(\hat{\mathcal{E}}_V)_{H,I_k}(\hat{\mathcal{E}}_W)_{\gamma^{-1}(I_k),L}^*Q(\rho)_L^* \\
&= \sum_{H,J,L} F_H(\hat{\mathcal{E}}_V)_{H,\gamma(J)}(\hat{\mathcal{E}}_W)_{J,L}^*Q(\rho)_L^*. \tag{15}
\end{aligned}$$

Hence, the algorithm may be modified as follows: Whenever a type II unitary U is encountered at step k , proceed deterministically, setting $I_k = \gamma(I_{k-1})$, $\|(\hat{\mathcal{E}}_{U_k})_{I_k,I_{k-1}}\|_1 = 1$ and $\text{Ph}((\hat{\mathcal{E}}_{U_k})_{I_k,I_{k-1}}) = 1$. Furthermore, complex conjugate all phases as $\text{Ph}(Q_{I_0}) \rightarrow \text{Ph}(Q_{I_0})^*$ and $\text{Ph}((\hat{\mathcal{E}}_{U_m})_{I_m,I_{m-1}}) \rightarrow \text{Ph}((\hat{\mathcal{E}}_{U_m})_{I_m,I_{m-1}})^*$ for all $m < k$. The rest of the algorithm proceeds as normal, with $\tilde{X}$ forming the estimate for $\text{Tr}(FU\rho U^\dagger)$. This modification directly accounts for the covariant transformations under type II, ensuring that the induced ℓ_1 norm of their superoperators does not contribute to $\mathcal{N}_I$.

Incorporating type III unitaries. For type III unitaries, there is an additional complication. As remarked in Lemma 3, such unitaries do not generally induce a covariant transformation on the KD distribution, and thus the induced nonpositivity satisfies $\|\hat{\mathcal{E}}_U\|_1 > 1$. On the other hand, as shown in Theorem 2, the type III unitary $U_\star$ exhibits covariance on KD-real inputs, permuting their entries as $Q(U_\star\rho U_\star^\dagger)_{ij} = Q(\rho)_{\gamma^{-1}(ij)}$ for some $\gamma^{-1} \in S_{d^2}$. The exact form of γ is given in Appendix D: the mapping is obtained via the Chinese remainder theorem (CRT) decompositions of (i, j) and modular arithmetic, which is computationally efficient to implement. Thus, if the state $(U_{k-1} \cdots U_1)\rho(U_{k-1} \cdots U_1)^\dagger$ is KD-real, type III unitaries can be incorporated into the estimation algorithm in a similar way to type II unitaries, i.e., by deterministically setting $\|(\hat{\mathcal{E}}_{U_k})_{I_k,I_{k-1}}\|_1 = \text{Ph}((\hat{\mathcal{E}}_{U_k})_{I_k,I_{k-1}}) = 1$ and $I_k = \gamma(I_{k-1})$ [cf. Eq. (15)] whenever they appear. On the other hand, if the input at step k is nonreal, covariance fails, and this modification is not possible. Instead, sampling from the columns of $\hat{\mathcal{E}}_U$ becomes necessary, contributing a multiplicative factor to $\mathcal{N}_I$ for each instance of a type III unitary. This leads to a sharp increase in sample complexity between KD-real and nonreal distributions. Consider, for example, a positivity-preserving circuit containing type III unitaries. If the input state is KD-positive (and thus KD-real), then the total induced nonpositivity $\mathcal{N}_I$ is at most $O(1)$, and the output probabilities can be efficiently estimated. However, if any $Q(\rho)_{ij} \in \mathbb{C}$ then

in the worst case $\mathcal{N}_I$ grows exponentially large in the number of type III unitaries, and efficient classical estimation fails (such circuits may still be efficiently simulable with other methods, however). In this sense, the presence of type III unitaries makes the induced nonpositivity of the circuit implicitly dependent on the reality of the input distribution. We find that classical simulation via KD distributions is a more intricate problem than in the Wigner case, where “conditional” covariance of gates does not occur.

Finally, we note that the above amendments can also be easily incorporated into the sampling algorithm by Mari and Eisert [4], which leverages covariance to efficiently sample from the output distribution of a quantum circuit with positive Wigner function inputs and Clifford gates. Hence, for circuits composed only of I, II, III unitaries, if the input state is KD-positive, then each deterministic modification can be applied, and the output distribution can be efficiently sampled. In circuits containing other gates, the type III unitary rule is only justified when the KD distribution of the state preceding the unitary is known to be real.

Consequences for resource theories. We conclude by combining the results of Secs. III and IV into a no-go result for resource theories of KD nonpositivity on $V = \text{DFT}_{pq}^{\otimes n}$.

Theorem 4. For KD distributions defined on $V = \text{DFT}_{pq}^{\otimes n}$, any resource theory that takes KD nonpositivity as a monotone cannot also declare all positivity-preserving, efficiently simulable unitaries to be free operations. In particular, it must either exclude the unitary $U_\star^{\otimes n}$ from its free operations, or else abandon monotonicity of KD nonpositivity under its free operations.

Proof. As proven in Lemma 3, for $d = pq$ the type III unitary $U_\star$ always exists. In Theorem 2 and Appendix D, we show that $U_\star$ preserves $\mathcal{N}(Q)$ for all KD-positive states. However, it does not generally preserve $\mathcal{N}(Q)$ for nonreal states. From $U_\star = P^\dagger(\mathbb{1}_p \otimes \text{DFT}_q)P$ [Eq. (11)] we also have that $U_\star^2$ is a permutation and $U_\star^4 = \mathbb{1}$. Suppose that $U_\star$ is included in the free operations of a resource theory of KD nonpositivity. If there exists a state ρ such that $\mathcal{N}(Q(U_\star\rho U_\star^\dagger)) < \mathcal{N}(Q(\rho))$, then (writing $\rho_k = U_\star^\dagger\rho(U_\star^\dagger)^k$) it must hold true that $\mathcal{N}(Q(U_\star\rho_k U_\star^\dagger)) > \mathcal{N}(Q(\rho_k))$ for some ρ_k ; otherwise, it would hold that $\mathcal{N}(Q(\rho)) = \mathcal{N}(Q(U_\star\rho_k U_\star^\dagger)) < \mathcal{N}(Q(\rho))$, which is a contradiction. Similarly, if $\mathcal{N}(Q(U_\star\rho U_\star^\dagger)) > \mathcal{N}(Q(\rho))$, there must exist a state ρ_k such that the total nonpositivity decreases under $U_\star$. Unless $U_\star$ is $\mathcal{N}$ preserving for all states (which we have shown is not the case), there will exist states such that the total nonpositivity increases under $U_\star$. Thus, $\mathcal{N}(Q)$ is not a monotone under the free operations. On the other hand, we have shown that for any KD-positive state ρ evolution by type I, II, III is classically efficiently simulable, as such unitaries are covariant with respect to positive KD distributions. Hence, if $U_\star$ is not included in the free operations, then there exist positivity-preserving, efficiently simulable unitaries which are not free, and the resource theory fails to capture the full set of classically simulable operations. ■

Theorem 4 implies that constructing resource theories of KD nonpositivity on the $V = \text{DFT}_{pq}^{\otimes n}$ family of KD distributions is likely to be challenging. We remark that as $U_\star$ is KD reality preserving, one possible avenue to bypass this no-go result is to consider the real part of the KD distribution as a resource, in effect working with the Margenau-Hill

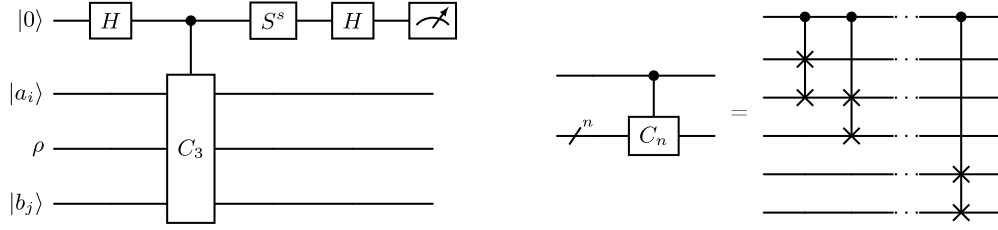


FIG. 1. (left): The cycle test for estimating $\text{Re}[Q(\rho)_{ij}]$ ($s = 0$), and $\text{Im}[Q(\rho)_{ij}]$ ($s = 1$). H is the Hadamard gate, and $S = \text{diag}(1, i)$. After many measurements, $Q(\rho)_{ij}$ is estimated from the outcome frequencies via $p(0)_{s=0} = \{1 + \text{Re}[Q(\rho)_{ij}]\}/2$ and $p(0)_{s=1} = \{1 + \text{Im}[Q(\rho)_{ij}]\}/2$. (right): The cycle gate may be implemented by a cascade of qudit controlled-SWAP gates.

distribution [52,53]. This forms an intriguing open question for future work.

Note added. Recently, the results of Remark 2 and Lemma 1 were introduced in a revised preprint of our paper. A revised version of Ref. [42] also appeared containing analogous results, obtained independently of ours in the Ph.D. thesis of one of its authors [54].

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DATA AVAILABILITY

There are no publicly available research data or software supporting this paper. Requests for further information or data should be sent to the authors.

APPENDIX A: ESTIMATING KD SUPEROPERATOR ELEMENTS

In this section, we extend the cycle test algorithm of Refs. [33,47] to provide a new method for experimental measurement of KD superoperator elements $(\hat{\mathcal{E}}_U)_{ij,kl}$ induced by an unknown unitary U and any informationally complete choice of bases $\mathcal{A}, \mathcal{B}$.

In general, it is not possible to directly sample from the KD distribution $Q(\rho)_{ij} = \text{Tr}(|b_j\rangle\langle b_j|a_i\rangle\langle a_i|\rho)$, since the outer products $\langle b_j|a_i\rangle\langle b_j|a_i\rangle$ are not positive semidefinite and thus cannot form POVM elements. However, a procedure was given in Ref. [33] for estimating the quasiprobabilities $Q(\rho)_{ij}$ using a generalization of the SWAP test, known as the cycle test [47]. The circuit is shown in Fig. 1. Similarly to the case of KD distributions, one can estimate elements $(\hat{\mathcal{E}}_U)_{ij,kl}$ of a KD superoperator induced by a unitary U , assuming $\mathcal{A}, \mathcal{B}$ are informationally complete. To do this, we can modify the cycle test algorithm. First, we rewrite the superoperator elements of Eq. (4) as

$$(\hat{\mathcal{E}}_U)_{ij,kl} = \frac{1}{|\langle b_l|a_k\rangle|^2} \text{Tr}(|a_i\rangle\langle a_i|U|a_k\rangle\langle a_k|U^\dagger \\ \times U|b_l\rangle\langle b_l|U^\dagger|b_j\rangle\langle b_j|).$$

The quantity $|\langle b_l|a_k\rangle|^2(\hat{\mathcal{E}}_U)_{ij,kl}$ then forms a Bargmann invariant, which (given access to U and the ability to prepare states from $\mathcal{A}, \mathcal{B}$) can be estimated using a four-state cycle gate C_4 , as shown in Fig. 2. One may estimate this quantity and divide by $|\langle b_l|a_k\rangle|^2$, which may also be estimated separately via the SWAP test if the states from $\mathcal{A}, \mathcal{B}$ are unknown. Unfortunately, as this method relies on an insertion of $U^\dagger U = \mathbb{1}$ it does not allow for the estimation of matrix elements of nonunitary completely positive and trace-preserving (CPTP) maps; we leave the extension of our procedure to nonunitary CPTP maps as an open question.

