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Frame representations of quantum mechanics and the necessity of negativity in quasi-probability representations

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Abstract
Several finite-dimensional quasi-probability representations of quantum states have been proposed to study various problems in quantum information theory and quantum foundations. These representations are often defined only on restricted dimensions and their physical significance in contexts such as drawing quantum-classical comparisons is limited by the non-uniqueness of the particular representation. Here we show how the mathematical theory of frames provides a unified formalism which accommodates all known quasi-probability representations of finite-dimensional quantum systems. Moreover, we show that any quasi-probability representation is equivalent to a frame representation and then prove that any such representation of quantum mechanics must exhibit either negativity or a deformed probability calculus.

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1. Introduction

The Wigner function [1] is a *quasi-probability* density on a classical phase space which represents a quantum state. The term quasi-probability refers to the fact that the function is not a true density as it takes on negative values for some quantum states. As is well known, the Wigner formalism can be lifted into a fully autonomous phase space theory which reproduces all the predictions of quantum mechanics [2].

In recent years various phase space and other quasi-probability representations of finite-dimensional quantum systems have been proposed. In the remainder of the paper, whenever we refer to a representation of quantum systems, we implicitly mean a representation of *finite-dimensional* quantum systems (of dimensional d). For example, the Wootters [3] phase space function is defined on a $d \times d$ lattice indexed by the integers modulo d for all d dimensional Hilbert spaces where d is prime—it is defined on the Cartesian product of these lattices whenever d is composite. Leonhardt [4] introduced a four-fold redundant phase space function on a $2d \times 2d$ lattice indexed by the integers modulo $2d$ which is valid for d an even integer. Heiss and Weigert [5] have defined a phase space function on d^2 points embedded in the sphere $\mathcal{S}^2$. Gibbons, Hoffman and Wootters [6] introduced a discrete Wigner function on a $d \times d$ lattice indexed by elements of a finite field of dimension d when d is a power of a prime number. There are several others (for a recent review see [7]). In addition to these discrete phase space functions, continuous phase space representations of finite-dimensional quantum state have also been introduced [8], as well as more general quasi-probability representations [9, 10], which are real-valued representations that do not necessarily reflect any preconceived classical phase space structure.

Such representations have provided insight into fundamental structures for finite-dimensional quantum systems. For example, the representation proposed by Wootters identifies sets of mutually unbiased bases [3, 6]. Inspired by the discovery that quantum resources lead to algorithms that dramatically outperform their classical counterparts, there has also been growing interest in the application of discrete phase representation to analyze the quantum-classical contrast for finite-dimensional systems, for example, quantum teleportation [11], the effect of decoherence on quantum walks [12], quantum Fourier transform and Grover's algorithm [13], conditions for exponential quantum computational speedup [14, 15] and quantum expanders [16].

A central concept in studies of the quantum-classical contrast in the quasi-probability formalisms of quantum mechanics is the appearance of *negativity*. A non-negative quasi-probability function is a true probability distribution, prompting some authors to suggest that the presence of negativity in this function is a defining signature of non-classicality. However, a quantum state can be negative in one representation and positive in another. This simple fact underscores the obvious problem that considering any one of these quasi-probability representations in the context of determining criteria for the non-classicality of a given quantum state is inadequate due to the non-uniqueness of that particular representation. Ideally one would like to determine whether the state can be expressed as a classical state in *any* quasi-probability representation. Indeed the sheer variety of proposed quasi-probability representations prompts the question of whether there is some shared underlying mathematical structure that might provide a means for identifying the full family of such representations. The first goal of the work presented here is to provide such a unifying formalism.

Moreover, from an operational point of view, states alone are an incomplete description of an experimental arrangement. For example, it is proved in [15] that, within the class of quasi-probability representations due to Gibbons *et al* [6], the only positive pure states are a subset of the so-called stabilizer states. The authors note that these states are 'classical' from the point of view of allowing an efficient classical simulation via the stabilizer formalism. However, this set of positive states includes the Bell states—states which (maximally) violate a Bell inequality—and hence these states are maximally *non-classical* according to a far more conventional criterion of classicality: locality.

The resolution of this paradox is that one must also consider the representation of measurements in the quasi-probability representation in order to assess the classicality of a complete *experimental procedure*. Hence, it is important to elucidate the ways in which a quasi-probability representation *of states alone* can be lifted to an autonomous quasi-probability representation of *both the states and measurements* defining a set of complete experimental configurations. Indeed, in the representation considered above, although the Bell state has a positive representation, one can show that the conditional probabilities representing the measurements assume negative values (and hence are non-classical in a sense we make precise below). Indeed, the second goal of this work is to determine the full set of possible quasi-probability representations of both states and measurements. Only by considering this full set of quasi-probability representations it is possible to establish a meaningful sense in which the appearance of negativity provides a rigorous notion of non-classicality, i.e., either the states or effects (or both) must exhibit negativity in all such representations (otherwise a classical representation does exist).

