New Journal of Physics
The open-access journal for physics

Framed Hilbert space: hanging the quasi-probability pictures of quantum theory

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New Journal of Physics **11** (2009) 063040 (33pp)
Received 27 March 2009
Published 22 June 2009
Online at http://www.njp.org/
doi:10.1088/1367-2630/11/6/063040

Abstract. Building on earlier work, we further develop a formalism based on the mathematical theory of frames that defines a set of possible phase-space or quasi-probability representations of finite-dimensional quantum systems. We prove that an alternate approach to defining a set of quasi-probability representations, based on a more natural generalization of a classical representation, is equivalent to our earlier approach based on frames, and therefore is also subject to our no-go theorem for a non-negative representation. Furthermore, we clarify the relationship between the contextuality of quantum theory and the necessity of negativity in quasi-probability representations and discuss their relevance as criteria for non-classicality. We also provide a comprehensive overview of known quasi-probability representations and their expression within the frame formalism.

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Contents

1. Introduction

One approach to establish a common ground between classical and quantum theory is phase space. Phase space is a natural concept in classical theory since it is equivalent to the state space. The idea of formulating quantum theory in phase space dates back to the early days of quantum theory when the so-called Wigner function was introduced [1]. The Wigner function is a *quasi-probability* distribution on a classical phase space[4]. The term quasi-probability refers to the fact that the function is not a true probability density as it takes on negative values for some quantum states. The Wigner function formalism can be lifted into a fully autonomous phase space theory that reproduces all the predictions of the standard quantum theory of infinite-dimensional systems [3]. In other words, this phase space formulation of quantum theory is equivalent to the usual abstract formalism of quantum theory in the same sense that Heisenberg's matrix mechanics and Schrodinger's wave mechanics are equivalent to the abstract formalism.

However, the Wigner function representation is non-unique, and, moreover, Wigner's approach is not applicable to describing quantum systems with a finite set of distinguishable states. In recent years, various analogues of the Wigner function for finite-dimensional quantum systems have been proposed. An important subclass of such quasi-probability representations are those defined on a *discrete phase space*. We will use the term *quasi-probability representation* to refer to the broader class of representations where the (ontic) state space is neither required to be discrete nor required to carry any classical phase space structure[5]. Such representations have provided insight into fundamental properties of finite-dimensional quantum systems. For example, the representation proposed by Wootters identifies sets of mutually unbiased bases [4, 5]. 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 space formalism to analyse the quantum-classical contrast for finite-dimensional systems. Examples include analyses of quantum teleportation [6], the effect of decoherence on quantum walks [7], quantum Fourier transform and Grover's algorithm [8], conditions for exponential quantum computational speedup [9, 10] and quantum expanders [11].

As noted above, a central concept in studies of the quantum-classical contrast in the quasi-probability formalisms of quantum theory 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. Unfortunately the application of any one of these quasi-probability representations in the context of determining criteria for the non-classicality of a given quantum task is limited in significance by the non-uniqueness of that particular representation. Ideally one would like to determine whether the task can be expressed as a classical process 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. Moreover, from an operational view, states alone are an incomplete description of an experimental arrangement. Hence, it is important to elucidate the ways in which a quasi-probability representation *of states alone* can be lifted into an autonomous quasi-probability representation of *both the states and measurements* defining any set of experimental configurations.

In an earlier paper [12], we introduced the concept of *frame representation* that mathematically unifies the known quasi-probability representations of quantum states. Once the frame is identified for a particular quasi-probability representation, we showed how any dual frame leads to an autonomous representation of the operational quantum formalism

[4] Note that the Wigner function is not the only such function. A review of the Wigner function and related representations appears in [2].

[5] The term *quasi-probability* is used to allow for the appearance of negative values in the states and/or measurements defined under the representation.

(i.e. including both states *and* measurements). Then we proved that such representation must possess negative values in either the states or measurements (or both). However, because this approach explicitly made use of dual frames to construct the autonomous formulation of quantum mechanics, it remained possible that negativity could be avoided through some other representation that is not explicitly defined via a selection of a dual frame. In this paper, we show that this is not possible. Specifically, we consider an alternative and more natural approach to the definition of the class of autonomous quasi-probability representations for finite-dimensional quantum mechanics and show that any such representation is equivalent to a frame representation and therefore cannot avoid negativity.

The outline of the paper is as follows. In section 2, we give a comprehensive overview of the known quasi-probability functions representing quantum states. In section 3, we review the results of [12] showing how the mathematical theory of frames provides a formalism that underlies all known quasi-probability representations of finite-dimensional quantum *states*. Furthermore, we explicitly construct the frames that give rise to several important quasi-probability representations. In section 4, we review the two ways, presented in [12], in which any frame 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 5, we propose a more natural approach to the definition of quasi-probability representations and show that this approach is equivalent to the approach obtained under frame representations and therefore does not admit a non-negative representation. In section 6, we look at the equivalence of non-negativity in quasi-probability representations and non-contextuality in ontological models. In section 7, we discuss the extension of our results to infinite-dimensional quantum systems and consider potential applications of our work in quantum information science.

2. Review of quasi-probability functions

Reviewed in this section are the existing quasi-probability representations of quantum states found in the literature. The original quasi-probability representation put forth by Wigner and later recognized as an equivalent formulation of the full quantum theory by Moyal [13] and others [3] is reviewed first. This *phase space* picture is only valid for infinite-dimensional Hilbert spaces, but it will be reviewed here because it has motivated all known generalizations for finite dimensions. Sections 2.1–2.6 are devoted to reviewing a representative sample of the known quasi-probability representations of finite-dimensional quantum states.

In section 2.7, a summary of these and a few other quasi-probability representations is presented in a more concise manner.

2.1. Wigner phase space representation

The position operator Q and momentum operator P are the central objects in the abstract formalism of infinite-dimensional quantum theory. The operators satisfy the canonical commutation relations

$$[Q, P] = i.$$

Since Q and P do not commute, the choice of the quantization map $g(q, p) \mapsto g(Q, P)$, for some function g, is not unique. This is the so-called 'ordering problem'. A class of solutions to this problem is the association $e^{i\xi q+i\eta p} \mapsto e^{i\xi Q+i\eta P} f(\xi,\eta)$ for some arbitrary function f (see table 1 of [2] for a review of the traditional choices for f).

Consider the classical particle phase space $\mathbb{R}^2$ and the continuous set of operators

$$F(q,p) := \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} d\xi\, d\eta\, e^{i\xi(q-Q)+i\eta(p-P)} f(\xi,\eta). \tag{1}$$

When $f(\xi,\eta)=1$, the distribution

$$\mu_\rho^{\text{Wigner}}(q,p) := \text{Tr}(\rho F(q,p)) \tag{2}$$

$$= \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2} d\xi\, d\eta\, \text{Tr}\left[\rho e^{i\xi(Q-q)+i\eta(P-p)}\right] \tag{3}$$

is the celebrated Wigner function [1]. The Wigner function is both positive and negative in general. However, it otherwise behaves as a classical probability density on the classical phase space. For these reasons, the Wigner function and others like it came to be called *quasi-probability* functions.

The Wigner function is the unique representation satisfying the properties [14]

Wig(1) For all ρ, $\mu_\rho^{\text{Wigner}}(q,p)$ is real.

Wig(2) For all ρ_1 and ρ_2,

$$\text{Tr}(\rho_1\rho_2) = 2\pi \int_{\mathbb{R}^2} d\xi\, d\eta\, \mu_{\rho_1}^{\text{Wigner}}(\xi,\eta)\, \mu_{\rho_2}^{\text{Wigner}}(\xi,\eta).$$

Wig(3) For all ρ, integrating μ_ρ^{Wigner} along the line $aq+bp=c$ in phase space yields the probability that a measurement of the observable $aQ+bP$ has the result c.