APPENDIX B: SELF-SIMILARITY OF KD DISTRIBUTIONS

During our study of Fourier-conjugate KD distributions we identified a self-similarity property, which allows for a more compressed representation of KD distributions. We present it here as a standalone result, which may be of independent interest.

Lemma 4. The multidimensional discrete Fourier transform $\hat{Q}$ of a Kirkwood-Dirac distribution on n qudits with transition matrix $V = \text{DFT}_d^{\otimes n}$ is self-similar, satisfying the constraint:

$$\hat{Q}(\mathbf{d} - \mathbf{x}, \mathbf{d} - \mathbf{y}) = \omega^{\mathbf{x} \cdot \mathbf{y}} [\hat{Q}(\mathbf{x}, \mathbf{y})]^*. \quad (\text{B1})$$

Proof. Substituting Eq. (2) into $\rho = \rho^\dagger$ and taking appropriate inner products, we obtain the following set of

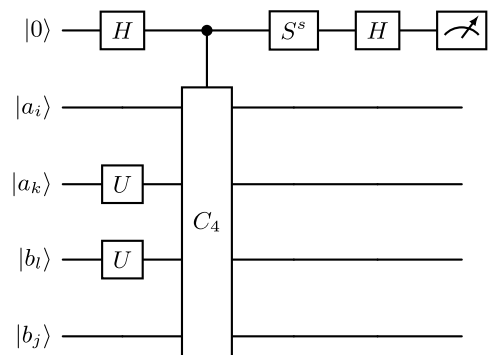


FIG. 2. Cycle test for estimating KD superoperator elements. The circuit estimates the quantity $|\langle b_l|a_k\rangle|^2(\hat{\mathcal{E}}_U)_{ij,kl}$, where $p(0)_{s=0} = \{1 + |\langle b_l|a_k\rangle|^2 \text{Re}[(\hat{\mathcal{E}}_U)_{ij,kl}]\}/2$, and $p(0)_{s=1} = \{1 + |\langle b_l|a_k\rangle|^2 \text{Im}[(\hat{\mathcal{E}}_U)_{ij,kl}]\}/2$.

constraints on Q_{ij} :

$$Q_{uv} = \sum_{ij} \frac{\langle a_i | b_v \rangle \langle b_v | a_u \rangle \langle a_u | b_j \rangle}{\langle a_i | b_j \rangle} Q_{ij}^*. \quad (\text{B2})$$

For the Fourier-conjugate KD distribution, we label the reference bases as follows:

$$\mathcal{A} = \{|\mathbf{i}\rangle = |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle \mid \mathbf{i} \in \mathbb{Z}_d^n\},$$

$$\mathcal{B} = \{\text{DFT}_d^{\otimes n} |\mathbf{j}\rangle = \text{DFT}_d |j_1\rangle \otimes \cdots \otimes \text{DFT}_d |j_n\rangle \mid \mathbf{j} \in \mathbb{Z}_d^n\},$$

where $\mathbf{i}, \mathbf{j} \in \mathbb{Z}_d^n$ are vectors with inner product

$$\mathbf{i} \cdot \mathbf{j} = \sum_{k=1}^n i_k j_k \pmod{d},$$

and entry-wise addition modulo d :

$$\mathbf{i} + \mathbf{j} = (i_1 + j_1 \pmod{d}, \dots, i_n + j_n \pmod{d}).$$

We also write $\mathbf{d} = (d, d, \dots, d)$ as a vector with d in each entry. The inner products then take the form

$$\langle a_i | b_j \rangle = d^{-n/2} \omega^{\mathbf{i} \cdot \mathbf{j}}, \quad \omega = e^{\frac{2\pi i}{d}}.$$

We write elements of the KD distribution as $Q(\mathbf{i}, \mathbf{j})$, where they take the explicit form:

$$Q(\mathbf{i}, \mathbf{j}) = d^{-n} \sum_{\mathbf{k} \in \mathbb{Z}_d^n} \omega^{\mathbf{k} \cdot \mathbf{j} - \mathbf{i} \cdot \mathbf{j}} \langle \mathbf{i} | \psi \rangle \langle \psi | \mathbf{k} \rangle. \quad (\text{B3})$$

The constraints of Eq. (B2) simplify into the following:

$$\begin{aligned} Q(\mathbf{u}, \mathbf{v}) &= d^{-n} \sum_{\mathbf{i}, \mathbf{j} \in \mathbb{Z}_d^n} \omega^{\mathbf{i} \cdot \mathbf{v} - \mathbf{u} \cdot \mathbf{v} + \mathbf{u} \cdot \mathbf{j} - \mathbf{i} \cdot \mathbf{j}} Q^*(\mathbf{i}, \mathbf{j}) \\ &= d^{-n} \sum_{\mathbf{i}, \mathbf{j} \in \mathbb{Z}_d^n} \omega^{-(\mathbf{i} - \mathbf{u}) \cdot (\mathbf{j} - \mathbf{v})} Q^*(\mathbf{i}, \mathbf{j}) \\ &= d^{-n} \sum_{\mathbf{a}, \mathbf{b} \in \mathbb{Z}_d^n} \omega^{-\mathbf{a} \cdot \mathbf{b}} Q^*(\mathbf{u} - \mathbf{a}, \mathbf{v} - \mathbf{b}), \end{aligned}$$

where we have set $\mathbf{i} - \mathbf{u} = -\mathbf{a}$ and $\mathbf{j} - \mathbf{v} = -\mathbf{b}$ in the penultimate sum. This is a convolution of $Q^*(\mathbf{u}, \mathbf{v})$ with a matrix Ω^* , where $\Omega(\mathbf{a}, \mathbf{b}) = d^{-n} \omega^{\mathbf{a} \cdot \mathbf{b}} = d^{-n/2} [\text{DFT}_d^{\otimes n}]_{\mathbf{a}, \mathbf{b}}$ (here, the superscript $*$ denotes complex conjugation whereas $\star$ denotes a convolution). Taking complex conjugates of both sides, we may write

$$Q^*(\mathbf{u}, \mathbf{v}) = \Omega \star Q(\mathbf{u}, \mathbf{v}).$$

The convolution theorem then implies that

$$\widehat{Q}^*(\mathbf{x}, \mathbf{y}) = \widehat{\Omega}(\mathbf{x}, \mathbf{y}) \widehat{Q}(\mathbf{x}, \mathbf{y}), \quad (\text{B4})$$

where $\widehat{Q}(\mathbf{x}, \mathbf{y})$ is the multidimensional, discrete Fourier transform of the KD distribution $Q(\mathbf{x}, \mathbf{y})$. To obtain Eq. (B1) we calculate $\widehat{\Omega}(\mathbf{x}, \mathbf{y})$ and $\widehat{Q}^*(\mathbf{x}, \mathbf{y})$:

$$\begin{aligned} \widehat{\Omega}(\mathbf{x}, \mathbf{y}) &= d^{-n} \sum_{\mathbf{a}, \mathbf{b} \in \mathbb{Z}_d^n} \omega^{\mathbf{a} \cdot \mathbf{b}} \omega^{-\mathbf{a} \cdot \mathbf{x} - \mathbf{b} \cdot \mathbf{y}} \\ &= d^{-n} \sum_{\mathbf{a} \in \mathbb{Z}_d^n} \omega^{-\mathbf{a} \cdot \mathbf{x}} \sum_{\mathbf{b} \in \mathbb{Z}_d^n} \omega^{-\mathbf{b} \cdot (\mathbf{y} - \mathbf{a})} \\ &= d^{-n} \sum_{\mathbf{a} \in \mathbb{Z}_d^n} \omega^{-\mathbf{a} \cdot \mathbf{x}} (d^n \delta_{\mathbf{y}, \mathbf{a}}) = \omega^{-\mathbf{x} \cdot \mathbf{y}}. \end{aligned} \quad (\text{B5})$$

Similarly, the DFT of $Q^*(\mathbf{a}, \mathbf{b})$ is given by

$$\begin{aligned} \widehat{Q}^*(\mathbf{x}, \mathbf{y}) &= \sum_{\mathbf{a}, \mathbf{b} \in \mathbb{Z}_d^n} \omega^{-\mathbf{a} \cdot \mathbf{x} - \mathbf{b} \cdot \mathbf{y}} Q^*(\mathbf{a}, \mathbf{b}) \\ &= \sum_{\mathbf{a}, \mathbf{b} \in \mathbb{Z}_d^n} \omega^{\mathbf{a} \cdot (\mathbf{d} - \mathbf{x}) + \mathbf{b} \cdot (\mathbf{d} - \mathbf{y})} Q^*(\mathbf{a}, \mathbf{b}) \\ &= \left(\sum_{\mathbf{a}, \mathbf{b} \in \mathbb{Z}_d^n} \omega^{-\mathbf{a} \cdot (\mathbf{d} - \mathbf{x}) - \mathbf{b} \cdot (\mathbf{d} - \mathbf{y})} Q(\mathbf{a}, \mathbf{b}) \right)^* \\ &= [\widehat{Q}(\mathbf{d} - \mathbf{x}, \mathbf{d} - \mathbf{y})]^*. \end{aligned} \quad (\text{B6})$$

Substituting Eqs. (B5) and (B6) into (B4) gives us the following:

$$[\widehat{Q}(\mathbf{d} - \mathbf{x}, \mathbf{d} - \mathbf{y})]^* = \omega^{-\mathbf{x} \cdot \mathbf{y}} \widehat{Q}(\mathbf{x}, \mathbf{y}), \quad (\text{B7})$$

and the complex conjugate of Eq. (B7) gives (B1). ■

Lemma 4 shows that $\widehat{Q}$ is determined by choosing one representative from each orbit of the involution $(x, y) \rightarrow (-x, -y)$. For example, if $n = 1$ this simplifies to $\widehat{Q}(d - x, d - y) = e^{\frac{2\pi i xy}{d}} [\widehat{Q}(x, y)]^*$ and the number of independent entries is approximately half of d^2 . For odd d , there is one fixed point $(0, 0)$, so one may choose $(d^2 + 1)/2$ representatives to describe $\widehat{Q}$. For even d , there are four fixed points $(0, 0)$, $(d/2, 0)$, $(0, d/2)$, $(d/2, d/2)$, so one may choose $(d^2 + 4)/2$ representatives. Then, the remainder of the matrix can be reconstructed through taking complex conjugates of the entries and multiplication by the relevant phase factors. In this sense, the discrete Fourier transform “compresses” the KD distribution.