The outline of this paper is as follows. In section 2, we show how the mathematical theory of frames, which has been developed in the context of signal analysis to devise methods of representing information redundantly in order to protect it against noise [17], provides a formalism which underlies all known quasi-probability representations of finite-dimensional quantum states. In section 3, we show that there are two ways in which any quasi-probability representation of states can be extended to include a representation of measurements, and hence lifted to a fully autonomous formulation of finite-dimensional quantum mechanics. In section 4, we prove that any representation that reproduces all of the predictions of quantum mechanics must either (i) exhibit negativity in the quasi-probability functions for either states or measurements or (ii) make use of a deformed probability calculus and then clarify in which sense these correspond to non-classical properties. We conclude in section 5 by discussing how our formalism can be applied to determine when non-classical resources are present in an experimental system or a given quantum information task which involve only a restricted set of preparations and measurements. In the discussion we also connect our results with recent independent work [18] which establishes negativity and contextuality as equivalent criteria of the non-classicality of quantum mechanics.

2. Frame representations of quantum states

From an operational point of view, the formulation of quantum mechanics requires only the Hermitian operators acting on a complex Hilbert space $\mathcal{H}$ with some finite dimension d [9]. The Hermitian operators themselves form a real Hilbert space Herm $(\mathcal{H})$ of dimension d^2 with inner product $\langle \hat{A}, \hat{B} \rangle := \mathrm{tr}(\hat{A}\hat{B})$.

A basis is a linearly independent set that spans Herm $(\mathcal{H})$. A *frame* is a generalization of the notion of a basis. Let Γ be some set with positive measure μ. The space of real-valued square integrable functions on Γ is denoted by $L^2(\Gamma, \mu)$. A *frame* for Herm $(\mathcal{H})$ is a mapping $\hat{F} : \Gamma \to \mathrm{Herm}\,(\mathcal{H})$ which satisfies

$$a\|\hat{A}\|^2 \leqslant \int_\Gamma \mathrm{d}\mu(\alpha) |\langle \hat{F}(\alpha), \hat{A} \rangle|^2 \leqslant b\|\hat{A}\|^2, \tag{1}$$

for all $\hat{A} \in \mathrm{Herm}\,(\mathcal{H})$ and some constants $a, b > 0$. Note that (for finite-dimensional Hilbert spaces) a frame is equivalent to a spanning set which need not be linearly independent. Such a linearly dependent spanning set is sometimes called an 'overcomplete basis'.

Definition 1. *A mapping* Herm $(\mathcal{H}) \to L^2(\Gamma, \mu)$ *of the form*

$$\hat{A} \mapsto A(\alpha) := \langle \hat{F}(\alpha), \hat{A} \rangle, \tag{2}$$

where $\hat{F}$ is a frame, is a frame representation of Herm $(\mathcal{H})$.

A *dual frame* is a frame $\hat{E} : \Gamma \to \mathrm{Herm}\,(\mathcal{H})$ which satisfies

$$\hat{A} = \int_\Gamma \mathrm{d}\mu(\alpha) \langle \hat{F}(\alpha), \hat{A} \rangle \hat{E}(\alpha), \tag{3}$$

for all $\hat{A} \in \mathrm{Herm}(\mathcal{H})$. When Γ is finite and $|\Gamma| = d^2$, the dual frame is the unique, otherwise there are infinitely many choices for a dual frame.

Here we present two examples of frames. Consider the operator $\hat{Z}$ whose spectrum is $\mathrm{spec}(\hat{Z}) = \left\{ \mathrm{e}^{\frac{2\mathrm{i}\pi}{d}k} : k \in \mathbb{Z}_d \right\}$. The eigenvectors form a basis for $\mathcal{H}$ and are denoted by $\{\phi_k : k \in \mathbb{Z}_d\}$. Consider also the operator defined by $\hat{X}\phi_k = \phi_{k+1}$, where all arithmetic is modulo d. The operators $\hat{Z}$ and $\hat{X}$ are often called *generalized Pauli operators* since they are indeed the usual Pauli operators when $d = 2$. The *parity operator* is defined by $\hat{P}\phi_k = \phi_{-k}$. Let $\Gamma = \mathbb{Z}_d \times \mathbb{Z}_d$ and μ be the counting measure and suppose d is prime. Consider the map $\hat{F} : \Gamma \to \mathrm{Herm}(\mathcal{H})$ defined by

$$\hat{F}(q, p) = \frac{1}{d^2} \hat{X}^{2q} \hat{Z}^{2p} \hat{P}\, \mathrm{e}^{\frac{4\mathrm{i}\pi}{d} qp}. \tag{4}$$