Note from equation (2) that the Wigner function is obtained from the set of operators in equation (1) (for $f=1$) via the trace. Thus, the properties Wig(1)–(3) can be transformed into properties on a set of operators $F(q,p)$ that uniquely specify the set in equation (1) for $f=1$. These properties are

Wig(4) $F(q,p)$ is Hermitian.

Wig(5) $2\pi\text{Tr}(F(q,p)F(q',p')) = \delta(q-q')\delta(p-p')$.

Wig(6) Let P_c be the projector onto the eigenstate of $aQ+bP$ with eigenvalue c. Then,

$$\int_{\mathbb{R}^2} dq\, dp\, F(q,p)\delta(aq+bp-c) = P_c.$$

The Wigner functions have many properties and applications [15] that are not of concern here. However, it is important to note that the wide variety of fruitful applications of the Wigner function is responsible for the interest in its generalization. The properties Wig(1)–(6) were presented here as most authors have aimed at a finite-dimensional analogy of the Wigner function defined such that it satisfies properties analogous to Wig(1)–(6) for discrete phase spaces. The remainder of the section is devoted to generalizing the definition of the Wigner function to finite-dimensional quantum systems.

2.2. Wootters discrete phase space representation

In [4], Wootters is interested in obtaining a discrete analogue of the Wigner function. Associated with each Hilbert space $\mathcal{H}$ of finite dimension d is a *discrete phase space*. First assume d is prime. The *prime phase space*, Φ_d, is a $d \times d$ array of points $\alpha = (q, p) \in \mathbb{Z}_d \times \mathbb{Z}_d$.

A *line*, λ, is the set of d points satisfying the linear equation $aq + bp = c$, where all arithmetic is modulo d. Two lines are *parallel* if their linear equations differ in the value of c. The prime phase space Φ_d contains $d + 1$ sets of d parallel lines called *striations*.

Assume that the Hilbert space $\mathcal{H}$ has composite dimension $d = d_1 d_2 \cdots d_k$. The discrete phase space of the entire d dimensional system is the Cartesian product of two-dimensional prime phase spaces of the subsystems. The phase space is thus a $(d_1 \times d_1) \times (d_2 \times d_2) \times \cdots \times (d_k \times d_k)$ array. Such a construction is formalized as follows: the *discrete phase space* is the multi-dimensional array $\Phi_d = \Phi_{d_1} \times \Phi_{d_2} \times \cdots \times \Phi_{d_k}$, where each Φ_{d_i} is a prime phase space. A *point* is the k-tuple $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_k)$ of points $\alpha_i = (q_i, p_i)$ in the prime phase spaces. A *line* is the k-tuple $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_k)$ of lines in the prime phase spaces. That is, a line is the set of d points satisfying the equation

$$(a_1 q_1 + b_1 p_1, a_2 q_2 + b_2 p_2, \ldots, a_k q_k + b_k p_k) = (c_1, c_2, \ldots, c_k),$$

which is symbolically written $aq + bp = c$. Two lines are *parallel* if their equations differ in the value c. As was the case for the prime phase spaces, parallel lines can be partitioned into sets, again called striations; the discrete phase space Φ_d contains $(d_1 + 1)(d_2 + 1) \cdots (d_k + 1)$ sets of d parallel lines.

The construction of the discrete phase space is now complete. To introduce Hilbert space into the discrete phase space formalism, Wootters chooses the following special basis for the space of Hermitian operators. The set of operators $\{A_\alpha : \alpha \in \Phi_d\}$ acting on a d dimensional Hilbert space are called *phase point operators* if the operators satisfy

- Woo(4) For each point α, A_α is Hermitian.
- Woo(5) For any two points α and β, $\mathrm{Tr}(A_\alpha A_\beta) = \mathrm{d}\delta_{\alpha\beta}$.
- Woo(6) For each line λ in a given striation, the operators $P_\lambda = \frac{1}{d} \sum_{\alpha \in \lambda} A_\alpha$ form a projective valued measurement (PVM): a set of d orthogonal projectors which sum to identity.

Note that these properties of the phase point operators Woo(4)–(6) are discrete analogues of the properties Wig(4)–(6) of the function F defining the original Wigner function. This definition suggests that the lines in the discrete phase space should be labelled with states of the Hilbert space. Since each striation is associated with a PVM, each of the d lines in a striation is labelled with an orthogonal state. For each Φ_d, there is a unique set of phase point operators up to unitary equivalence.

Although the sets of phase point operators are unitarily equivalent, the induced labelling of the lines associated with the chosen set of phase point operators are not equivalent. This is clear from the fact that unitarily equivalent PVMs do not project onto the same basis.

The choice of phase point operators in [4] will be adopted. For d prime, the phase point operators are

$$A_\alpha = \frac{1}{d} \sum_{j,m=0}^{d-1} \omega^{pj - qm + (jm/2)} X^j Z^m, \tag{4}$$

where ω is a dth root of unity and X and Z are the generalized Pauli operators (see appendix A). For composite d, the phase point operator in Φ_d associated with the point $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_k)$ is given by

$$A_\alpha = A_{\alpha_1} \otimes A_{\alpha_2} \otimes \cdots \otimes A_{\alpha_k}, \tag{5}$$

where each A_{α_i} is the phase point operator of the point α_i in Φ_{d_i}.

The d^2 phase point operators are linearly independent and form a basis for the space of Hermitian operators acting on a d dimensional Hilbert space. Thus, any density operator ρ can be decomposed as

$$\rho = \sum_{q,p} \mu_\rho^{\text{Wootters}}(q, p) A(q, p),$$

where the real coefficients are explicitly given by

$$\mu_\rho^{\text{Wootters}}(q, p) = \frac{1}{d}\operatorname{Tr}(\rho A(q, p)). \tag{6}$$

This discrete phase space function is the Wootters *discrete Wigner function*. This discrete quasi-probability function satisfies the following properties that are the discrete analogies of the properties Wig(1)–(3) the original continuous Wigner function satisfies.

- Woo(1) For all ρ, $\mu_\rho^{\text{Wootters}}(q, p)$ is real.
- Woo(2) For all ρ_1 and ρ_2,

$$\operatorname{Tr}(\rho_1\rho_2) = d \sum_{q,p} \mu_{\rho_1}^{\text{Wootters}}(q, p)\mu_{\rho_2}^{\text{Wootters}}(q, p).$$

- Woo(3) For all ρ, summing $\mu_\rho^{\text{Wootters}}$ along the line λ in phase space yields the probability that a measurement of the PVM associated with the striation that contains λ has the outcome associated with λ.

2.3. Odd dimensional discrete Wigner functions

In [16], Cohendet *et al* define a discrete analogue of the Wigner function that is valid for integer spin. That is, $\dim(\mathcal{H}) = d$ is assumed to be odd. Whereas Wootters builds up a discrete phase space before defining a Wigner function, the authors of [16] implicitly define a discrete phase space through the definition of their Wigner function.

Consider the operators

$$W_{mn}\phi_k = \omega^{2n(k-m)}\phi_{k-2m},$$

with $m, n \in \mathbb{Z}_d$ and ϕ_k are the eigenvectors of Z (see appendix A). Then, the *discrete Wigner function* of a density operator ρ is

$$\mu_\rho^{\text{odd}}(q, p) = \frac{1}{d}\operatorname{Tr}(\rho W_{qp} P), \tag{7}$$

where P is the parity operator (see appendix A).