In addition to showing the self-similarity of $\widehat{Q}$, we can relate this object to the discrete Wigner distribution. Here, it is convenient to use a slightly different convention to Eqs. (B1) and (B6). We denote the multidimensional Fourier transform by $\tilde{Q}(\mathbf{a}, \mathbf{b})$ instead. From Eq. (B3), this is given by

$$\begin{aligned} \tilde{Q}(\mathbf{a}, \mathbf{b}) &= d^{-n} \sum_{\mathbf{i}, \mathbf{j} \in \mathbb{Z}_d^n} \omega^{-\mathbf{i} \cdot \mathbf{a} + \mathbf{j} \cdot \mathbf{b}} Q(\mathbf{i}, \mathbf{j}) \\ &= d^{-2n} \sum_{\mathbf{i}, \mathbf{j}, \mathbf{k} \in \mathbb{Z}_d^n} \omega^{-\mathbf{i} \cdot \mathbf{a} + \mathbf{j} \cdot \mathbf{b} + \mathbf{k} \cdot \mathbf{j} - \mathbf{i} \cdot \mathbf{j}} \langle \mathbf{i} | \psi \rangle \langle \psi | \mathbf{k} \rangle \\ &= d^{-2n} \sum_{\mathbf{i}, \mathbf{k} \in \mathbb{Z}_d^n} \langle \mathbf{i} | \psi \rangle \langle \psi | \mathbf{k} \rangle \omega^{-\mathbf{i} \cdot \mathbf{a}} \underbrace{\sum_{\mathbf{j}} \omega^{\mathbf{j} \cdot (\mathbf{k} + \mathbf{b} - \mathbf{i})}}_{\mathbf{k} + \mathbf{b} - \mathbf{i} = \mathbf{0} \pmod{d}} \\ &= d^{-n} \sum_{\mathbf{k} \in \mathbb{Z}_d^n} \langle \mathbf{k} + \mathbf{b} | \psi \rangle \langle \psi | \mathbf{k} \rangle \omega^{-\mathbf{a} \cdot (\mathbf{k} + \mathbf{b})} \\ &= d^{-n} \sum_{\mathbf{m} \in \mathbb{Z}_d^n} \langle \mathbf{m} | \psi \rangle \langle \psi | \mathbf{m} - \mathbf{b} \rangle \omega^{-\mathbf{a} \cdot \mathbf{m}} \\ &= d^{-n} \text{Tr}[\langle \psi | (X^{\mathbf{b}})^{\dagger} (Z^{\mathbf{a}})^{\dagger}], \end{aligned}$$

where all of the bit-string addition and subtraction is performed modulo d , and $Z^{\mathbf{a}}, X^{\mathbf{b}}$ are the Weyl-Heisenberg unitaries, defined for single qudits as

$$Z = \sum_{m=0}^{d-1} \omega^m |m\rangle \langle m|, \quad X = \sum_{m=0}^{d-1} |m+1\rangle \langle m|,$$

and for n qudits as

$$Z^{\mathbf{a}} = Z^{a_1} \otimes \cdots \otimes Z^{a_n} = \sum_{\mathbf{m} \in \mathbb{Z}_d^n} \omega^{\mathbf{a} \cdot \mathbf{m}} |\mathbf{m}\rangle \langle \mathbf{m}|,$$

$$X^{\mathbf{b}} = X^{b_1} \otimes \cdots \otimes X^{b_n} = \sum_{\mathbf{m} \in \mathbb{Z}_d^n} |\mathbf{m} + \mathbf{b}\rangle \langle \mathbf{m}|.$$

Once we take the complex conjugate of the final expression, the DFT of our KD distribution forms a matrix of expectation values of $|\psi\rangle$ with respect to the Weyl-Heisenberg

unitaries, $[Q(\mathbf{a}, \mathbf{b})]^* = d^{-n} \text{Tr}(|\psi\rangle \langle \psi| Z^{\mathbf{a}} X^{\mathbf{b}})$. We then multiply each entry of the resulting matrix by a phase $\omega^{-(\mathbf{a} \cdot \mathbf{b})2^{-1}}$, where 2^{-1} is the multiplicative inverse modulo d (for odd d). The resulting matrix $T(\mathbf{a}, \mathbf{b})$ contains elements of “phased” Weyl-Heisenberg unitaries:

$$T(\mathbf{a}, \mathbf{b}) = \omega^{-(\mathbf{a} \cdot \mathbf{b})2^{-1}} [\tilde{Q}(\mathbf{a}, \mathbf{b})]^*$$

$$= d^{-n} \text{Tr}(|\psi\rangle \langle \psi| \omega^{-(\mathbf{a} \cdot \mathbf{b})2^{-1}} Z^{\mathbf{a}} X^{\mathbf{b}}).$$

Taking the symplectic Fourier transform of this matrix, we obtain a new matrix with elements:

$$W(\mathbf{p}, \mathbf{q}) = d^{-n} \sum_{\mathbf{r}, \mathbf{s} \in \mathbb{Z}_d^n} \omega^{\mathbf{p} \cdot \mathbf{s} - \mathbf{q} \cdot \mathbf{r}} T(\mathbf{r}, \mathbf{s}) = d^{-2n} \sum_{\mathbf{r}, \mathbf{s} \in \mathbb{Z}_d^n} \omega^{\mathbf{p} \cdot \mathbf{s} - \mathbf{q} \cdot \mathbf{r}} \text{Tr}(|\psi\rangle \langle \psi| \omega^{-(\mathbf{r} \cdot \mathbf{s})2^{-1}} Z^{\mathbf{r}} X^{\mathbf{s}})$$

$$= d^{-n} \text{Tr} \left(|\psi\rangle \langle \psi| d^{-n} \sum_{\mathbf{r}, \mathbf{s} \in \mathbb{Z}_d^n} \omega^{\mathbf{p} \cdot \mathbf{s} - \mathbf{q} \cdot \mathbf{r}} (\omega^{-(\mathbf{r} \cdot \mathbf{s})2^{-1}} Z^{\mathbf{r}} X^{\mathbf{s}}) \right) = d^{-n} \text{Tr}(|\psi\rangle \langle \psi| A^{\mathbf{p}, \mathbf{q}}), \quad (\text{B8})$$

which for odd d are precisely the elements of the discrete Wigner distribution [5,55], i.e., expectation values of $|\psi\rangle$ with respect to the phase point operators $A^{\mathbf{p}, \mathbf{q}}$ [defined implicitly in the last line of (B8)]. Performing the inverse of the above similarly allows one to start with a Wigner distribution and obtain the KD distribution for $V = \text{DFT}_d^{\otimes n}$. Thus, the two representations of quantum states are related by an invertible sequence of DFTs and diagonal phase multiplications. This was previously shown for the continuous case in Refs. [56,57].

APPENDIX C: BOUNDS ON KD QUASIPROBABILITIES

Here, we offer some general bounds on the magnitude of Kirkwood-Dirac quasiprobabilities, which may be of independent interest. The first result is a general bound on the magnitude of quasiprobabilities in any informationally complete KD distribution. To this end, we define $m_{\mathcal{A}, \mathcal{B}}$ and $M_{\mathcal{A}, \mathcal{B}}$ as the smallest and largest absolute values of inner products between $\mathcal{A}, \mathcal{B}$:

$$m_{\mathcal{A}, \mathcal{B}} = \min_{(i, j) \in [[d]]^2} |\langle a_i | b_j \rangle|, \quad M_{\mathcal{A}, \mathcal{B}} = \max_{(i, j) \in [[d]]^2} |\langle a_i | b_j \rangle|.$$

These relate as $0 \leq m_{\mathcal{A}, \mathcal{B}} \leq 1/\sqrt{d} \leq M_{\mathcal{A}, \mathcal{B}} \leq 1$ [44]. We also make use of the support uncertainties $n_{\mathcal{A}}, n_{\mathcal{B}}$, defined in Eq. (3).

Lemma 5. The magnitudes of all Kirkwood-Dirac quasiprobabilities $Q(\psi)_{ij}$ for a pure state $|\psi\rangle$ with support uncertainties $(n_{\mathcal{A}}, n_{\mathcal{B}})$ are upper bounded as

$$|Q(\psi)_{ij}| \leq M_{\mathcal{A}, \mathcal{B}}^3 \sqrt{n_{\mathcal{A}} n_{\mathcal{B}}}. \quad (\text{C1})$$

For KD-positive distributions, we also have the lower bound on the nonzero elements $Q(\psi)_{ij}$:

$$m_{\mathcal{A}, \mathcal{B}}^3 \leq Q(\psi)_{ij}.$$

Proof. We make use of a pair of projectors onto the support of $|\psi\rangle$ in $\mathcal{A}$ and $\mathcal{B}$:

$$\Pi_{\mathcal{A}} = \sum_{|a_i\rangle \in S_{\mathcal{A}}} |a_i\rangle \langle a_i|, \quad \Pi_{\mathcal{B}} = \sum_{|b_j\rangle \in S_{\mathcal{B}}} |b_j\rangle \langle b_j|.$$

Clearly, the rank of $\Pi_{\mathcal{A}}$ is $n_{\mathcal{A}}$, the rank of $\Pi_{\mathcal{B}}$ is $n_{\mathcal{B}}$, and $\Pi_{\mathcal{A}}|\psi\rangle = \Pi_{\mathcal{B}}|\psi\rangle = |\psi\rangle$. Inserting these into the expression for $|Q_{ij}|$, we get

$$|Q(\psi)_{ij}| = |\langle b_j | a_i \rangle| |\langle a_i | \Pi_{\mathcal{B}} | \psi \rangle| |\langle \psi | \Pi_{\mathcal{A}} | b_j \rangle|$$

$$= |\langle b_j | a_i \rangle| \left| \sum_{|b_k\rangle \in S_{\mathcal{B}}} \langle a_i | b_k \rangle \langle b_k | \psi \rangle \right| \left| \sum_{|a_l\rangle \in S_{\mathcal{A}}} \langle \psi | a_l \rangle \langle a_l | b_j \rangle \right|$$

$$\leq M_{\mathcal{A}, \mathcal{B}}^3 \left(\sum_{|b_k\rangle \in S_{\mathcal{B}}} |\langle b_k | \psi \rangle| \right) \left(\sum_{|a_l\rangle \in S_{\mathcal{A}}} |\langle \psi | a_l \rangle| \right)$$

$$\leq M_{\mathcal{A}, \mathcal{B}}^3 \sqrt{n_{\mathcal{A}} n_{\mathcal{B}}},$$

where we have used the triangle inequality and definition of $M_{\mathcal{A}, \mathcal{B}}$ in the third line, and the Cauchy-Schwarz inequality in the fourth.