This map is a frame for $\mathrm{Herm}(\mathcal{H})$. It is also an orthogonal basis for $\mathrm{Herm}(\mathcal{H})$ and thus the dual frame is unique. Now let $\Gamma = \mathbb{Z}_{2d} \times \mathbb{Z}_{2d}$ and μ be the counting measure and suppose d is even. Consider the map $\hat{F} : \Gamma \to \mathrm{Herm}(\mathcal{H})$ defined by

$$\hat{F}(q, p) = \frac{1}{4d^2} \hat{X}^{q} \hat{Z}^{p} \hat{P}\, \mathrm{e}^{\frac{\mathrm{i}\pi}{d} qp}. \tag{5}$$

This map is also a frame. However $|\Gamma| = 4d^2$ and thus the dual frame cannot be unique.

We propose the following as a minimal requirement for the definition of a quasi-probability representation of quantum *states*.

Definition 2. *A quasi-probability representation of quantum states is any map* $\mathrm{Herm}(\mathcal{H}) \to L^2(\Gamma, \mu)$ *that is linear and invertible.*

Given this definition, any phase space representation is then a particular type of quasi-probability representation. In particular, if there exists symmetry group on Γ, G, carrying a unitary representation $\hat{U} : G \to U(\mathcal{H})$ and a quasi-probability representation satisfying the covariance property $\hat{U}_g \hat{A} \hat{U}_g^\dagger \mapsto \{A(g(\alpha))\}_{\alpha\in\Gamma}$ for all $\hat{A} \in \mathrm{Herm}(\mathcal{H})$ and $g \in G$, then $\hat{A} \mapsto A(\alpha)$ is a *phase space representation*. All phase space functions (that we are aware of) in the literature correspond to quasi-probability representations that satisfy this additional covariance condition.

It is clear that a frame representation defined by equation (2) is a linear bijection and hence a quasi-probability representation. Thus, the frames defined by equations (4) and (5) are quasi-probability representations. Indeed, equation (4) defines the phase space quasi-probability function defined by Wootters [3] while equation (5) defines the phase space quasi-probability function defined by Leonhardt [4]. It is less obvious that the converse is also true. Nevertheless, the following theorem verifies this fact.

Theorem 1. *If A mapping W is a quasi-probability representation, then it is a frame representation for a unique frame* $\hat{F}$.

Proof. Linearity and the Riesz representation theorem implies that $W(\hat{A})(\alpha) = \langle \hat{F}(\alpha), \hat{A}\rangle$ for some unique mapping $\hat{F} : \Gamma \to \mathrm{Herm}(\mathcal{H})$ (not necessarily a frame). Since $\mathrm{Herm}(\mathcal{H})$ is finite-dimensional, the inverse W^{-1} is bounded. Thus, W is bounded below by the bounded inverse theorem. That is, there exists a constant $a > 0$ such that

$$a\|\hat{A}\|^2 \leqslant \int_\Gamma \mathrm{d}\mu(\alpha) |\langle \hat{F}(\alpha), \hat{A}\rangle|^2.$$

Since $\langle \hat{F}(\alpha), \hat{A}\rangle \in L^2(\Gamma, \mu)$, there exists a constant $b > 0$ such that

$$\int_\Gamma \mathrm{d}\mu(\alpha) |\langle \hat{F}(\alpha), \hat{A}\rangle|^2 \leqslant b\|\hat{A}\|^2.$$

Hence $\hat{F}$ is a frame. □

3. Frame representations of quantum mechanics

Most proposed phase space functions (of finite-dimensional quantum systems) are representations of quantum states alone. Here we show that there are two approaches within the frame formalism to lift any representation of states to a fully autonomous representation of finite-dimensional quantum mechanics.

An operational set of axioms [9] of quantum mechanics are the following:

(i) There exists a Hilbert space $\mathcal{H}$, $\dim \mathcal{H} = d$.
(ii) A preparation (state) is represented by a density operator $\hat{\rho}$ satisfying $\langle \psi, \hat{\rho}\psi \rangle \geqslant 0$, for all $\psi \in \mathcal{H}$, and $\mathrm{tr}(\hat{\rho}) = 1$.
(iii) A measurement is represented by a set of effects $\{\hat{M}_k\}$, i.e., positive operator valued measure (POVM), satisfying $0 \leqslant \langle \psi, \hat{M}_k \psi \rangle \leqslant 1$, for all $\psi \in \mathcal{H}$, and $\sum_k \hat{M}_k = \hat{\mathbb{1}}$.
(iv) For a system with density operator $\hat{\rho}$ subject to the measurement $\{\hat{M}_k\}$, the probability of obtaining outcome k is given by the Born rule

$$\Pr(k) = \mathrm{tr}(\hat{M}_k \hat{\rho}). \tag{6}$$

Hence to construct an autonomous formulation of quantum mechanics we need a set of functions $\{M_k\}$ on phase space representing the set of measurement operators $\{\hat{M}_k\}$ as well as a prescription for calculating the probabilities that are prescribed by the Born rule.