The authors call the operators $\triangle_{qp} = W_{qp}P$ *Fano operators* and note that they satisfy

$$\triangle_{qp}^{\dagger} = \triangle_{qp}, \qquad \triangle_{qp}^{2} = \mathbb{1},$$
$$\mathrm{Tr}(\triangle_{qp}\triangle_{q'p'}) = \mathrm{d}\delta_{qq'}\delta_{pp'}, \qquad W_{xk}^{\dagger}\triangle_{qp}W_{xk} = \triangle_{q-2xp-2k}.$$

The Fano operators play a role similar to Wootters' phase point operators; they form a complete basis of the space of Hermitian operators. The phase space implicitly defined through the definition of the discrete Wigner function (7) is $\mathbb{Z}_d \times \mathbb{Z}_d$. When d is an odd prime, this phase space is equivalent to Wootters discrete phase space. In this case, the Fano operators are $\triangle_{qp} = A_{(-q,p)}$. This can seen by writing the Wootters phase point operators as

$$A_{(q,p)} = \frac{1}{d}X^{2q}Z^{2p}P\omega^{2qp}.$$

2.4. Even dimensional discrete Wigner functions

In [17], Leonhardt defines discrete analogues of the Wigner function for both odd and even dimensional Hilbert spaces. In a later paper [18], Leonhardt discusses the need for separate definitions for the odd and even dimension cases. Naively applying his definition, or that of Cohendet *et al*, of the discrete Wigner function for odd dimensions to even dimensions yields unsatisfactory results. The reason for this is the discrete Wigner function carries redundant information for even dimensions, which is insufficient to specify the state uniquely. The solution is to enlarge the phase space until the information in the phase space function becomes sufficient to specify the state uniquely.

Suppose $\dim(\mathcal{H}) = d$ is odd. Leonhardt defines the discrete Wigner function as

$$\mu_{\rho}^{\mathrm{Leonhardt}}(q,p) = \frac{1}{d}\mathrm{Tr}(\rho X^{2q}Z^{2p}P\omega^{2qp}).$$

Leonhardt's definition of an odd dimensional discrete Wigner function is unitarily equivalent to the Cohendet *et al* definition. That is, $\mu_{\rho}^{\mathrm{Leonhardt}}(q,p) = \mu_{\rho}^{\mathrm{odd}}(-q,p)$. To define a discrete Wigner function for even dimensions, Leonhardt takes half-integer values of q and p. This amounts to enlarging the phase space to $\mathbb{Z}_{2d} \times \mathbb{Z}_{2d}$. Thus the *even dimensional* discrete Wigner function is

$$\mu_{\rho}^{\mathrm{even}}(q,p) = \frac{1}{2d}\mathrm{Tr}(\rho X^{q}Z^{p}P\omega^{qp/2}),$$

where the operators

$$\triangle_{qp}^{\mathrm{even}} = \frac{1}{2d}X^{q}Z^{p}P\omega^{qp/2}$$

could be called the even dimensional Fano or phase point operators. Of course, these operators do not satisfy all the criteria that the Fano operators (in the case of Cohendet *et al*) or the phase point operators (in the case of Wootters) satisfy; they are not orthogonal. Moreover, they are not even linearly independent which can easily be inferred since there are $4d^2$ of them and a set of linearly independent operators contains a maximum of d^2 operators.

2.5. Wigner functions on the sphere

In [19], Heiss and Weigert are concerned with a set of postulates put forth by Stratonovich [20]. The aim of Stratonovich was to find a Wigner function type mapping, analogous to that of an infinite-dimensional system on $\mathbb{R}^2$, of a d dimensional system on the sphere $\mathbb{S}^2$. The first postulate is linearity and is always satisfied if the Wigner functions on the sphere satisfy

$$\mu_\rho^{\text{sphere}}(\mathbf{n}) = \mathrm{Tr}(\rho\triangle(\mathbf{n})), \tag{8}$$

where $\mathbf{n}$ is a point on $\mathbb{S}^2$. The remaining postulates on this quasi-probability mapping are

$$\mu_\rho^{\text{sphere}}(\mathbf{n})^* = \mu_\rho^{\text{sphere}}(\mathbf{n}),$$

$$\frac{d}{4\pi}\int_{\mathbb{S}^2} \mathrm{d}\mathbf{n}\ \mu_\rho^{\text{sphere}}(\mathbf{n}) = 1,$$

$$\frac{d}{4\pi}\int_{\mathbb{S}^2} \mathrm{d}\mathbf{n}\ \mu_{\rho_1}^{\text{sphere}}(\mathbf{n})\mu_{\rho_2}^{\text{sphere}}(\mathbf{n}) = \mathrm{Tr}(\rho_1\rho_2),$$

$$\mu_{(g\cdot\rho)}^{\text{sphere}}(\mathbf{n}) = \mu_\rho^{\text{sphere}}(\mathbf{n})^g, \quad g \in SU(2),$$

where $g\cdot\rho$ is the image of $U_g\rho U_g^\dagger$ and $U : SU(2) \to \mathbb{U}(\mathcal{H})$ is an irreducible unitary representation of the group $SU(2)$. These postulates are analogous to Wig(1)–(3) for the Wigner function modulo the second normalization condition (which could have been included in the Wigner function properties).

The continuous set of operators $\triangle(\mathbf{n})$ is called a *kernel* and plays the role of the phase point and Fano operators of the previous sections. Requiring that equation (8) hold changes the postulates to new conditions on the kernel

$$\triangle(\mathbf{n})^\dagger = \triangle(\mathbf{n}), \tag{9}$$

$$\frac{d}{4\pi}\int_{\mathbb{S}^2} \mathrm{d}\mathbf{n}\ \triangle(\mathbf{n}) = \mathbb{1}, \tag{10}$$

$$\frac{d}{4\pi}\int_{\mathbb{S}^2} \mathrm{d}\mathbf{n}\ \mathrm{Tr}(\triangle(\mathbf{n})\triangle(\mathbf{m}))\triangle(\mathbf{n}) = \triangle(\mathbf{m}), \tag{11}$$

$$\triangle(g\cdot\mathbf{n}) = U_g\triangle(\mathbf{n})U_g^\dagger, \quad g \in SU(2). \tag{12}$$

These postulates are the spherical analogies of properties Wig(4)–(6) (again, modulo the normalization condition). Heiss and Weigert provide a derivation of 2^{2s}, where $s = (d-1)/2$ is the *spin*, unique kernels satisfying these postulates. They are

$$\triangle(\mathbf{n}) = \sum_{m=-s}^{s}\sum_{l=0}^{2s} \epsilon_l \frac{2l+1}{2s+1} C_{m\,0\,m}^{s\,l\,s}\phi_m(\mathbf{n})\phi_m^*(\mathbf{n}), \tag{13}$$

where C denotes the so-called *Clebsch–Gordon coefficients*; $\phi_m(\mathbf{n})$ are the eigenvectors of the operator $\mathbf{S}\cdot\mathbf{n}$, where $\mathbf{S} = (X, Y, Z)$; and $\epsilon_l = \pm 1$, for $l = 1\ldots 2s$ and $\epsilon_0 = 1$.