For the lower bound, we use an argument similar to that of Ref. [44]. Using the global phase invariance of the KD distribution, we can adjust the phases and indices of the basis vectors in $\mathcal{A}, \mathcal{B}$ so that $\langle a_i | \psi \rangle$ and $\langle b_j | \psi \rangle$ are real and positive for $i, j \in [[n_{\mathcal{A}}]] \times [[n_{\mathcal{B}}]]$ and zero otherwise. It follows that if the KD distribution is positive, the inner products $\langle a_i | b_j \rangle$ are real and non-negative for $|a_i\rangle \in S_{\mathcal{A}}, |b_j\rangle \in S_{\mathcal{B}}$. We can thus write

$$Q(\psi)_{ij} = \langle b_j | a_i \rangle \sum_{|b_k\rangle \in S_{\mathcal{B}}} \langle a_i | b_k \rangle \langle b_k | \psi \rangle \sum_{|a_l\rangle \in S_{\mathcal{A}}} \langle \psi | a_l \rangle \langle a_l | b_j \rangle$$

$$\geq m_{\mathcal{A}, \mathcal{B}}^3 \left(\sum_{|b_k\rangle \in S_{\mathcal{B}}} \langle b_k | \psi \rangle \right) \left(\sum_{|a_l\rangle \in S_{\mathcal{A}}} \langle \psi | a_l \rangle \right) \geq m_{\mathcal{A}, \mathcal{B}}^3,$$

where the last line follows from the ℓ_1 - ℓ_2 norm inequality $\|\psi\|_1 \geq \|\psi\|_2$. ■

The upper bound given in Lemma 5 generically constrains the maximum attainable magnitudes of pure state quasiprobabilities in any (including informationally incomplete) KD distribution in terms of the value of $M_{\mathcal{A}, \mathcal{B}}$ of the distribution, as well as the support size $n_{\mathcal{A}} n_{\mathcal{B}}$ of the state. Recent work characterizing Bargmann invariants [58–61] (which KD quasiprobabilities form an instance of) implies that when more fine-grained information about $Q(\rho)_{ij}$ is known—

namely, the phase $\theta = \arg(Q(\rho)_{ij}) \in [0, 2\pi)$ —a more precise bound may also be constructed:

$$|Q(\psi)_{ij}| \leq \cos^3\left(\frac{\pi}{3}\right) \sec^3\left(\frac{\theta - \pi}{3}\right). \quad (\text{C2})$$

Thus, the bounds (C1) and (C2) are complementary, and may be used at will depending on information available about $Q(\rho)$. An example of their consequence is given below:

Remark 3. Let $Q(\psi)$ be a Kirkwood-Dirac distribution of a pure state defined on a pair of MUBs. If $\mathcal{N}(Q(\psi)) = 1$, then all its nonzero quasiprobabilities are uniformly $Q_{ij} = 1/d$.

Proof. Here $M_{A,B} = 1/\sqrt{d}$, and for MUBs all pure KD-positive states satisfy $n_A n_B = d$. Substituting these into Eq. (C1) we get $|Q(\psi)_{ij}| = Q(\psi)_{ij} \leq 1/d$. The number of nonzero $Q(\psi)_{ij}$ is also given by $n_A n_B = d$. Because the quasiprobabilities must also sum to 1, this can all be satisfied only if (C1) is saturated, so $Q(\psi)_{ij} = 1/d$ or 0. ■

Remark 3 further implies that all nonzero amplitudes of KD-positive states on MUBs satisfy $|\langle\psi|a_i\rangle| = \sqrt{1/n_A}$ and $|\langle\psi|b_j\rangle| = \sqrt{1/n_B}$. Because we can write the inner product between any two pure states $|\psi\rangle, |\phi\rangle$ as

$$|\langle\psi|\phi\rangle|^2 = \sum_{ij} \frac{Q_{ij}^*(\psi)Q_{ij}(\phi)}{|\langle a_i|b_j\rangle|^2},$$

the inner product of any two KD-positive states on MUBs satisfies

$$|\langle\psi|\phi\rangle| = \sqrt{\frac{k}{d}}, \quad (\text{C3})$$

where the integer k is the overlap of the support of their distributions. Note that the above holds true for all MUBs, not just the case of $V = \text{DFT}_d$.

Taking an MUB system of n qudits, Remark 3 tells us that every pure KD-positive state is a uniform mixture on its support with the nonzero quasiprobabilities reading $1/d^n$. In particular, this implies that the distribution becomes exponentially large, with exponentially small probabilities. In the discrete Wigner distribution setting, the exact same property is satisfied by the stabilizer states, i.e., all pure Wigner-positive states [62,63]. In a recent result, Gross, Nezami, and Walter [63] have used this to devise an efficient property test for whether an unknown state is a stabilizer state. Whether such tests exist for the $V = \text{DFT}_d^{\otimes n}$ KD distribution (or in general) remains an open question. Finally, we note that Eq. (C3) closely resembles Theorem 11 of Ref. [64] satisfied by stabilizer states.

APPENDIX D: PROOFS FOR TYPE III UNITARIES

1. Extended proof of Theorem 2

Here, we prove Theorem 2 for the general case of $V = \text{DFT}_d$ where $d = pq$ for any pair of distinct primes p, q .

Proof. The strategy is the same as in the $d = 6$ case. We write $|a_i\rangle \in \mathcal{A}$, $|b_j\rangle \in \mathcal{B}$, $|x, y\rangle_{p,q} \in \mathcal{C}_{p,q}$ and $|u, v\rangle_{q,p} \in \mathcal{C}_{q,p}$. The linear decomposition of any ρ such that $Q(\rho)_{ij} \in \mathbb{R}$ (established in Ref. [48]) then becomes

$$\rho = \sum_i \alpha_i |a_i\rangle\langle a_i| + \sum_j \beta_j |b_j\rangle\langle b_j|$$

$$+ \sum_{x,y} \gamma_{x,y} |x, y\rangle\langle x, y|_{p,q} + \sum_{u,v} \varepsilon_{u,v} |u, v\rangle\langle u, v|_{q,p}.$$

Similarly, by linearity of (1) we may write $Q(\rho)$ as a linear combination of the pure state KD distributions:

$$Q(\rho) = \sum_i \alpha_i Q(a_i) + \sum_j \beta_j Q(b_j) + \sum_{x,y} \gamma_{x,y} Q((x, y)_{p,q}) + \sum_{u,v} \varepsilon_{u,v} Q((u, v)_{q,p}).$$

From Eqs. (1) and (8), the pure state distributions can be shown to satisfy

$$Q(a_i)_{kl} = d^{-1} \delta_{ki},$$

$$Q(b_j)_{kl} = d^{-1} \delta_{lj},$$

$$Q((x, y)_{p,q})_{kl} = d^{-1} \delta_{x,k \bmod p} \delta_{y,l \bmod q},$$

$$Q((u, v)_{q,p})_{kl} = d^{-1} \delta_{u,k \bmod q} \delta_{v,l \bmod p}.$$

Therefore, assuming $\rho \in \mathcal{E}_{\text{KD}+}$, we get d^2 linear equations of the form:

$$Q(\rho)_{kl} = \frac{1}{d} (\alpha_k + \beta_l + \gamma_{k \bmod p, l \bmod q} + \varepsilon_{k \bmod q, l \bmod p}).$$

Recall that $U_\star = P^\dagger(\mathbb{1}_p \otimes \text{DFT}_q)P$. We know from Lemma 3 that $U_\star|a_i\rangle \propto |i \bmod p, p i \bmod q\rangle_{p,q}$ and $U_\star|b_j\rangle \propto |-\bar{p} j \bmod q, j \bmod p\rangle_{q,p}$, where $\bar{p} = p^{-1} \bmod q$ and $\bar{q} = q^{-1} \bmod p$. We can explicitly calculate the action of $U_\star$ on $|x, y\rangle_{p,q}$:

$$\begin{aligned} P|x, y\rangle_{p,q} &= \frac{1}{\sqrt{q}} \sum_{k=0}^{q-1} e^{\frac{2\pi i}{q} ky} P|a_{kp+x}\rangle \\ &= \frac{1}{\sqrt{q}} \sum_{k=0}^{q-1} e^{\frac{2\pi i}{q} ky} |kp+x \bmod p\rangle \otimes |kp+x \bmod q\rangle \\ &= |x\rangle \otimes \frac{1}{\sqrt{q}} \sum_{k=0}^{q-1} e^{\frac{2\pi i}{q} ky} |kp+x \bmod q\rangle. \end{aligned}$$

Now set $t = kp + x \bmod q$ so that $k = \bar{p}(t - x) \bmod q$. Redefining the sum, we get

$$\begin{aligned} P|x, y\rangle_{p,q} &= |x\rangle \otimes \frac{1}{\sqrt{q}} \sum_{t=0}^{q-1} e^{\frac{2\pi i}{q} y \bar{p}(t-x)} |t\rangle \\ &\propto |x\rangle \otimes \text{DFT}_q |\bar{p} y\rangle. \end{aligned}$$

Hence,

$$\begin{aligned} U_\star|x, y\rangle_{p,q} &= P^\dagger(\mathbb{1}_p \otimes \text{DFT}_q)P|x, y\rangle_{p,q} \\ &\propto P^\dagger(|x\rangle \otimes \text{DFT}_q^2 |\bar{p} y\rangle) \\ &\propto P^\dagger(|x\rangle \otimes |-\bar{p} y\rangle) \\ &\propto |a_{xq\bar{q}-\bar{p}y p\bar{p}}\rangle, \end{aligned}$$

where $xq\bar{q} + (-\bar{p}y)p\bar{p} \bmod d$ is of the form in Eq. (10). Similarly for states in $\mathcal{C}_{q,p}$:

$$P|u, v\rangle_{q,p} = \frac{1}{\sqrt{p}} \sum_{k=0}^{p-1} e^{\frac{2\pi i}{p} kv} P|a_{kq+u}\rangle$$

$$\begin{aligned}
&= \frac{1}{\sqrt{p}} \sum_{k=0}^{p-1} e^{\frac{2\pi i}{p} kv} |kq + u \bmod p\rangle \otimes |kq + u \bmod q\rangle \\
&= \left(\frac{1}{\sqrt{p}} \sum_{k=0}^{p-1} e^{\frac{2\pi i}{p} kv} |kq + u \bmod p\rangle \right) \otimes |u\rangle \\
&\propto \text{DFT}_p |\bar{q} v\rangle \otimes |u\rangle,
\end{aligned}$$

so that by Eq. (12)

$$\begin{aligned}
U_\star |u, v\rangle_{q,p} &\propto P^\dagger (\text{DFT}_p |\bar{q} v\rangle \otimes \text{DFT}_q |u\rangle) \\
&\propto |b_v q\bar{q} + p u p\bar{p}\rangle.
\end{aligned}$$