3.1. Deformed probability representations

The first frame representation approach to an autonomous formulation of quantum mechanics consists of mapping both states and measurements to $L^2(\Gamma, \mu)$ via the same frame $\hat{F}$, i.e. $\hat{\rho} \mapsto \rho(\alpha) := \langle \hat{\rho}, \hat{F}(\alpha) \rangle$ and $\hat{M}_i \mapsto M_i(\alpha) := \langle \hat{M}_i, \hat{F}(\alpha) \rangle$. The functions in the range of this frame representation, when the domain is restricted to the density operators, are called *quasi-probability densities*. Similarly, the functions in the range of the frame representation, when the domain is restricted to the effects, are called *conditional quasi-probabilities*. Then the axioms of quantum mechanics become the following:

(i) There is a measurable set of allowed properties Γ endowed with a positive measure μ.
(ii) A preparation (state) is represented by a quasi-probability density $\rho(\alpha) \in \mathbb{R}$ which satisfies the normalization condition $\int_\Gamma \mathrm{d}\mu(\alpha)\rho(\alpha) = 1$.
(iii) A measurement is represented by a set of conditional quasi-probabilities $\{M_k(\alpha) \in \mathbb{R}\}$ which satisfies $\sum_k M_k(\alpha) = 1$ for all $\alpha \in \Gamma$.
(iv) For a system with quasi-probability density ρ subject to the measurement $\{M_k\}$, the probability of obtaining outcome k is given by

$$\Pr(k) = \int_\Gamma \mathrm{d}\mu(\alpha, \beta)\rho(\alpha) M_k(\beta) \langle \hat{E}(\alpha), \hat{E}(\beta) \rangle, \tag{7}$$

where $\hat{E}$ is any frame dual to $\hat{F}$.

As will become clear in the next section, equation (7) is a *deformed* version of the usual law of total probability and hence we call this first approach a *deformed probability representation of quantum mechanics*. This is not the only possibility. Indeed, below we will see a different approach.

3.2. Quasi-probability representations

Note that the deformed probability calculus, equation (7), can be written as

$$\Pr(k) = \int_\Gamma \mathrm{d}\mu(\alpha)\rho(\alpha)\tilde{M}_k(\alpha), \tag{8}$$

where

$$\tilde{M}_k(\alpha) = \int_\Gamma \mathrm{d}\mu(\beta) M_k(\beta)\langle \hat{E}(\alpha), \hat{E}(\beta)\rangle. \tag{9}$$

Recall that M_k is the frame representation of $\hat{M}_k$ for the frame $\hat{F}$. Hence $\tilde{M}_k$ can be identified as the frame representation of $\hat{M}_k$ using a frame $\hat{E}$ that is dual to $\hat{F}$. The second frame representation approach to an autonomous formulation consists of mapping density operators to functions in $L^2(\Gamma, \mu)$ via a particular choice of frame $\hat{F}$ and effects to functions in $L^2(\Gamma, \mu)$ via a frame $\hat{E}$ that is dual to $\hat{F}$, i.e. $\hat{\rho} \mapsto \rho(\alpha) := \langle \hat{\rho}, \hat{F}(\alpha)\rangle$ and $\hat{M}_k \mapsto M_k(\alpha) := \langle \hat{M}_k, \hat{E}(\alpha)\rangle$. As above we define the former functions to be quasi-probability densities and the latter functions to be conditional quasi-probabilities. The axioms of quantum mechanics can be reformulated once again as follows:

(i) There is a set of allowed properties Γ with a positive measure μ.
(ii) A preparation (state) is represented by a quasi-probability density $\rho(\alpha) \in \mathbb{R}$ which satisfies the normalization condition $\int_\Gamma \mathrm{d}\mu(\alpha)\rho(\alpha) = 1$.
(iii) A measurement is represented by a set of conditional quasi-probabilities $\{\tilde{M}_k(\alpha) \in \mathbb{R}\}$ which satisfies $\sum_k \tilde{M}_k(\alpha) = 1$ for all $s \in \Gamma$.
(iv) For a system with probability density ρ subject to the measurement $\{\tilde{M}_k\}$, the probability of obtaining outcome k is given by equation (8).

As will become clear in the next section, the probability calculus equation (8) given in condition (iv) is now just the usual law of total probability, although the preparation and measurement functions are not necessarily positive semi-definite. Hence, we call this second approach a *quasi-probability representations of quantum mechanics* (i.e., a quasi-probability representation of both states *and* measurements).