Heiss and Weigert relax the postulates equations (9)–(12) on the kernel $\triangle(\mathbf{n})$ to allow for a pair of kernels $\triangle^{\mathbf{n}}$ and $\triangle_{\mathbf{m}}$. The pair individually satisfy equation (9), while one of them satisfies equation (10) and the other equation (12). Together, the pair must satisfy the generalization of equation (11)

$$\frac{d}{4\pi}\int_{\mathbb{S}^2} \mathrm{d}\mathbf{n}\,\mathrm{Tr}(\triangle^{\mathbf{n}}\triangle_{\mathbf{m}})\triangle^{\mathbf{n}} = \triangle_{\mathbf{m}}. \tag{14}$$

A pair of kernels, together satisfying equation (14), is given by

$$\triangle_{\mathbf{n}} = \sum_{m=-s}^{s}\sum_{l=0}^{2s} \gamma_l \frac{2l+1}{2s+1} C^{s\,l\,s}_{m\,0\,m}\phi_m(\mathbf{n})\phi_m^*(\mathbf{n}),$$

$$\triangle^{\mathbf{n}} = \sum_{m=-s}^{s}\sum_{l=0}^{2s} \gamma_l^{-1} \frac{2l+1}{2s+1} C^{s\,l\,s}_{m\,0\,m}\phi_m(\mathbf{n})\phi_m^*(\mathbf{n}),$$

where $\gamma_l = \pm 1$ for $l = 1\ldots 2s$ and $\gamma_0 = 1$. The original postulates are satisfied when $\gamma_l = \gamma_l^{-1} \equiv \epsilon_l$.

The major contribution of [19] is the derivation of a *discrete* kernel $\triangle_\nu := \triangle_{\mathbf{n}_\nu}$, for $\nu = 1\ldots d^2$ that satisfies the discretized postulates

$$\triangle_\nu^\dagger = \triangle_\nu, \tag{15}$$

$$\frac{1}{d}\sum_{\nu=1}^{d^2} \triangle^\nu = \mathbb{1}, \tag{16}$$

$$\frac{1}{d}\sum_{\nu=1}^{d^2} \mathrm{Tr}(\triangle_\nu\triangle^\mu)\triangle_\nu = \triangle^\mu, \tag{17}$$

$$\triangle_{g\cdot\nu} = U_g\triangle_\nu U_g^\dagger, \qquad g\in SU(2). \tag{18}$$

The subset of points $\mathbf{n}_\nu$ is called a *constellation*. The linearity postulate is not explicitly stated since it is always satisfied under the assumption

$$\rho \to \mu_\rho^{\text{constellation}}(\nu) = \mathrm{Tr}(\rho\triangle_\nu). \tag{19}$$

Equation (17) is called a *duality* condition. That is, it is only satisfied if $\triangle_\nu$ and $\triangle^\mu$ are *dual bases* for $\mathbb{H}(\mathcal{H})$. In particular,

$$\frac{1}{d}\mathrm{Tr}(\triangle_\nu\triangle^\mu) = \delta_{\nu\mu}.$$

Although the explicit construction of a pair of discrete kernels satisfying equations (15)–(18) might be computationally hard, their existence is a trivial exercise in linear algebra. Indeed, so long as $\triangle_\nu$ is a basis for $\mathbb{H}(\mathcal{H})$, its dual, $\triangle^\mu$, is uniquely determined by

$$\triangle^\mu = \sum_{\nu=1}^{d^2} \mathtt{G}^{-1}_{\nu\mu}\,\triangle_\nu,$$

where the Gram matrix $\mathtt{G}$ is given by

$$\mathtt{G}_{\nu\mu} = \mathrm{Tr}(\triangle_\nu\triangle_\mu).$$

The authors of [19] note that almost any constellation leads to a discrete kernel $\triangle_\nu$ forming a basis for $\mathbb{H}(\mathcal{H})$. The term *almost any* here means that a randomly selected discrete kernel will form, with probability 1, a basis for $\mathbb{H}(\mathcal{H})$.

2.6. Finite fields discrete phase space representation

Recall that when $\dim(\mathcal{H}) = d$ is prime, Wootters defines the discrete phase space as a $d \times d$ lattice indexed by the group $\mathbb{Z}_d$. In [21], Wootters generalizes his original construction of a discrete phase space to allow the $d \times d$ lattice to be indexed by a finite field $\mathbb{F}_d$ which exists when $d = p^n$ is an integer power of a prime number. This approach is discussed at length in the paper [5] authored by Gibbons, Hoffman and Wootters (GHW).

Similar to his earlier approach, Wootters defines the *phase space*, Φ_d, as a $d \times d$ array of points $\alpha = (q, p) \in \mathbb{F}_d \times \mathbb{F}_d$. A *line*, λ, is the set of d points satisfying the linear equation $aq + bp = c$, where all arithmetic is done in $\mathbb{F}_d$. Two lines are *parallel* if their linear equations differ in the value of c.

The mathematical structure of $\mathbb{F}_d$ is appealing because lines defined as above have the following useful properties: (i) given any two points, exactly one line contains both points, (ii) given a point α and a line λ not containing α, there is exactly one line parallel to λ that contains α, and (iii) two non-parallel lines intersect at exactly one point. Note that these are usual properties of lines in Euclidean space. As before, the d^2 points of the phase space Φ_d can be partitioned into $d + 1$ sets of d parallel lines called *striations*. The line containing the point (q, p) and the origin $(0, 0)$ is called a *ray* and consists of the points (sq, sp), where s is a parameter taking values in $\mathbb{F}_d$. We choose each ray, specified by the equation $aq + bp = 0$, to be the representative of the striation it belongs to.

A translation in phase space, $\mathcal{T}_{\alpha_0}$, adds a constant vector, $\alpha_0 = (q_0, p_0)$, to every phase space point: $\mathcal{T}_{\alpha_0}\alpha = \alpha + \alpha_0$. Each line, λ, in a striation is invariant under a translation by any point contained in its ray, parameterized by the points (sq, sp). That is,

$$\tau_{(sq,sp)}\lambda = \lambda. \tag{20}$$

The discrete Wigner function is

$$\mu_\rho^{\text{field}}(q, p) = \frac{1}{d}\mathrm{Tr}(\rho A_{(q,p)}),$$

where now the Hermitian *phase point operators* satisfy the following properties for a projector valued function Q, called a *quantum net*, to be defined later.

- GHW(4) For each point α, A is Hermitian.
- GHW(5) For any two points α and β, $\mathrm{Tr}(A_\alpha A_\beta) = \mathrm{d}\delta_{\alpha\beta}$.
- GHW(6) For any line λ, $\sum_{\alpha\in\lambda} A_\alpha = \mathrm{d}Q(\lambda)$.

The projector valued function Q assigns quantum states to lines in phase space. This mapping is required to satisfy the special property of *translational covariance*, which is defined after a short, but necessary, mathematical digression. Note first that properties GHW(4) and GHW(5) are identical to Woo(4) and Woo(4). Also note that if GHW(6) is to be analogous to Woo(6), the property of translation covariance must be such that the set $\{Q(\lambda)\}$ when λ ranges over a striation forms a PVM.

The set of elements $E = \{e_0, \ldots, e_{n-1}\} \subset \mathbb{F}_d$ is called a *field basis* for $\mathbb{F}_d$ if any element, x, in $\mathbb{F}_d$ can be written

$$x = \sum_{i=0}^{n-1} x_i e_i, \tag{21}$$

where each x_i is an element of the prime field $\mathbb{Z}_p$. The *field trace*[6] of any field element is given by

$$\mathrm{tr}(x) = \sum_{i=0}^{n-1} x^{p^i}. \tag{22}$$

There exists a unique field basis, $\tilde{E} = \{\tilde{e}_0, \ldots, \tilde{e}_{n-1}\}$, such that $\mathrm{tr}(\tilde{e}_i e_j) = \delta_{ij}$. We call $\tilde{E}$ the *dual* of E.