In summary, we have

$$\begin{aligned}
U_\star |a_i\rangle &\propto |i \bmod p, p i \bmod q\rangle_{p,q}, \\
U_\star |b_j\rangle &\propto |-\bar{p} j \bmod q, j \bmod p\rangle_{q,p}, \\
U_\star |x, y\rangle_{p,q} &\propto |a_{x q\bar{q} - \bar{p} y p\bar{p}}\rangle, \\
U_\star |u, v\rangle_{q,p} &\propto |b_{v q\bar{q} + p u p\bar{p}}\rangle.
\end{aligned}$$

Hence,

$$\begin{aligned}
Q(U_\star \rho U_\star^\dagger) &= \sum_i \alpha_i Q((i \bmod p, p i \bmod q)_{p,q}) \\
&\quad + \sum_j \beta_j Q((- \bar{p} j \bmod q, j \bmod p)_{q,p}) \\
&\quad + \sum_{x,y} \gamma_{x,y} Q(a_{x q\bar{q} - \bar{p} y p\bar{p}}) \\
&\quad + \sum_{u,v} \varepsilon_{u,v} Q(b_{v q\bar{q} + p u p\bar{p}}).
\end{aligned}$$

Therefore, the entries of $Q(U_\star \rho U_\star^\dagger)$ are given by

$$\begin{aligned}
Q(U_\star \rho U_\star^\dagger)_{kl} &= \frac{1}{d} \sum_i \alpha_i \delta_{i \bmod p, k \bmod p} \delta_{p i \bmod q, l \bmod q} \\
&\quad + \frac{1}{d} \sum_j \beta_j \delta_{-\bar{p} j \bmod q, k \bmod q} \delta_{j \bmod p, l \bmod p} \\
&\quad + \frac{1}{d} \sum_{x,y} \gamma_{x,y} \delta_{k, x q\bar{q} - \bar{p} y p\bar{p}} \\
&\quad + \frac{1}{d} \sum_{u,v} \varepsilon_{u,v} \delta_{l, v q\bar{q} + p u p\bar{p}}.
\end{aligned}$$

We may simplify the sum into the following:

$$\begin{aligned}
Q(U_\star \rho U_\star^\dagger)_{kl} &= \frac{1}{d} (\alpha_{k'} + \beta_{l'} + \gamma_{k \bmod p, -p k \bmod q} \\
&\quad + \varepsilon_{\bar{p} l \bmod q, l \bmod p}),
\end{aligned}$$

where we have set

$$\begin{aligned}
k' &= (k \bmod p) q\bar{q} + (\bar{p} l \bmod q) p\bar{p}, \\
l' &= (l \bmod p) q\bar{q} + (-p k \bmod q) p\bar{p}.
\end{aligned} \quad (\text{D1})$$

Our choice of indices (k', l') satisfies

$$\begin{aligned}
k' \bmod p &= k \bmod p, \quad k' \bmod q = \bar{p} l \bmod q, \\
l' \bmod p &= l \bmod p, \quad l' \bmod q = -p k \bmod q.
\end{aligned}$$

Giving $Q(U_\star \rho U_\star^\dagger)_{kl} = Q(\rho)_{k'l'}$. Therefore, conjugating ρ by $U_\star$ corresponds to a permutation of the entries of $Q(\rho)$ as $(k, l) \rightarrow (k', l')$ via the bijective mapping defined in Eqs. (D1). Assuming $\rho \in \mathcal{E}_{\text{KD}+}$, we have $Q(\rho)_{kl} \geq 0$ for all k, l , even if some of the coefficients $(\alpha, \beta, \gamma, \varepsilon)$ are negative. Therefore, $Q(U_\star \rho U_\star^\dagger)_{kl} \geq 0$ for all k, l . Hence, $U_\star \rho U_\star^\dagger \in \mathcal{E}_{\text{KD}+}$, and the KD positivity of ρ is preserved under conjugation by $U_\star$. Finally, note that for our proof it does not matter whether $\mathcal{E}_{\text{KD}+} = \text{conv}(\mathcal{E}_{\text{KD}+}^{\text{pure}})$ holds, or not. For $d = pq \neq 6$, to the best of our knowledge, this remains an open question. Similarly to Lemma 3, by symmetry the above also applies to $U'_\star = P^\dagger (\text{DFT}_p \otimes \mathbb{1}_q) P$, which is another type III unitary. ■

2. Multiqudit systems

We now prove that Theorem 2 generalizes to the multiqudit case of $V = \text{DFT}_{pq}^{\otimes n}$. Although for such distributions there may exist positivity-preserving unitaries beyond types I, II, and III, here we show that the unitary $U_\star^{\otimes n}$ acts covariantly and preserves the total nonpositivity for any KD-real distribution $Q(\rho)$, and so Theorem 4 remains valid for $n > 1$.

Theorem 5. For $V = \text{DFT}_{pq}^{\otimes n}$, the unitary $U_\star^{\otimes n}$ acts covariantly on any KD-real distribution $Q(\rho)$. As a consequence, it is positivity preserving.

Proof. We begin similarly to Lemma 3, and rewrite the action of $U_\star^{\otimes n}$ on the state ρ in the $V = \text{DFT}_{pq}^{\otimes n}$ distribution as the action by $\tilde{U}_\star = \mathbb{1}_p^{\otimes n} \otimes \text{DFT}_q^{\otimes n}$ on an identical distribution obtained by a global change of basis by $P^{\otimes n}$. In the new distribution, we write the basis states as $\mathcal{A} = \{|\mathbf{i}_p\rangle \otimes |\mathbf{i}_q\rangle\}$ and $\mathcal{B} = \{\text{DFT}_p^{\otimes n} |\bar{q} \mathbf{j}_p\rangle \otimes \text{DFT}_q^{\otimes n} |\bar{p} \mathbf{j}_q\rangle\}$, where

$$\begin{aligned}
|\mathbf{i}_p\rangle &= |(i_1)_p\rangle \otimes \cdots \otimes |(i_n)_p\rangle \in (\mathbb{C}^p)^{\otimes n}, \\
|\bar{p} \mathbf{j}_q\rangle &= |\bar{p}(j_1)_q\rangle \otimes \cdots \otimes |\bar{p}(j_n)_q\rangle \in (\mathbb{C}^q)^{\otimes n},
\end{aligned}$$

and similarly for $|\mathbf{i}_q\rangle, |\bar{q} \mathbf{j}_p\rangle$. The transformation under $\tilde{U}_\star$ straightforwardly generalizes from Eq. (13):

$$Q_{\mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q} \rightarrow \frac{1}{q^n} \sum_{\mathbf{s}_q, \mathbf{t}_q \in \mathbb{Z}_q^n} e^{\frac{2\pi i}{q} (\mathbf{i}_q + \bar{p} \mathbf{t}_q) \cdot (\mathbf{s}_q - \bar{p} \mathbf{j}_q)} Q_{\mathbf{i}_p, \mathbf{s}_q; \mathbf{j}_p, \mathbf{t}_q}. \quad (\text{D2})$$

Next, we make use of general constraints on quasiprobability distributions from Appendix B. We assume that the quasiprobability distribution is KD-real, so that $Q_{\mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q}$ is equal to its complex conjugate. Equation (B2) then takes on the form:

$$Q_{\mathbf{u}_p, \mathbf{u}_q; \mathbf{v}_p, \mathbf{v}_q} = \sum_{\mathbf{i}_p, \mathbf{j}_p \in \mathbb{Z}_p^n} \sum_{\mathbf{i}_q, \mathbf{j}_q \in \mathbb{Z}_q^n} (\hat{\mathcal{K}}_{\mathbf{u}_p, \mathbf{u}_q; \mathbf{v}_p, \mathbf{v}_q}^{\mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q} Q_{\mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q},$$

where $\hat{\mathcal{K}}$ is a superoperator matrix on $\mathbb{C}^{d^{2n} \times d^{2n}}$ with entries

$$\begin{aligned} (\hat{\mathcal{K}})_{\mathbf{u}_p, \mathbf{u}_q; \mathbf{v}_p, \mathbf{v}_q}^{\mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q} &= \frac{1}{d^n} e^{\frac{2\pi i}{p} (\mathbf{v}_p - \mathbf{j}_p) \cdot (\mathbf{i}_p - \mathbf{u}_p)} e^{\frac{2\pi i}{q} (\mathbf{v}_q - \mathbf{j}_q) \cdot (\mathbf{i}_q - \mathbf{u}_q)} \\ &= \frac{1}{p^n} e^{\frac{2\pi i}{p} (\mathbf{v}_p - \mathbf{j}_p) \cdot (\mathbf{i}_p - \mathbf{u}_p)} \frac{1}{q^n} e^{\frac{2\pi i}{q} (\mathbf{v}_q - \mathbf{j}_q) \cdot (\mathbf{i}_q - \mathbf{u}_q)} \\ &= (\hat{\mathcal{K}}^{(p)})_{\mathbf{u}_p, \mathbf{v}_p}^{\mathbf{i}_p, \mathbf{j}_p} \otimes (\hat{\mathcal{K}}^{(q)})_{\mathbf{u}_q, \mathbf{v}_q}^{\mathbf{i}_q, \mathbf{j}_q}. \end{aligned}$$

Taking $Q_{\mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q}$ as a real-valued vector in $\mathbb{C}^{d^{2n}}$, we can write the above in the vectorized picture:

$$\hat{\mathcal{K}}|Q\rangle\rangle = \hat{\mathcal{K}}^{(p)} \otimes \hat{\mathcal{K}}^{(q)}|Q\rangle\rangle = |Q\rangle\rangle. \quad (\text{D3})$$

Therefore, by our assumption that $Q(\rho)$ is KD-real we have obtained a linear eigenvector equation (D3) for the quasiprobability distribution vector. This implies that any KD-real $|Q\rangle\rangle$ resides in the +1 eigenspace of $\hat{\mathcal{K}}$, and we may isolate its eigenvectors to obtain the general form of KD-real distributions. Furthermore, since $\hat{\mathcal{K}}$ factorizes into a tensor product of two superoperators, the +1 eigenspace of $\hat{\mathcal{K}}$ is spanned by the tensor products of eigenspaces of $\hat{\mathcal{K}}^{(p)}$ and $\hat{\mathcal{K}}^{(q)}$ with reciprocal eigenvalues.