Note that in this quasi-probability representation approach a second frame $\hat{E}$, which is dual to $\hat{F}$, is required. Recall that the frames given in equations (4) and (5) defined the phase space quasi-probability functions of Wootters and Leonhardt. For the Wootters case, the dual frame is unique and is given by

$$\hat{E}(q, p) = \frac{1}{d}\hat{X}^{2q}\hat{Z}^{2p}\hat{P}\,\mathrm{e}^{\frac{4\mathrm{i}\pi}{d}qp}.$$

For the Leonhardt case, the frame in equation (5) is not a basis and the dual is not unique. However, a quasi-probability representation of quantum mechanics only requires *a* dual frame. One such dual frame is

$$\hat{E}(q, p) = \frac{1}{2d}\hat{X}^{q}\hat{Z}^{p}\hat{P}\,\mathrm{e}^{\frac{\mathrm{i}\pi}{d}qp}.$$

4. Non-classicality: negative quasi-probability or a deformed law of total probability

Let the set Γ represent the properties of a classical system and the function $\rho(\alpha) > 0$ represent the probabilistic knowledge of these properties. Note that these probability densities form a convex set with the Dirac measures as its extreme points. A measurement is a partitioning of the space Γ into disjoint subsets $\{\triangle_j\}$. The probability of the system to have properties in $\triangle_j$ (we will call this 'outcome j') is

$$\Pr(j) = \int_{\triangle_j} \mathrm{d}\mu(\alpha)\rho(\alpha) = \int_{\Gamma} \mathrm{d}\mu(\alpha)\chi_j(\alpha)\rho(\alpha),$$

where $\chi_j(\alpha) \in \{0, 1\}$ is the indicator function of $\triangle_j$. The measurement is equivalently specified by the set $\{\chi_j(\alpha)\}$, which is interpreted as the conditional probability of outcome k given the systems is known to have the properties α. A measurement of this type is deterministic: it reveals with certainty the properties of the system. Consider now an indeterministic measurement specified by the conditional probabilities $\{M_k(\alpha) \in [0, 1]\}$. These can always be thought of as a convex combination of indicator functions. That is, the measurement functions form a convex set with the indicator functions as its extreme points. We summarize the above description with the following definition.

Definition 3. *Any statistical or operational model of a set of experimental configurations is classical if all of the following properties hold:*

(i) There is a set of allowed properties Γ with a positive measure μ.
(ii) A preparation (state) is represented by a probability density $\rho(\alpha) \geqslant 0$ which satisfies the normalization condition $\int_\Gamma \mathrm{d}\mu(\alpha)\rho(\alpha) = 1$.
(iii) A measurement is represented by a set $\{M_k(\alpha) \in [0, 1]\}$ which satisfies $\sum_k M_k(\alpha) = 1$ for all $\alpha \in \Gamma$.
(iv) For a system with probability density ρ subject to the measurement $\{M_k\}$, the probability of obtaining outcome k is given by the law of total probability

$$\Pr(k) = \int_{\Gamma} \mathrm{d}\mu(\alpha)\rho(\alpha)M_k(\alpha). \tag{10}$$

Consider now a frame representation defined via a *positive* frame $\hat{F}$. Applying the deformed probability representation (the first approach of the previous section) to map quantum mechanics to the space of functions $L^2(\Gamma, \mu)$, we find that the representations of the preparations and measurements satisfy the criteria of the *classical* model because they are guaranteed to be non-negative function when the frame $\hat{F}$ is positive. However, as noted previously, the calculation of probabilities, equation (7), is *deformed* when compared to the classical one, equation (10). Hence under this approach the associated frame representations do not meet the criteria of a classical model.

Now, applying instead the quasi-probability representation (the second approach of the previous section) the probability calculus, equation (8), is the same as the classical one, equation (10). Furthermore the preparations are represented by non-negative functions (because the frame $\hat{F}$ is positive) and therefore also meet the criteria set out by condition (ii). However, in this case the measurements must be represented via a frame $\hat{E}$ which is dual to the frame $\hat{F}$ that is used for representing preparations. It is not immediately obvious that any quasi-probability representation of quantum mechanics following this second approach is also unable to meet the criteria of a classical operational model, in particular condition (iii) which requires non-negative conditional probabilities. We now show that this is impossible by proving that there does not exist a dual frame of positive operators for a frame of positive operators.