The construction presented in [5] is physically significant for a system of n objects (called *particles*) having a p dimensional Hilbert space. A translation operator, T_α associated with a point in phase space $\alpha = (q, p)$ must act independently on each particle in order to preserve the tensor product structure of the composite system's Hilbert space. We expand each component of the point α into its field basis decomposition as in equation (21)

$$q = \sum_{i=0}^{n-1} q_i e_i \tag{23}$$

and

$$p = \sum_{i=0}^{n-1} p_i f \tilde{e}_i, \tag{24}$$

with f any element of $\mathbb{F}_d$. Note that the basis we choose for p is a multiple of the dual of that chosen for q. Now, the translation operator associated with the point (q, p) is

$$T_{(q,p)} = \bigotimes_{i=0}^{n-1} X^{q_i} Z^{p_i}. \tag{25}$$

Since X and Z are unitary, T_α is unitary.

We assign with each line in phase space a pure quantum state. The quantum net Q is defined such that for each line, λ, $Q(\lambda)$ is the operator that projects onto the pure state associated with λ. As a consequence of the choice of basis for p in equation (24), the state assigned to the line $\tau_\alpha \lambda$ is obtained through

$$Q(\tau_\alpha \lambda) = T_\alpha Q(\lambda) T_\alpha^\dagger. \tag{26}$$

This is the condition of translational covariance and it implies that each striation is associated with an orthonormal basis of the Hilbert space. To see this, recall the property in equation (20). From equation (26), this implies that, for each $s \in \mathbb{F}_d$, $T_{(sq,sp)}$ must commute with $Q(\lambda)$, where the line λ is any line in the striation defined by the ray consisting of the points (sq, sp). That is, the states associated with the lines of the striation must be common eigenstates of the unitary translation operator $T_{(sq,sp)}$, for each $s \in \mathbb{F}_d$. Thus, the states are orthogonal and form a basis for the Hilbert space. That is, their projectors form a PVM that makes GHW(6) identical to Woo(6) when d is prime.

In [5], the author's note that, although the association between states and vertical and horizontal lines is fixed, the quantum net is not unique. In fact, there are d^{d-1} quantum nets that satisfy equation (20). When d is prime, one of these quantum nets corresponds exactly to the original discrete Wigner function defined by Wootters in section 2.2.

[6] Note that we will distinguish the field trace, $\mathrm{tr}(\cdot)$, from the usual trace of a Hilbert space operator, $\mathrm{Tr}(\cdot)$, by the case of the first letter.

Table 1. Finite quasi-probability representations.

Author(s)	Year	Valid dimensions	Phase space	Index field	Redundancy	Quantum theory scope
Stratonovich [20]	1957	Any	Sphere	Polar coordinates	Continuous	States
Wootters [4]	1987	Prime[a]	$d \times d$ lattice	$\mathbb{Z}_d$	No	Standard
Cohendet *et al* [16]	1987	Odd	$d \times d$ lattice	$\mathbb{Z}_d$	No	States
Leonhardt [17]	1995	Even[b]	$2d \times 2d$ lattice	$\mathbb{Z}_{2d}$	Four-fold	States
Heiss and Weigert [19]	2000	Any	Sphere[c]	Arbitrary	No	States
Hardy [23]	2001	Any	None	n/a	No	Operational
Havel [24]	2003	Any	None	n/a	No	States
Gibbons *et al* [5]	2004	Power of prime	$d \times d$ lattice	$\mathbb{F}_d$	No	States
Ruzzi *et al* [25]	2005	Odd	$d \times d$ lattice	$\mathbb{Z}_d$	No	States
Chaturvedi *et al* [26]	2006	Any	$d \times d$ lattice	$\mathbb{Z}_d$	No	States
Gross [27]	2006	Odd	$d \times d$ lattice	$\mathbb{Z}_d$	No	States

[a]Wootters' original discrete Wigner function [4] is usually understood to be valid for prime dimension but, as discussed in section 2.2, is easily extended to any dimension by combining prime dimensional phase spaces.
[b]Leonhardt [17] also defines a discrete Wigner function valid for odd dimensional, which is equivalent to the other odd dimensional cases [16].
[c]The phase space of Heiss and Weigert is any subset of d points on the sphere that can be indexed arbitrarily.

2.7. Summary of existing quasi-probability representations of quantum states

The phase space functions reviewed in sections 2.2–2.6 form only a subset of the literature on finite-dimensional phase space functions; there are indeed several others (for a recent review see [22]). More generally, there exist *quasi-probability representations* given by real-valued representations that do not necessarily reflect any preconceived classical phase space structure. For example in [23] Hardy shows that five axioms are sufficient to imply a special quasi-probabilistic representation that is equivalent to an operational form of quantum theory. In [24] Havel also proposes an kind of analogue of the Wigner function called the 'real density matrix'.

An overview of all of the quasi-probability representations for finite-dimensional quantum systems reviewed above (as well as a couple more) is presented in table 1. The table identifies the ontic space structure and the mathematical field that indexes it (if applicable). The second to last column indicates whether or not the representation contains redundant information. The last column reveals the scope of quantum theory the paper aims to cover (note that typically only states are considered).

3. Frame representations of quantum states

In the previous section, we reviewed some of the quasi-probability representations of quantum states found in the literature. In section 3.1, we unify these known quasi-probability representations of quantum states into one concise mathematical definition.

Section 3.2 contains an introduction to the mathematical theory of frames. In section 3.3, it is shown that frame theory is both necessary and sufficient to define any quasi-probability representation of quantum states. The frames for each of the quasi-probability representations reviewed in section 2 are given in section 3.4.

3.1. Unification of existing quasi-probability representations of quantum states

Each of the quasi-probability functions discussed in section 2 are *linear* representations of the density operator. These representations are also *invertible* as the density operator can be obtained from any quasi-probability function. Each quasi-probability function is also a member of the function space $L^2(\Lambda)$, where Λ represents a classical state space (e.g. the phase space, where applicable). These three properties will constitute the following minimal definition of a quasi-probability representation of *quantum states alone* [12]:

Definition 1. *A quasi-probability representation of quantum states is any map* $\mathbb{H}(\mathcal{H}) \to L^2(\Lambda)$ *that is linear and invertible.*

This definition was chosen since all the known quasi-probability representations of states satisfy it. One might object that the restrictions imposed on this map are too strong. Indeed there is no mention of linearity, invertibility, or L^2 spaces in any notion of classical probability. However, a classical probabilistic description describes an entire experimental arrangement. In section 5.3, we show that these ad hoc requirements follow from more natural assumptions on a representation on a complete experimental description. That is, definition 1 is satisfied on the part of this more natural definition, which represents quantum states.

Given definition 1, any phase space function is then a particular type of quasi-probability representation.

Definition 2. *If there exists a symmetry group on* Λ, G, *carrying a unitary representation* $U : G \to \mathbb{U}(\mathcal{H})$ *and a quasi-probability representation satisfying the covariance property* $U_g \rho U_g^\dagger \mapsto \{\mu_\rho(g(\lambda))\}_{\lambda\in\Lambda}$ *for all* $\rho \in \mathbb{D}(\mathcal{H})$ *and* $g \in G$, *then* $\rho \mapsto \mu_\rho(\lambda)$ *is a phase space representation of quantum states.*

All phase space functions in the literature correspond to quasi-probability representations that satisfy this additional covariance condition.

Table 1 shows that the range of validity in the Hilbert space dimension of these functions are often disjoint. Moreover, the construction of the phase spaces use varying mathematical structures: integers, finite fields and points on a sphere. Coupled with the fact that at least two known representations required redundancy, it may seem at first that definition 1 is as far as one can go in unifying the quasi-probability functions. However, a much stronger result is possible. In [12], it was shown that the mathematical theory of *frames* is both sufficient *and necessary* to describe any representation of quantum states satisfying definition 1.