We next find the eigenbasis for $\hat{\mathcal{K}}^{(p)}$. Due to the tensor product structure, its eigenvectors reside in $\mathbb{C}^{p^{2n}}$. Consider the vectors $|\phi_{\mathbf{l}_p, \mathbf{m}_p}\rangle\rangle$ with entries:

$$\langle\langle \mathbf{i}_p, \mathbf{j}_p | \phi_{\mathbf{l}_p, \mathbf{m}_p} \rangle\rangle = \frac{1}{p^n} e^{\frac{2\pi i}{p} (\mathbf{i}_p \cdot \mathbf{l}_p + \mathbf{j}_p \cdot \mathbf{m}_p)}.$$

There are $p^n \times p^n$ such vectors; as they are orthonormal, they form a basis for $\mathbb{C}^{p^{2n}}$:

$$\begin{aligned} \langle\langle \phi_{\mathbf{l}_p, \mathbf{m}_p} | \phi_{\mathbf{l}'_p, \mathbf{m}'_p} \rangle\rangle &= \frac{1}{p^{2n}} \sum_{\mathbf{i}_p, \mathbf{j}_p} e^{\frac{2\pi i}{p} [\mathbf{i}_p \cdot (\mathbf{l}'_p - \mathbf{l}_p) + \mathbf{j}_p \cdot (\mathbf{m}'_p - \mathbf{m}_p)]} \\ &= \frac{1}{p^{2n}} \sum_{\mathbf{i}_p} e^{\frac{2\pi i}{p} \mathbf{i}_p \cdot (\mathbf{l}'_p - \mathbf{l}_p)} \sum_{\mathbf{j}_p} e^{\frac{2\pi i}{p} \mathbf{j}_p \cdot (\mathbf{m}'_p - \mathbf{m}_p)} \\ &= \delta_{\mathbf{l}_p, \mathbf{l}'_p} \delta_{\mathbf{m}_p, \mathbf{m}'_p}. \end{aligned}$$

Each vector $|\phi_{\mathbf{l}_p, \mathbf{m}_p}\rangle\rangle$ forms an eigenvector of $\hat{\mathcal{K}}^{(p)}$:

$$\begin{aligned} \hat{\mathcal{K}}^{(p)}|\phi_{\mathbf{l}_p, \mathbf{m}_p}\rangle\rangle &= \sum_{\mathbf{i}_p, \mathbf{j}_p} \langle\langle \mathbf{i}_p, \mathbf{j}_p | \phi_{\mathbf{l}_p, \mathbf{m}_p} \rangle\rangle \hat{\mathcal{K}}^{(p)}|\mathbf{i}_p, \mathbf{j}_p\rangle\rangle = \sum_{\mathbf{u}_p, \mathbf{v}_p} \sum_{\mathbf{i}_p, \mathbf{j}_p} \langle\langle \mathbf{i}_p, \mathbf{j}_p | \phi_{\mathbf{l}_p, \mathbf{m}_p} \rangle\rangle (\hat{\mathcal{K}}^{(p)})_{\mathbf{u}_p, \mathbf{v}_p}^{\mathbf{i}_p, \mathbf{j}_p} |\mathbf{u}_p, \mathbf{v}_p\rangle\rangle \\ &= \frac{1}{p^{2n}} \sum_{\mathbf{u}_p, \mathbf{v}_p} \sum_{\mathbf{i}_p, \mathbf{j}_p} e^{\frac{2\pi i}{p} [(\mathbf{v}_p - \mathbf{j}_p) \cdot (\mathbf{i}_p - \mathbf{u}_p) + (\mathbf{i}_p \cdot \mathbf{l}_p + \mathbf{j}_p \cdot \mathbf{m}_p)]} |\mathbf{u}_p, \mathbf{v}_p\rangle\rangle = \frac{1}{p^{2n}} \sum_{\mathbf{u}_p, \mathbf{v}_p} \sum_{\mathbf{i}_p, \mathbf{j}_p} e^{\frac{2\pi i}{p} [\mathbf{i}_p \cdot (\mathbf{l}_p + \mathbf{v}_p - \mathbf{j}_p) - \mathbf{u}_p \cdot (\mathbf{v}_p - \mathbf{j}_p) + \mathbf{j}_p \cdot \mathbf{m}_p]} |\mathbf{u}_p, \mathbf{v}_p\rangle\rangle \\ &= \frac{1}{p^n} \sum_{\mathbf{u}_p, \mathbf{v}_p} \sum_{\mathbf{j}_p} \delta_{\mathbf{j}_p, \mathbf{l}_p + \mathbf{v}_p} e^{\frac{2\pi i}{p} [\mathbf{j}_p \cdot (\mathbf{m}_p + \mathbf{u}_p) - \mathbf{u}_p \cdot \mathbf{v}_p]} |\mathbf{u}_p, \mathbf{v}_p\rangle\rangle = \frac{1}{p^n} \sum_{\mathbf{u}_p, \mathbf{v}_p} e^{\frac{2\pi i}{p} (\mathbf{l}_p \cdot \mathbf{m}_p + \mathbf{u}_p \cdot \mathbf{l}_p + \mathbf{v}_p \cdot \mathbf{m}_p)} |\mathbf{u}_p, \mathbf{v}_p\rangle\rangle = e^{\frac{2\pi i}{p} \mathbf{l}_p \cdot \mathbf{m}_p} |\phi_{\mathbf{l}_p, \mathbf{m}_p}\rangle\rangle. \end{aligned}$$

Similarly, for $\hat{\mathcal{K}}^{(q)}$ each vector $|\psi_{\mathbf{l}_q, \mathbf{m}_q}\rangle\rangle$ with entries $\langle\langle \mathbf{i}_q, \mathbf{j}_q | \psi_{\mathbf{l}_q, \mathbf{m}_q} \rangle\rangle = q^{-n} e^{\frac{2\pi i}{q} (\mathbf{i}_q \cdot \mathbf{l}_q + \mathbf{j}_q \cdot \mathbf{m}_q)}$ is an eigenvector with eigenvalue $e^{\frac{2\pi i}{q} \mathbf{l}_q \cdot \mathbf{m}_q}$. Therefore, the +1 eigenspace of $\hat{\mathcal{K}}$ is spanned by the tensor products $|\phi_{\mathbf{l}_p, \mathbf{m}_p}\rangle\rangle \otimes |\psi_{\mathbf{l}_q, \mathbf{m}_q}\rangle\rangle$, such that

$$e^{\frac{2\pi i}{p} \mathbf{l}_p \cdot \mathbf{m}_p} e^{\frac{2\pi i}{q} \mathbf{l}_q \cdot \mathbf{m}_q} = 1.$$

Since p and q are coprime, this condition is equivalent to requiring that $\mathbf{l}_p \cdot \mathbf{m}_p = 0 \pmod{p}$ and $\mathbf{l}_q \cdot \mathbf{m}_q = 0 \pmod{q}$. Therefore, a +1 eigenvector of $\hat{\mathcal{K}}$ is a tensor product of +1 eigenvectors of $\hat{\mathcal{K}}^{(p)}$ and $\hat{\mathcal{K}}^{(q)}$.

Next, we study the action of the superoperator $\hat{\mathcal{E}}_{\hat{U}_*}$ on the +1 eigenspace of $\hat{\mathcal{K}}$. From Eq. (D2) the superoperator elements are given by

$$\begin{aligned} (\hat{\mathcal{E}}_{\hat{U}_*})_{\mathbf{u}_p, \mathbf{u}_q; \mathbf{v}_p, \mathbf{v}_q}^{\mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q} &= (\hat{\mathbb{1}}^{(p)})_{\mathbf{u}_p, \mathbf{v}_p}^{\mathbf{i}_p, \mathbf{j}_p} \otimes (\hat{\mathcal{T}}^{(q)})_{\mathbf{u}_q, \mathbf{v}_q}^{\mathbf{i}_q, \mathbf{j}_q} \\ &= (\hat{\mathbb{1}}^{(p)})_{\mathbf{u}_p, \mathbf{v}_p}^{\mathbf{i}_p, \mathbf{j}_p} \otimes \frac{1}{q^n} e^{\frac{2\pi i}{q} (\mathbf{u}_q + \bar{p}\mathbf{j}_q) \cdot (\mathbf{i}_q - \bar{p}\mathbf{v}_q)}. \end{aligned}$$

We only need to consider the eigenstates $|\psi_{\mathbf{l}_q, \mathbf{m}_q}\rangle\rangle$:

$$\begin{aligned} \hat{\mathcal{T}}^{(q)}|\psi_{\mathbf{l}_q, \mathbf{m}_q}\rangle\rangle &= \sum_{\mathbf{i}_q, \mathbf{j}_q} \langle\langle \mathbf{i}_q, \mathbf{j}_q | \psi_{\mathbf{l}_q, \mathbf{m}_q} \rangle\rangle \hat{\mathcal{T}}^{(q)}|\mathbf{i}_q, \mathbf{j}_q\rangle\rangle = \sum_{\mathbf{u}_q, \mathbf{v}_q} \sum_{\mathbf{i}_q, \mathbf{j}_q} \langle\langle \mathbf{i}_q, \mathbf{j}_q | \psi_{\mathbf{l}_q, \mathbf{m}_q} \rangle\rangle (\hat{\mathcal{T}}^{(q)})_{\mathbf{u}_q, \mathbf{v}_q}^{\mathbf{i}_q, \mathbf{j}_q} |\mathbf{u}_q, \mathbf{v}_q\rangle\rangle \\ &= \frac{1}{q^{2n}} \sum_{\mathbf{u}_q, \mathbf{v}_q} \sum_{\mathbf{i}_q, \mathbf{j}_q} e^{\frac{2\pi i}{q} [\mathbf{i}_q \cdot (\mathbf{l}_q + \mathbf{u}_q + \bar{p}\mathbf{j}_q) + \mathbf{j}_q \cdot \mathbf{m}_q - \bar{p}\mathbf{v}_q \cdot (\mathbf{u}_q + \bar{p}\mathbf{j}_q)]} |\mathbf{u}_q, \mathbf{v}_q\rangle\rangle = \frac{1}{q^{2n}} \sum_{\mathbf{u}_q, \mathbf{v}_q} \sum_{\mathbf{i}_q, \mathbf{j}_q} e^{\frac{2\pi i}{q} [\mathbf{i}_q \cdot (\mathbf{l}_q + \mathbf{u}_q + \bar{p}\mathbf{j}_q) + \mathbf{j}_q \cdot \mathbf{m}_q - \bar{p}\mathbf{v}_q \cdot (\mathbf{u}_q + \bar{p}\mathbf{j}_q)]} |\mathbf{u}_q, \mathbf{v}_q\rangle\rangle \\ &= \frac{1}{q^n} \sum_{\mathbf{u}_q, \mathbf{v}_q} \sum_{\mathbf{j}_q} \delta_{\mathbf{j}_q, -p(\mathbf{l}_q + \mathbf{u}_q)} e^{\frac{2\pi i}{q} [\mathbf{j}_q \cdot \mathbf{m}_q - \bar{p}\mathbf{v}_q \cdot (\mathbf{u}_q + \bar{p}\mathbf{j}_q)]} |\mathbf{u}_q, \mathbf{v}_q\rangle\rangle = \frac{1}{q^n} \sum_{\mathbf{u}_q, \mathbf{v}_q} e^{\frac{2\pi i}{q} [-p(\mathbf{l}_q + \mathbf{u}_q) \cdot \mathbf{m}_q + \bar{p}\mathbf{v}_q \cdot \mathbf{l}_q]} |\mathbf{u}_q, \mathbf{v}_q\rangle\rangle \\ &= \frac{1}{q^n} e^{\frac{-2\pi i}{q} p\mathbf{l}_q \cdot \mathbf{m}_q} \sum_{\mathbf{u}_q, \mathbf{v}_q} e^{\frac{2\pi i}{q} [\mathbf{u}_q \cdot (-p\mathbf{m}_q) + \mathbf{v}_q \cdot (\bar{p}\mathbf{l}_q)]} |\mathbf{u}_q, \mathbf{v}_q\rangle\rangle = e^{\frac{-2\pi i}{q} p\mathbf{l}_q \cdot \mathbf{m}_q} |\psi_{-p\mathbf{m}_q, \bar{p}\mathbf{l}_q}\rangle\rangle. \end{aligned}$$

In general, this is a phased permutation of the eigenbasis of $\hat{\mathcal{K}}^{(q)}$. However, if $|\psi_{\mathbf{l}_q, \mathbf{m}_q}\rangle$ is a $+1$ eigenvector, then $\mathbf{l}_q \cdot \mathbf{m}_q = 0 \bmod q$, and the phase factor is unity. The resulting vector $|\psi_{-p\mathbf{m}_q, \bar{p}\mathbf{l}_q}\rangle$ is also a $+1$ eigenvector of $\hat{\mathcal{K}}^{(q)}$, since $(-p\mathbf{m}_q) \cdot (\bar{p}\mathbf{l}_q) = -p\bar{p}(\mathbf{m}_q \cdot \mathbf{l}_q) = 0 \bmod q$. Therefore, the superoperator $\hat{\mathcal{E}}_{\tilde{U}_*}$ permutes the $+1$ eigenspace of $\hat{\mathcal{K}}$ and preserves KD reality.

Finally, we explicitly show that the action of $\hat{\mathcal{E}}_{\tilde{U}_*}$ permutes the entries of any KD-real distribution. The entries of a KD distribution are given by

$$Q(\tilde{\rho})_{\mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q} = \langle \langle \mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q | Q(\tilde{\rho}) \rangle \rangle.$$

Then,

$$\begin{aligned} Q(\tilde{U}_* \tilde{\rho} \tilde{U}_*^\dagger)_{\mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q} &= \langle \langle \mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q | Q(\tilde{U}_* \tilde{\rho} \tilde{U}_*^\dagger) \rangle \rangle \\ &= \langle \langle \mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q | \hat{\mathcal{E}}_{\tilde{U}_*} | Q(\tilde{\rho}) \rangle \rangle. \end{aligned}$$

Since $Q(\tilde{\rho})$ is KD-real, it expands over the $+1$ eigenvectors of $\hat{\mathcal{K}}$ as

$$|Q(\tilde{\rho})\rangle = \sum_{\substack{\mathbf{l}_p \cdot \mathbf{m}_p = 0 \bmod p, \\ \mathbf{l}_q \cdot \mathbf{m}_q = 0 \bmod q}} c_{\mathbf{l}_p, \mathbf{m}_p, \mathbf{l}_q, \mathbf{m}_q} |\phi_{\mathbf{l}_p, \mathbf{m}_p}\rangle \otimes |\psi_{\mathbf{l}_q, \mathbf{m}_q}\rangle.$$

It follows that

$$\begin{aligned} \hat{\mathcal{E}}_{\tilde{U}_*} |Q(\tilde{\rho})\rangle &= \hat{\mathbb{1}}^{(p)} \otimes \hat{\mathcal{T}}^{(q)} |Q(\tilde{\rho})\rangle \\ &= \sum_{\substack{\mathbf{l}_p \cdot \mathbf{m}_p = 0, \\ \mathbf{l}_q \cdot \mathbf{m}_q = 0}} c_{\mathbf{l}_p, \mathbf{m}_p, \mathbf{l}_q, \mathbf{m}_q} |\phi_{\mathbf{l}_p, \mathbf{m}_p}\rangle \otimes |\psi_{-p\mathbf{m}_q, \bar{p}\mathbf{l}_q}\rangle. \end{aligned}$$

Furthermore, we have

$$\begin{aligned} \langle \langle \mathbf{i}_q, \mathbf{j}_q | \psi_{-p\mathbf{m}_q, \bar{p}\mathbf{l}_q} \rangle \rangle &= q^{-n} e^{\frac{2\pi i}{q} (-p\mathbf{i}_q \cdot \mathbf{m}_q + \bar{p}\mathbf{j}_q \cdot \mathbf{l}_q)} \\ &= \langle \langle \bar{p}\mathbf{j}_q, -p\mathbf{i}_q | \psi_{\mathbf{l}_q, \mathbf{m}_q} \rangle \rangle. \end{aligned}$$

Putting everything together, we obtain

$$\begin{aligned} Q(\tilde{U}_* \tilde{\rho} \tilde{U}_*^\dagger)_{\mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q} &= \langle \langle \mathbf{i}_p, \mathbf{i}_q; \mathbf{j}_p, \mathbf{j}_q | \hat{\mathcal{E}}_{\tilde{U}_*} | Q(\tilde{\rho}) \rangle \rangle \\ &= \sum_{\substack{\mathbf{l}_p \cdot \mathbf{m}_p = 0, \\ \mathbf{l}_q \cdot \mathbf{m}_q = 0}} c_{\mathbf{l}_p, \mathbf{m}_p, \mathbf{l}_q, \mathbf{m}_q} \langle \langle \mathbf{i}_p, \mathbf{j}_p | \phi_{\mathbf{l}_p, \mathbf{m}_p} \rangle \rangle \langle \langle \mathbf{i}_q, \mathbf{j}_q | \psi_{-p\mathbf{m}_q, \bar{p}\mathbf{l}_q} \rangle \rangle \\ &= \sum_{\substack{\mathbf{l}_p \cdot \mathbf{m}_p = 0, \\ \mathbf{l}_q \cdot \mathbf{m}_q = 0}} c_{\mathbf{l}_p, \mathbf{m}_p, \mathbf{l}_q, \mathbf{m}_q} \langle \langle \mathbf{i}_p, \mathbf{j}_p | \phi_{\mathbf{l}_p, \mathbf{m}_p} \rangle \rangle \langle \langle \bar{p}\mathbf{j}_q, -p\mathbf{i}_q | \psi_{\mathbf{l}_q, \mathbf{m}_q} \rangle \rangle \\ &= Q(\tilde{\rho})_{\mathbf{i}_p, \bar{p}\mathbf{j}_q; \mathbf{j}_p, -p\mathbf{i}_q}. \end{aligned}$$

This is a permutation of the index set. A permutation of entries preserves the total nonpositivity as well as KD-reality; hence, the total nonpositivity of a KD-real $Q(\tilde{\rho})$ —and equivalently of a KD-real $Q(\rho)$ —is preserved under the action of $\tilde{U}_*$. This proves that $U_*^{\otimes n}$ is positivity preserving for the $V = \text{DFT}_{pq}^{\otimes n}$ distribution. The induced bijection Γ^{-1} between indices takes on the same form entrywise as in the $n = 1$ case [Eq. (D1)]:

$$\Gamma^{-1}(\mathbf{i}, \mathbf{j}) = (\mathbf{i}_p q \bar{q} + \bar{p} \mathbf{j}_q p \bar{p}, \mathbf{j}_p q \bar{q} - p \mathbf{i}_q p \bar{p}).$$

■

- [1] D. Gottesman, The Heisenberg representation of quantum computers, in *Group22: Proceedings of the XXII International Colloquium on Group Theoretical Methods in Physics*, edited by S. P. Corney, R. Delbourgo, and P. D. Jarvis (International Press, Cambridge, MA, 1999), pp. 32–43.
- [2] R. W. Spekkens, Negativity and contextuality are equivalent notions of nonclassicality, *Phys. Rev. Lett.* **101**, 020401 (2008).
- [3] A. Ferraro and M. G. A. Paris, Nonclassicality criteria from phase-space representations and information-theoretical constraints are maximally inequivalent, *Phys. Rev. Lett.* **108**, 260403 (2012).
- [4] A. Mari and J. Eisert, Positive Wigner functions render classical simulation of quantum computation efficient, *Phys. Rev. Lett.* **109**, 230503 (2012).
- [5] D. Gross, Hudson's theorem for finite-dimensional quantum systems, *J. Math. Phys.* **47**, 122107 (2006).
- [6] C. Ferrie and J. Emerson, Frame representations of quantum mechanics and the necessity of negativity in quasi-probability representations, *J. Phys. A: Math. Theor.* **41**, 352001 (2008).
- [7] V. Veitch, C. Ferrie, D. Gross, and J. Emerson, Negative quasi-probability as a resource for quantum computation, *New J. Phys.* **14**, 113011 (2012).
- [8] E. F. Galvão, Discrete Wigner functions and quantum computational speedup, *Phys. Rev. A* **71**, 042302 (2005).
- [9] V. Veitch, S. A. Hamed Mousavian, D. Gottesman, and J. Emerson, The resource theory of stabilizer quantum computation, *New J. Phys.* **16**, 013009 (2014).
- [10] N. Delfosse, P. Allard Guerin, J. Bian, and R. Raussendorf, Wigner function negativity and contextuality in quantum computation on rebits, *Phys. Rev. X* **5**, 021003 (2015).
- [11] M. Howard and E. Campbell, Application of a resource theory for magic states to fault-tolerant quantum computing, *Phys. Rev. Lett.* **118**, 090501 (2017).
- [12] R. Raussendorf, J. Bermejo-Vega, E. Tyhurst, C. Okay, and M. Zurel, Phase-space-simulation method for quantum computation with magic states on qubits, *Phys. Rev. A* **101**, 012350 (2020).
- [13] C. Weedbrook, S. Pirandola, R. García-Patrón, N. J. Cerf, T. C. Ralph, J. H. Shapiro, and S. Lloyd, Gaussian quantum information, *Rev. Mod. Phys.* **84**, 621 (2012).
- [14] H. Pashayan, J. J. Wallman, and S. D. Bartlett, Estimating outcome probabilities of quantum circuits using quasiprobabilities, *Phys. Rev. Lett.* **115**, 070501 (2015).
- [15] R. Jozsa and A. Miyake, Matchgates and classical simulation of quantum circuits, *Proc. R. Soc. London, Ser. A* **464**, 3089 (2008).
- [16] S. Aaronson and A. Arkhipov, The computational complexity of linear optics, in *STOC'11: Proceedings of the forty-third annual ACM symposium on Theory of computing* (Association for Computing Machinery, New York, NY, 2011), pp. 333–342.
- [17] B. M. Terhal and D. P. DiVincenzo, Adaptive quantum computation, constant depth quantum circuits and Arthur-Merlin games, *Quant. Inf. Comp.* **4**, 134 (2004).
- [18] J. G. Kirkwood, Quantum statistics of almost classical assemblies, *Phys. Rev.* **44**, 31 (1933).