Theorem 2. *There does not exist a dual frame of positive operators for a frame of positive operators.*

Proof. Consider the mapping

$$\tilde{\Phi}(\hat{A}) = \int_{\Gamma} \mathrm{d}\mu(\alpha)\langle \hat{F}(\alpha), \hat{A}\rangle \hat{E}(\alpha). \tag{11}$$

If $\tilde{\Phi}$ were the identity super-operator, then by definition $\hat{E}$ would be the dual frame of $\hat{F}$. We will show that this is not possible when both $\hat{F}$ and $\hat{E}$ are positive frames. Let $\{|\phi_i\rangle\langle\phi_j| : i, j \in \mathbb{Z}_{\mathrm{d}}\}$ be the standard basis for $\mathrm{L}(\mathcal{H})$. Then, the Choi–Jamiolkowski [19] representation of $\tilde{\Phi}$ is

$$J(\tilde{\Phi}) = \sum_{i,j\in\mathbb{Z}_{\mathrm{d}}} \tilde{\Phi}(|\phi_i\rangle\langle\phi_j|) \otimes |\phi_i\rangle\langle\phi_j| \tag{12}$$

$$= \int_{\Gamma} \mathrm{d}\mu(\alpha) \left(\sum_{i,j\in\mathbb{Z}_{\mathrm{d}}} \langle\phi_j|\hat{F}(\alpha)|\phi_i\rangle \hat{E}(\alpha) \otimes |\phi_i\rangle\langle\phi_j| \right) \tag{13}$$

$$= \int_{\Gamma} \mathrm{d}\mu(\alpha) \left(\hat{E}(\alpha) \otimes \sum_{i,j\in\mathbb{Z}_{\mathrm{d}}} \langle\phi_j|\hat{F}(\alpha)|\phi_i\rangle |\phi_i\rangle\langle\phi_j| \right) \tag{14}$$

$$= \int_{\Gamma} \mathrm{d}\mu(\alpha)(\hat{E}(\alpha) \otimes \hat{F}(\alpha)), \tag{15}$$

which is a separable operator (a convex combination of positive operators of the form $\hat{A} \otimes \hat{B}$) on $\mathcal{H} \otimes \mathcal{H}$ when both $\hat{F}$ and $\hat{E}$ are positive frames. However, $J(\tilde{\mathbb{1}})$ is not a separable operator on $\mathcal{H} \otimes \mathcal{H}$ and thus $\tilde{\Phi}$ cannot be the identity super-operator. Hence $\hat{E}$ cannot be a dual frame of $\hat{F}$. □

This theorem can also be proven using the results of [20]. Theorem 2 of that paper shows that the channel $\tilde{\Phi}$ defined by equation (11) for positive operators $\hat{F}$ and $\hat{E}$ is the so-called *entanglement breaking*. However, theorem 6 of [20] states that if $\tilde{\Phi}$ has fewer than d Kraus operators, it is *not* entanglement breaking. Since the identity super-operator has fewer than d Kraus operators, $\tilde{\Phi}$ is not entanglement breaking and therefore $\hat{E}$ is not the dual of $\hat{F}$.

Hence, although quantum states can always be represented as non-negative probabilities, measurement functions must then take on negative values or vice-versa. In this way we have a direct proof that there does not exist any choice of quasi-probability representation of quantum mechanics that can be made consistent with the non-negativity conditions associated with a classical model of statistical events.

5. Discussion

Our results prove that the full spectrum of experimental statistics prescribed by finite-dimensional quantum theory cannot be described by any classical model consisting of the usual rules of probability applied over an arbitrary choice of property (or hidden variable) space. Equivalently stated, there does not exist a space of events upon which one can formulate a non-negative quasi-probability representation of quantum mechanics.

A promising application of the formalism we have developed is to address the question of whether a restricted set of preparations and measurements involves non-classical resources. This question has arisen in the context of the degree of coherent control over quantum systems, for example, in experiments involving nuclear magnetic resonance or super-conducting devices, where the quantum states and effects that can be achieved are restricted due to thermalization and decoherence. Our formalism leads to a broadly enabling and rigorous approach to determining the extent to which quantum effects are indeed present in those systems. Another context in which this question arises is the field of quantum information and computation. One has a task which can be achieved with a restricted set of quantum preparations and effects and one would like to know whether non-classical resources are actually required for that task. In both of these contexts, if we can identify a particular frame and a dual which can represent the restricted set of states and measurements as non-negative functions then we can show that the task or process can be represented as a classical statistical process, and hence prove that it does not require quantum resources. Conversely, if one can prove that no such choice of frames exists, then one can prove that quantum resources are indeed necessary.

Finally, we conclude by addressing the question of how the notion of non-classicality established by the absence of non-negative quasi-probability representation relates to another fundamental notion of non-classicality in quantum mechanics, namely, *contextuality*. The traditional definition of contextuality comes from a theorem due to Kochen and Specker [21]. The Kochen–Specker theorem establishes a contradiction between a set of plausible assumptions associated with the idea that quantum systems possess pre-existing values for the outcomes of measurements, as is the case in the classical world. Assuming that physical systems do possess pre-existing values that are revealed via measurements, the Kochen–Specker theorem leads to the following counterintuitive property that such pre-existing values must satisfy [22]: suppose three operators $\hat{A}$, $\hat{B}$ and $\hat{C}$ satisfy $[\hat{A}, \hat{B}] = 0 = [\hat{A}, \hat{C}]$, but $[\hat{B}, \hat{C}] \neq 0$, then the pre-existing value of the observable A will depend on whether observable B or C is measured along with A. That is, the pre-existing value of A depends on the *context* of the measurement. We note that the notion of context independence is at the heart of Bell-type inequalities, where the pre-existing values of the commuting operators in question are required to be context independent by appealing to local causality.