3.2. The mathematical theory of frames

A *frame* can be thought of as a generalization of an orthonormal basis [28]. However, the particular Hilbert space under consideration here is not $\mathcal{H}$. Considered here is a generalization of a basis for $\mathbb{H}(\mathcal{H})$, which is the set of Hermitian operators on a complex Hilbert space of dimension d. With the trace inner product (or Hilbert–Schmidt inner product) $\langle A, B\rangle := \mathrm{Tr}(AB)$, $\mathbb{H}(\mathcal{H})$ forms a Hilbert space itself of dimension d^2. Let Λ be some measure space[7].

[7] For brevity, the σ-algebra and measure are left implied.

Definition 3. *A frame for* $\mathbb{H}(\mathcal{H})$ *is a set of operators* $\mathcal{F} := \{F(\lambda)\} \subset \mathbb{H}(\mathcal{H})$ *that satisfies*

$$a\|A\|^2 \leqslant \int_\Lambda \mathrm{d}\lambda\, |\langle F(\lambda), A\rangle|^2 \leqslant b\|A\|^2, \tag{27}$$

for all $A \in \mathbb{H}(\mathcal{H})$ *and some constants* $a, b > 0$.

This definition generalizes a defining condition for an orthogonal basis $\{B_k\}_{k=1}^{d^2}$

$$\sum_{k=1}^{d^2} |\langle B_k, A\rangle|^2 = \|A\|^2, \tag{28}$$

for all $A \in \mathbb{H}(\mathcal{H})$.

Definition 4. *A frame* $\mathcal{D} := \{D(\lambda)\}$ *that satisfies*

$$A = \int_\Lambda \mathrm{d}\lambda\, \langle F(\lambda), A\rangle D(\lambda), \tag{29}$$

for all $A \in \mathbb{H}(\mathcal{H})$*, is a dual frame (to* $\mathcal{F}$*).*

The *frame operator* associated with the frame $\mathcal{F}$ is defined as

$$S(A) := \int_\Lambda \mathrm{d}\lambda\, \langle F(\lambda), A\rangle F(\lambda).$$

If the frame operator satisfies $S = a\tilde{\mathbb{1}}$, the frame is called *tight*. The frame operator is invertible and thus every operator has a representation

$$A = S^{-1}SA = \int_\Lambda \mathrm{d}\lambda\, \langle F(\lambda), A\rangle S^{-1}F(\lambda). \tag{30}$$

The frame $S^{-1}\mathcal{F}$ is called the *canonical dual frame*. When $|\Lambda| = d^2$, the canonical dual frame is the unique dual, otherwise there are infinitely many choices for a dual.

A tight frame is ideal from the perspective that its canonical dual is proportional to the frame itself. Hence, the reconstruction is given by the convenient formula

$$A = S^{-1}SA = \frac{1}{a}\int_\Lambda \mathrm{d}\lambda\, \langle F(\lambda), A\rangle F(\lambda),$$

which is to be compared with

$$A = \sum_{k=1}^{d^2} \langle B_k, A\rangle B_k,$$

which defines $\{B_k\}_{k=1}^{d^2}$ as an orthonormal basis.

The mapping $A \mapsto \langle F(\lambda), A\rangle$ is usually called the *analysis operation* in the frame literature as it encodes the signal in terms of the frame. Here the notion of a signal is not appropriate and a more suggestive name has been chosen and formalized in the following definition.

Definition 5. *A mapping* $\mathbb{H}(\mathcal{H}) \to L^2(\Lambda)$ *of the form*

$$A \mapsto \langle F(\lambda), A\rangle, \tag{31}$$

where $\{F(\lambda)\}$ *is a frame, is a frame representation of* $\mathbb{H}(\mathcal{H})$*.*

3.3. *Equivalence of the quasi-probability and frame representation of quantum states*

Since each frame has at least a canonical dual, a frame representation (definition 5) can always be inverted according to the reconstruction formula in equation (30). A frame representation is defined such that it exists in $L^2(\Lambda)$. It is clear that a frame representation is linear by virtue of the linearity of the inner product. Thus each frame representation is guaranteed to be a quasi-probability representation of quantum states (definition 1). However, it is not immediately clear that the converse is true: every quasi-probability representation of quantum states is a frame representation. Indeed, the following lemma establishes the equivalence between frame representations and quasi-probability representations of quantum states.

Lemma 1. *A mapping $\mathbb{H}(\mathcal{H}) \to L^2(\Lambda)$ is quasi-probability representation of quantum states (definition 1) if and only if it is a frame representation for some unique frame $\mathcal{F}$.*

Proof. The proof of this lemma also appears in [12]. As noted above, it is clear that a frame representation is a quasi-probability representation. So assume the mapping $W : \mathbb{H}(\mathcal{H}) \to L^2(\Lambda)$ is a quasi-probability representation. Linearity and the Riesz representation theorem imply that $W(A)(\lambda) = \langle F(\lambda), A\rangle$ for some unique set $\mathcal{F} := \{F(\lambda)\}$ (not necessarily a frame). Since $\mathbb{H}(\mathcal{H})$ 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

$$a\|A\|^2 \leqslant \int_\Lambda \mathrm{d}\lambda\, |\langle F(\lambda), A\rangle|^2.$$

Since $\langle F(\lambda), A\rangle \in L^2(\Lambda)$, there exists a constant $b > 0$ such that

$$\int_\Lambda \mathrm{d}\lambda\, |\langle F(\lambda), A\rangle|^2 \leqslant b\|A\|^2.$$

Hence $\mathcal{F}$ is a frame. □

Thus, there is a unique frame that defines each of the quasi-probability functions reviewed in section 2. In the cases, where the representation of the density operator is not redundant, the frame is just a basis. In the redundant cases, Leonhardt's even dimensional representation (section 2.4) for example, the formalism of frame theory is necessary as a basis will not suffice.

3.4. *Examples of quasi-probability representations of quantum states*

The frames for each of the quasi-probability representations of quantum states reviewed in section 2 are now given.

3.4.1. Wootters discrete Wigner function. Let d be a prime number. Here $\Lambda = \mathbb{Z}_d \times \mathbb{Z}_d$. Consider the frame $\mathcal{F}^{\text{Wootters}} = \{F^{\text{Wootters}}(q, p)\}$, where

$$F^{\text{Wootters}}(q, p) = \frac{1}{d^2} X^{2q} Z^{2p} P \omega^{2qp}.$$

The quasi-probability function $\mu_\rho^{\text{Wootters}}$ is a frame representation given by the frame $\mathcal{F}^{\text{Wootters}}$. The frame operator of $\mathcal{F}^{\text{Wootters}}$ is $S = d^{-1}\tilde{\mathbb{1}}$. The unique dual frame of $\mathcal{F}^{\text{Wootters}}$ is given by

$S^{-1}\mathcal{F}^{\text{Wootters}}$, where $S^{-1} = d\tilde{\mathbb{1}}$. Comparing this result with equation (5), the dual frame to $\mathcal{F}^{\text{Wootters}}$ is a set of phase point operators.