- [19] P. A. M. Dirac, On the analogy between classical and quantum mechanics, *Rev. Mod. Phys.* **17**, 195 (1945).
- [20] M. Lostaglio, A. Belenchia, A. Levy, S. Hernández-Gómez, N. Fabbri, and S. Gherardini, Kirkwood-Dirac quasiprobability approach to the statistics of incompatible observables, *Quantum* **7**, 1128 (2023).
- [21] L. M. Johansen, Quantum theory of successive projective measurements, *Phys. Rev. A* **76**, 012119 (2007).
- [22] C. Bamber and J. S. Lundeen, Observing Dirac's classical phase space analog to the quantum state, *Phys. Rev. Lett.* **112**, 070405 (2014).
- [23] D. R. M. Arvidsson-Shukur, N. Y. Halpern, H. V. Lepage, A. A. Lasek, C. H. W. Barnes, and S. Lloyd, Quantum advantage in postselected metrology, *Nat. Commun.* **11**, 3775 (2020).
- [24] S. Das, S. Modak, and M. N. Bera, Saturating quantum advantages in postselected metrology with the positive Kirkwood-Dirac distribution, *Phys. Rev. A* **107**, 042413 (2023).
- [25] N. Lupu-Gladstein, Y. B. Yilmaz, D. R. Arvidsson-Shukur, A. Brodutch, A. O. Pang, A. M. Steinberg, and N. Y. Halpern, Negative quasiprobabilities enhance phase estimation in quantum-optics experiment, *Phys. Rev. Lett.* **128**, 220504 (2022).
- [26] D. R. M. Arvidsson-Shukur, J. C. Drori, and N. Y. Halpern, Conditions tighter than noncommutation needed for nonclassicality, *J. Phys. A: Math. Theor.* **54**, 284001 (2021).
- [27] N. Y. Halpern, Jarzynski-like equality for the out-of-time-ordered correlator, *Phys. Rev. A* **95**, 012120 (2017).
- [28] A. E. Allahverdyan, Nonequilibrium quantum fluctuations of work, *Phys. Rev. E* **90**, 032137 (2014).
- [29] H. J. D. Miller and J. Anders, Time-reversal symmetric work distributions for closed quantum dynamics in the histories framework, *New J. Phys.* **19**, 062001 (2017).
- [30] A. Levy and M. Lostaglio, Quasiprobability distribution for heat fluctuations in the quantum regime, *PRX Quantum* **1**, 010309 (2020).
- [31] M. Lostaglio, Certifying quantum signatures in thermodynamics and metrology via contextuality of quantum linear response, *Phys. Rev. Lett.* **125**, 230603 (2020).
- [32] J. R. González Alonso, N. Y. Halpern, and J. Dressel, Out-of-time-ordered-correlator quasiprobabilities robustly witness scrambling, *Phys. Rev. Lett.* **122**, 040404 (2019).
- [33] R. Wagner, Z. Schwartzman-Nowik, I. L. Paiva, A. Te'eni, A. Ruiz-Molero, R. S. Barbosa, E. Cohen, and E. F. Galvão, Quantum circuits for measuring weak values, Kirkwood-Dirac quasiprobability distributions, and state spectra, *Quantum Sci. Technol.* **9**, 015030 (2024).
- [34] D. Schmid, R. D. Baldijão, Y. Ying, R. Wagner, and J. H. Selby, Kirkwood-Dirac representations beyond quantum states (and their relation to noncontextuality), *Phys. Rev. A* **110**, 052206 (2024).
- [35] M. F. Pusey, Anomalous weak values are proofs of contextuality, *Phys. Rev. Lett.* **113**, 200401 (2014).
- [36] N. S. Williams and A. N. Jordan, Weak values and the Leggett-Garg inequality in solid-state qubits, *Phys. Rev. Lett.* **100**, 026804 (2008).
- [37] H. F. Hofmann, Statistical signatures of quantum contextuality, *Entropy* **26**, 725 (2024).
- [38] D. R. M. Arvidsson-Shukur, W. F. Braasch, Jr, S. De Bièvre, J. Dressel, A. N. Jordan, C. Langrenetz, M. Lostaglio, J. S. Lundeen, and N. Y. Halpern, Properties and applications of the Kirkwood-Dirac distribution, *New J. Phys.* **26**, 121201 (2024).
- [39] R. Raussendorf, D. E. Browne, N. Delfosse, C. Okay, and J. Bermejo-Vega, Contextuality and Wigner-function negativity in qubit quantum computation, *Phys. Rev. A* **95**, 052334 (2017).
- [40] S. De Bièvre, C. Langrenetz, and D. Radchenko, The Kirkwood-Dirac representation associated to the Fourier transform for finite Abelian groups: Positivity, *Ann. Henri Poincaré* **27**, 3093 (2026).
- [41] M. Spriet, Characterizing the Kirkwood-Dirac positivity on second countable LCA groups, [arXiv:2507.23628](https://arxiv.org/abs/2507.23628).
- [42] C. Langrenetz, W. Salmon, S. De Bièvre, J. J. Thio, C. K. Long, and D. R. M. Arvidsson-Shukur, Almost sure minimality of the set of experiments with classical Kirkwood-Dirac representations, *Phys. Rev. A* **113**, 062215 (2026).
- [43] C. Langrenetz, D. R. M. Arvidsson-Shukur, and S. De Bièvre, Characterizing the geometry of the Kirkwood-Dirac-positive states, *J. Math. Phys.* **65**, 072201 (2024).
- [44] S. De Bièvre, Complete incompatibility, support uncertainty, and Kirkwood-Dirac nonclassicality, *Phys. Rev. Lett.* **127**, 190404 (2021).
- [45] J. Xu, Kirkwood-Dirac classical pure states, *Phys. Lett. A* **510**, 129529 (2024).
- [46] Y.-H. Yang, S. Yao, S.-J. Geng, X.-L. Wang, and P.-Y. Chen, Geometry of Kirkwood-Dirac classical states: A case study based on discrete Fourier transform, *J. Phys. A: Math. Theor.* **57**, 435303 (2024).
- [47] M. Oszmaniec, D. J. Brod, and E. F. Galvão, Measuring relational information between quantum states, and applications, *New J. Phys.* **26**, 013053 (2024).
- [48] J. Xu, Hermitian Kirkwood-Dirac-real operators for discrete fourier transformations, *J. Math. Phys.* **66**, 102104 (2025).
- [49] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/rsy9-12fx> for a Mathematica notebook containing calculations supporting Theorem 2.
- [50] J. Ding and N. H. Rhee, Teaching tip: When a matrix and its inverse are stochastic, *The College Mathematics Journal* **44**, 108 (2013).
- [51] J. J. Thio, S. Yang, N. Y. Halpern, S. De Bièvre, C. H. W. Barnes, and D. R. M. Arvidsson-Shukur, Kirkwood-Dirac nonpositivity is a necessary resource for quantum computing, *Phys. Rev. Lett.* **137**, 080601 (2026).
- [52] G. Francica, Most general class of quasiprobability distributions of work, *Phys. Rev. E* **106**, 054129 (2022).
- [53] J.-H. Pei, J.-F. Chen, and H. T. Quan, Exploring quasiprobability approaches to quantum work in the presence of initial coherence: Advantages of the Margenau-Hill distribution, *Phys. Rev. E* **108**, 054109 (2023).
- [54] C. Langrenetz, La distribution de Kirkwood-Dirac comme outil de l'information quantique, Ph.D. thesis, Université de Lille, 2025.
- [55] M. Zurel and A. Heimendahl, Efficient classical simulation of quantum computation beyond Wigner positivity, [arXiv:2407.10349](https://arxiv.org/abs/2407.10349).
- [56] R. O'Connell and L. Wang, A new parametrized quantum distribution function and its time development, *Phys. Lett. A* **107**, 9 (1985).

- [57] R. F. O'Connell, Quantum distribution functions in non-equilibrium statistical mechanics, in *Frontiers of Nonequilibrium Statistical Physics*, edited by G. T. Moore and M. O. Scully (Springer, US, Boston, MA, 1986), pp. 83–95.
- [58] M.-S. Li and Y.-X. Tan, Bargmann invariants for quantum imaginarity, [Phys. Rev. A **111**, 022409 \(2025\)](#).
- [59] L. Zhang, B. Xie, and B. Li, Geometry of sets of Bargmann invariants, [Phys. Rev. A **111**, 042417 \(2025\)](#).
- [60] S. S. Pratapsi, J. Gouveia, L. Novo, and E. F. Galvão, Elementary characterization of Bargmann invariants, [Phys. Rev. A **112**, 042421 \(2025\)](#).
- [61] J. Xu, Numerical ranges of Bargmann invariants, [Phys. Lett. A **565**, 131091 \(2026\)](#).
- [62] D. Gross and M. Walter, Stabilizer information inequalities from phase space distributions, [J. Math. Phys. **54**, 082201 \(2013\)](#).
- [63] 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, [Commun. Math. Phys. **385**, 1325 \(2021\)](#).
- [64] H. J. García, I. L. Markov, and A. W. Cross, On the geometry of stabilizer states, [Quantum Inf. Comput. **14**, 683 \(2014\)](#).