Spekkens has generalized the notion of *non-contextuality* from the idea that outcomes of individual measurements are independent of the measurement context to the requirement that the *probabilities* for outcomes of measurements are independent of the measurement context [23]. This is achieved by formulating a definition of contextuality for an arbitrary operational theory and includes a notion of contextuality for preparation procedures (states) as well as measurements. In [18], Spekkens has shown that a quasi-probability representation of quantum mechanics which excludes negativity is equivalent to the generalized notion of non-contextuality that he proposed in [23] and has obtained an independent proof of the impossibility of constructing a non-negative quasi-probability representation. Interestingly, in light of this connection our direct proof of the non-existence of a positive dual frame to a positive frame gives a new independent proof of the generalized contextuality of quantum mechanics.

In this paper we have shown that using frame theory provides a formalism that unifies the known quasi-probability representations of quantum *states*. We have shown two different ways (the *deformed* and *quasi-probability* approach) to lift a quasi-probability representation of states to a consistent and equivalent formulation of quantum mechanics. We have also proved that these quasi-probability representations of quantum states and *measurements* require either negativity or a deformation of the rule for calculating probabilities. We have thus given a mathematically rigorous set of criteria that establish the (long suspected) connection between negativity and non-classicality. While the results of this paper have been proven only for finite-dimensional Hilbert spaces (although allowing for either finite or continuous representation spaces), we conjecture that the results continue to hold also for infinite-dimensional quantum systems (i.e., all separable Hilbert spaces).

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Appendix

For completeness we describe here how to formulate quantum mechanics directly in either the deformed or quasi-probability representations without appealing to the axioms of quantum mechanics in their usual formulation (i.e., in terms of positive linear operators on finite-dimensional Hilbert space). Recall that previously, in the deformed probability representation, a quasi-probability density was defined as a function in the range of a frame representation when the domain is restricted to the density operators. Similarly, the conditional quasi-probabilities were those functions in the range of a frame representation when the domain is restricted to the effects. Of course, for a particular choice of frame, not every function in $L^2(\Gamma, \mu)$ will correspond to a valid quantum state or effect. Hence we need a set of *internal* conditions, without appealing to the nature of the linear operators in the standard formulation of quantum theory, which characterize the valid state and measurement functions in $L^2(\Gamma, \mu)$. The conditions can be found by simply noting that the frame representation, equation (2), is an isometric and algebraic isomorphism from Herm $(\mathcal{H})$ to $L^2(\Gamma, \mu)$ equipped with inner product

$$\langle A, B\rangle_{\mathtt{F}} := \int_{\Gamma^2} \mathrm{d}\mu(\alpha, \beta) A(\alpha) B(\beta) \mathtt{F}(\alpha, \beta),$$

where $\mathtt{F}(\alpha, \beta) := \langle \hat{E}(\alpha), \hat{E}(\beta)\rangle$, and algebraic multiplication

$$(A \star_{\mathfrak{F}} B)(\alpha) := \int_{\Gamma^2} \mathrm{d}\mu(\beta, \gamma) A(\beta) B(\gamma) \mathfrak{F}(\alpha, \beta, \gamma),$$

where $\mathfrak{F}(\alpha, \beta, \gamma) = \langle \hat{F}(\alpha), \hat{E}(\beta)\hat{E}(\gamma)\rangle$.

Using the above, we first state the conditions for a function in $L^2(\Gamma, \mu)$ to be a valid state or effect in the deformed probability representation. A *pure state* is a function $\rho_{\mathrm{pure}} \in L^2(\Gamma, \mu)$ satisfying $\rho_{\mathrm{pure}} \star_{\mathfrak{F}} \rho_{\mathrm{pure}} = \rho_{\mathrm{pure}}$. A general *state* is a function $\rho \in L^2(\Gamma, \mu)$ satisfying $\langle \rho, \rho_{\mathrm{pure}}\rangle_{\mathtt{F}} \geqslant 0$ for all pure states and $\int_\Gamma \mathrm{d}\mu(\alpha)\rho(\alpha) = 1$. A *measurement* is represented by a set $\{M_k \in L^2(\Gamma, \mu)\}$ of *effects* which satisfies $\langle M_k, \rho_{\mathrm{pure}}\rangle_{\mathtt{F}} \geqslant 0$ for all pure states and for which $\sum_k M_k = \mathbb{1}$, where $\mathbb{1}$ is the identity element in $L^2(\Gamma, \mu)$ with respect to the algebra defined by $\star_{\mathfrak{F}}$.