Consider the group of translations on Λ with unitary representation $T_{(q,p)} = X^q Z^p$. Then,

$$\begin{aligned} T_{(q,p)} F^{\text{Wootters}}(q', p') T^{\dagger}_{(q,p)} &= \frac{1}{d^2} X^q Z^p X^{2q'} Z^{2p'} P Z^{-p} X^{-q} \omega^{2q'p'} \\ &= \frac{1}{d^2} X^{2(q+q')} Z^{2(p+p')} P \omega^{2(q+q')(p+p')} \\ &= F^{\text{Wootters}}(q+q', p+p'). \end{aligned}$$

Thus, by definition, the Wootters representation is a phase space representation.

Recall from section 2.2 that Wootters also considered non-prime dimensions. In that case, the phase point operators (equation (5)) were a tensor product of phase point operators (equation (4)) for prime dimensions. The same is true here for the frame in composite dimensions. When d is composite with prime decomposition $d = d_1 d_2 \cdots d_k$. Let $\Lambda = \Lambda_1 \times \Lambda_2 \times \cdots \times \Lambda_k$ where each $\Lambda_i = \mathbb{Z}_{d_i} \times \mathbb{Z}_{d_i}$. When d is composite the frame is $\mathcal{F}^{\text{Wootters}} = \{F^{\text{Wootters}}(q_{(i)}, p_{(i)})\}$, where

$$F^{\text{Wootters}}(q_{(i)}, p_{(i)}) = F^{\text{Wootters}}(q_{(1)}, p_{(1)}) \otimes F^{\text{Wootters}}(q_{(2)}, p_{(2)}) \otimes \cdots \otimes F^{\text{Wootters}}(q_{(k)}, p_{(k)})$$

and each $F^{\text{Wootters}}(q_{(i)}, p_{(i)})$ is a frame as in equation (section 3.4.1).

3.4.2. Odd dimensional discrete Wigner functions. Let d be an odd integer. Here $\Lambda = \mathbb{Z}_d \times \mathbb{Z}_d$. Consider the frame $\mathcal{F}^{\text{odd}} = \{F^{\text{odd}}(q, p)\}$, where

$$F^{\text{odd}}(q, p) = \frac{1}{d^2} X^{-2q} Z^{2p} P \omega^{-2qp}.$$

The quasi-probability function μ^{odd}_{ρ} is a frame representation given by the frame $\mathcal{F}^{\text{odd}}$. The frame operator of $\mathcal{F}^{\text{odd}}$ is $S = d^{-1}\tilde{\mathbb{1}}$. The unique dual frame of $\mathcal{F}^{\text{odd}}$ is given by $S^{-1}\mathcal{F}^{\text{odd}}$, where $S^{-1} = d\tilde{\mathbb{1}}$. The dual frame to $\mathcal{F}^{\text{odd}}$ is what Cohendet *et al* call a set of Fano operators.

Consider the group of translations on Λ with unitary representation $T_{(q,p)} = X^{-q} Z^p$. Then,

$$T_{(q,p)} F^{\text{odd}}(q', p') T^{\dagger}_{(q,p)} = F^{\text{odd}}(q+q', p+p').$$

By definition, this odd dimensional representation is a phase space representation.

3.4.3. Even dimensional discrete Wigner functions. Let d be an even integer. Then $\Lambda = \mathbb{Z}_{2d} \times \mathbb{Z}_{2d}$. Consider the frame $\mathcal{F}^{\text{even}} = \{F^{\text{even}}(q, p)\}$, where

$$F^{\text{even}}(q, p) = \frac{1}{4d^2} X^q Z^p P \omega^{qp/2}.$$

The quasi-probability function μ^{even}_{ρ} is a frame representation given by the frame $\mathcal{F}^{\text{even}}$. The frame operator of $\mathcal{F}^{\text{even}}$ is $S = (2d)^{-1}\tilde{\mathbb{1}}$. However, this implies the frame is only tight; it is not a basis and the dual is not unique. The canonical dual frame of $\mathcal{F}^{\text{even}}$ is given by $S^{-1}\mathcal{F}^{\text{even}}$, where $S^{-1} = 2d\tilde{\mathbb{1}}$. The canonical dual frame to $\mathcal{F}^{\text{even}}$ is what was called a set of even dimensional Fano operators.

Consider the group of translations on Λ with unitary representation $T_{(q,p)} = X^{q/2}Z^{p/2}$. Then,

$$T_{(q,p)}F^{\text{even}}(q', p')T^{\dagger}_{(q,p)} = F^{\text{even}}(q+q', p+p').$$

Thus, by definition, this odd dimensional representation is a phase space representation.

3.4.4. Wigner functions on the sphere. Let d be any integer. Here the phase space is $\Lambda = \mathbb{S}^2$. Consider the frame $\mathcal{F}^{\text{sphere}} := \{F^{\text{sphere}}(\mathbf{n})\}$ given by

$$F^{\text{sphere}}(\mathbf{n}) = \triangle(\mathbf{n}),$$

where $\triangle(\mathbf{n})$ is the same kernel given in equation (13). The quasi-probability function μ_ρ^{sphere} is a frame representation given by the frame $\mathcal{F}^{\text{sphere}}$. From equation (11), it follows that the frame operator of $\mathcal{F}^{\text{sphere}}$ is $S = 4\pi d^{-1}\tilde{\mathbb{1}}$. Thus, the frame is tight. Equation (12) is the group covariance property defining a phase space representation for the group $SU(2)$.

Now consider the discrete representation on sphere defined by Heiss and Weigert. Now the phase space Λ is a subset of points on the sphere that form a valid constellation. Consider the frame $\mathcal{F}^{\text{constellation}} := \{F^{\text{constellation}}(\nu)\}$, where

$$F^{\text{constellation}}(\nu) = \triangle_\nu,$$

where $\triangle_\nu$ is a kernel satisfying the postulates (15)–(16). The quasi-probability function $\mu_\rho^{\text{constellation}}$ is a frame representation given by the frame $\mathcal{F}^{\text{constellation}}$. As was the case for the other discrete representation in the previous examples, the frame operator of $\mathcal{F}^{\text{constellation}}$ is $S = d^{-1}\tilde{\mathbb{1}}$. The unique dual frame of $\mathcal{F}^{\text{constellation}}$ is given by $S^{-1}\mathcal{F}^{\text{constellation}}$, where $S^{-1} = d\tilde{\mathbb{1}}$. Thus, the dual frame to $\mathcal{F}^{\text{constellation}}$ is what Heiss and Weigert call a dual kernel. Again, from equation (18), this representation satisfies definition of a phase space representation.

3.4.5. Finite fields discrete phase space representation. Let d be a power of a prime number. Here $\Lambda = \mathbb{F}_d \times \mathbb{F}_d$. Consider the frame $\mathcal{F}^{\text{field}} = \{F^{\text{field}}(q, p)\}$, where

$$F^{\text{field}}(q, p) = \frac{1}{d}\left(\sum_{(q,p)\in\lambda} Q(\lambda) - \mathbb{1}\right),$$

where Q is a quantum net. The quasi-probability function μ_ρ^{field} is a frame representation given by the frame $\mathcal{F}^{\text{field}}$. The frame operator of $\mathcal{F}^{\text{field}}$ is $S = d^{-1}\tilde{\mathbb{1}}$. The unique dual frame of $\mathcal{F}^{\text{field}}$ is given by $S^{-1}\mathcal{F}^{\text{field}}$, where $S^{-1} = d\tilde{\mathbb{1}}$. The dual frame to $\mathcal{F}^{\text{field}}$ is a set of phase point operators.

Equation (26) shows this particular representation is constructed to be translationally covariant and is thus a phase space representation.