For quasi-probability representations of quantum mechanics, the term quasi-probability density has the same meaning as in the deformed probability representation. Similarly, the conditional quasi-probabilities are those functions in the range of the frame representation of the measurements (i.e. the frame representation defined via the dual $\hat{E}$) when the domain is restricted to the effects. In this representation states and measurements in $L^2(\Gamma, \mu)$ must again meet certain criteria to be valid. The conditions are similar to those in the deformed probability representation. In particular, the pure states and general states are equivalently characterized. However, a measurement is now represented by a set $\{M_k \in L^2(\Gamma, \mu)\}$ which satisfies $\langle M_k, \rho_{\mathrm{pure}}\rangle \geqslant 0$ (now the usual pointwise inner product) for all pure states and for which $\sum_k M_k = \mathbb{1}$, where $\mathbb{1}$ is the identity element in $L^2(\Gamma, \mu)$ with respect to the algebra defined by $\star_{\mathfrak{E}}$ (which is defined in the same way as $\star_{\mathfrak{F}}$ with the roles of the frame and its dual reversed).

References

[1] Wigner E 1932 On the quantum correction for thermodynamic equilibrium *Phys. Rev.* **40** 0749
[2] Baker G A 1958 Formulation of quantum mechanics based on the quasi-probability distribution induced on phase space *Phys. Rev.* **109** 2198
[3] Wootters W K 1987 A Wigner-function formulation of finite-state quantum mechanics *Ann. Phys.* **176** 1
[4] Leonhardt U 1995 Quantum state tomography and discrete Wigner functions *Phys. Rev. Lett.* **74** 4101
[5] Heiss S and Weigert S 2000 Discrete Moyal-type representations for a spin *Phys. Rev.* A **63** 012105
[6] Gibbons K S, Hoffman M J and Wootters W K 2004 Discrete phase space based on finite fields *Phys. Rev.* A **70** 062101 (http://arxiv.org/abs/quant-ph/0401155v6)
[7] Vourdas A 2004 Quantum systems with finite Hilbert space *Rep. Prog. Phys.* **67** 267
[8] Várilly J C and Gracia-Bondía J M 1972 The Moyal representation for spin *Ann. Phys, NY* **190** 107
[9] Hardy L 2001 Quantum theory from five reasonable axioms (http://arxiv.org/abs/quant-ph/0101012v4)
[10] Havel T F 2003 The real density matrix *Quantum Inform. Process.* **1** 511 (http://arxiv.org/abs/quant-ph/0302176v5)
[11] Paz J P 2002 Discrete Wigner functions and the phase-space representation of quantum teleportation *Phys. Rev.* A **65** 062311 (http://arxiv.org/abs/quant-ph/0204150v1)
[12] López C C and Paz J P 2003 Phase-space approach to the study of decoherence in quantum walks *Phys. Rev.* A **68** 0052305 (http://arxiv.org/abs/quant-ph/0308104v3)
[13] Miquel C, Paz J P and Saraceno M 2002 Quantum computers in phase space *Phys. Rev.* A **65** 062309
[14] Galvao E F 2005 Discrete Wigner functions and quantum computational speedup *Phys. Rev.* A **71** 042302 (http://arxiv.org/abs/quant-ph/0405070v2)
[15] Cormick C, Galvao E F, Gottesman D, Paz J P and Pittenger A O 2006 Classicality in discrete Wigner functions *Phys. Rev.* A **73** 012301
[16] Gross D and Eisert J 2007 Quantum Margulis expanders (http://arxiv.org/abs/quant-ph/0710.0651v1)
[17] Christensen O 2003 *Introduction to Frames and Riesz Bases* (Boston: Birkhäuser)
[18] Spekkens R 2007 Negativity and contextuality are equivalent notions of nonclassicality (http://arxiv.org/abs/quant-ph/0710.5549v1)
[19] Jamiolkoski A 1972 Linear transformations which preserve trace and positive semidefiniteness of operators *Rep. Math. Phys.* **3** 275
[20] Horodecki M, Shor P W and Ruskai M B 2003 Entanglement breaking channels *Rev. Math. Phys.* **15** 269 (http://arxiv.org/abs/quant-ph/0302031v2)
[21] Kochen S and Specker E 1967 The problem of hidden variables in quantum mechanics *J. Math. Mech.* **17** 59
[22] Isham C J 1995 *Lectures on Quantum Theory: Mathematical and Structural Foundations* (London: Imperial College Press)
[23] Spekkens R W 2005 Contextuality for preparations, transformations, and unsharp measurements *Phys. Rev.* A **71** 052108