4. Frame representations of quantum theory

Quantum theory is an operational theory where each preparation is associated with a density operator $\rho \in \mathbb{D}(\mathcal{H})$. This association is not required to be injective; different preparations may lead to the same density operator. However, the mapping is assumed to be surjective; there exists a preparation that leads to each density operator. Similarly, each measurement procedure and outcome k is associated with an effect $E_k \in \mathbb{E}(\mathcal{H})$. Again, this mapping need not be injective but it is surjective. Quantum theory prescribes the probability of outcome k via the Born rule $\Pr(k) = \mathrm{Tr}(\rho E_k)$. Since the set of outcomes is mutually exclusive and exhaustive, each measurement procedure together with all the outcomes $\{E_k\}$ forms a positive operator valued measure (POVM).

Table 1 shows that most proposed quasi-probability representations are representations of quantum states alone. In sections 4.1 and 4.2, 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 theory. In section 4.3, a set of internal consistency conditions for each of the two approaches is given that allows one to formulate quantum theory independently of the standard operator theoretic formalism. A short detour is taken in section 4.4 to show that an operational formulation of quantum theory including *transformations* can be accommodated within the scope of the frame formalism. Finally in section 4.5, a novel quasi-probability representation based on *SIC-POVMs* is presented that relates the frame formalism to a recent research topic in quantum information.

4.1. Deformed probability representations of quantum theory

The first frame representation approach consists of mapping both states and measurements to $L^2(\Lambda)$ via a particular choice of frame $\mathcal{F}$. Formally, we have the following definition:

Definition 6. *Suppose that the frame $\{F(\lambda)\}$ consists of positive operators that satisfies $\int_\Lambda \mathrm{d}\lambda\, F(\lambda) = \mathbb{1}$ (a normalization condition). Together, the mappings*

$$\rho \mapsto \langle F(\lambda), \rho\rangle,$$
$$E \mapsto \langle F(\lambda), E\rangle,$$

for all $\rho \in \mathbb{D}(\mathcal{H})$ and $E \in \mathbb{E}(\mathcal{H})$, are called a deformed probability representation of quantum theory.

The reason for the qualifier *deformed* is apparent from the following proposition:

Proposition 1. *A deformed probability representation of quantum theory is a pair of mappings (call them $\mu_\rho := \langle F, \rho\rangle$ and $\xi_E = \langle F, E\rangle$) which satisfy, for all $\lambda \in \Lambda$, all $\rho \in \mathbb{D}(\mathcal{H})$ and all $E \in \mathbb{E}(\mathcal{H})$,*

(a) $\mu_\rho(\lambda) \geqslant 0$ *and* $\xi_E(\lambda) \in [0, 1]$*;*
(b) $\int_\Lambda \mathrm{d}\lambda\, \mu_\rho(\lambda) = 1$*; and,*
(c) $\mathrm{Tr}(\rho E) = \int_{\Lambda^2} \mathrm{d}\lambda\, \mathrm{d}\gamma\, \mu_\rho(\lambda)\xi_E(\gamma)\langle D(\lambda), D(\gamma)\rangle$,

where $\{D(\lambda)\}$ is a frame dual to $\{F(\lambda)\}$.

Property (c) is a *deformed* law of total probability. It can be thought of as a deformation of the usual law of total probability. Recall from lemma 1 that all quasi-probability representations of states are frame representations. Given a quasi-probability representation (of states), one can identify the unique frame that gives rise to it. Then, using that frame to represent the measurement operators, one obtains a deformed probability representation of quantum theory.

4.2. Frame representations of quantum theory

Note that the deformed probability calculus (proposition 1(c)) can be written

$$\mathrm{Tr}(\rho E) = \int_\Lambda \mathrm{d}\lambda\ \mu_\rho(\lambda)\xi'_E(\lambda), \tag{32}$$

where

$$\xi'_E(\lambda) = \int_\Lambda \mathrm{d}\gamma\ \xi_E(\gamma)\langle D(\lambda), D(\gamma)\rangle. \tag{33}$$

Recall that ξ_E is the frame representation of E for the frame $\mathcal{F}$. Hence ξ'_E can be identified as the frame representation of E using a frame $\mathcal{D}$ that is dual to $\mathcal{F}$. The second frame representation approach consists of mapping states to $L^2(\Lambda)$ via a particular choice of frame $\mathcal{F}$ and measurements to $L^2(\Lambda)$ via a frame $\mathcal{D}$ that is dual to $\mathcal{F}$. Formally, we have the following definition:

Definition 7. *Suppose that the frames $\{F(\lambda)\}$ and $\{D(\lambda)\}$ are dual and $\int_\Lambda \mathrm{d}\lambda\ F(\lambda) = \mathbb{1}$ (normalization). Together, the mappings*

$$\rho \mapsto \langle F(\lambda), \rho\rangle,$$
$$E \mapsto \langle D(\lambda), E\rangle,$$

for all $\rho \in \mathbb{D}(\mathcal{H})$ and $E \in \mathbb{E}(\mathcal{H})$, are called a frame representation of quantum theory.

A frame representation of quantum theory satisfies properties similar to those of a deformed probability representation.

Proposition 2. *A frame representation of quantum theory is a pair of mappings (call them $\mu_\rho := \langle F, \rho\rangle$ and $'_E := \langle D, E\rangle$) that satisfy, for all $\lambda \in \Lambda$, all $\rho \in \mathbb{D}(\mathcal{H})$ and all $E \in \mathbb{E}(\mathcal{H})$,*

(a) $\mu_\rho(\lambda) \in \mathbb{R}$ *and* $\xi'_E(\lambda) \in \mathbb{R}$;
(b) $\int_\Lambda \mathrm{d}\lambda\, \mu_\rho(\lambda) = 1$; *and,*
(c) $\mathrm{Tr}(\rho E) = \int_\Lambda \mathrm{d}\lambda\, \mu_\rho(\lambda)\xi'_E(\lambda)$.

Property (c) is formally identical to the usual law of total probability although the functions in the integrand are not presumed to be non-negative. Indeed, in [12] it was shown that a pair of dual frames cannot both consist solely of positive operators.

Recall from lemma 1 that all quasi-probability representations of states are frame representations. Given a quasi-probability representation of states, one can identify the unique frame that gives rise to it. Then, using a *dual frame* to represent the measurement operators, one obtains a frame representation of quantum theory.

4.3. Internal consistency conditions

Consider first the deformed probability representations. Of course, for a particular choice of frame, not every function in $L^2(\Lambda)$ will correspond to a valid quantum state or effect. Here a set of *internal* conditions is provided, independent of the standard axioms of quantum theory that characterize the valid functions in $L^2(\Lambda)$. The conditions can be found by noting that the frame representation equation (31) is an isometric and algebraic isomorphism from $\mathbb{H}(\mathcal{H})$ to $L^2(\Lambda)$

equipped with inner product

$$\langle \mu_1, \mu_2 \rangle_{\mathtt{D}} := \int_{\Lambda^2} \mathrm{d}\lambda\, \mathrm{d}\gamma\ \mu_1(\lambda)\mu_2(\gamma)\mathtt{D}(\lambda, \gamma),$$

where $\mathtt{D}(\lambda, \gamma) := \langle D(\lambda), D(\gamma)\rangle$, and algebraic multiplication

$$(\mu_1 \star_{\mathfrak{F}} \mu_2)(\lambda) := \int_{\Lambda^2} \mathrm{d}\gamma\, \mathrm{d}\eta\ \mu_1(\gamma)\mu_2(\eta)\mathfrak{F}(\lambda, \gamma, \eta),$$

where $\mathfrak{F}(\lambda, \gamma, \eta) = \langle F(\lambda), D(\gamma)D(\eta)\rangle$.

Now the condition for a function in $L^2(\Lambda)$ to be a valid state or effect can be stated. A *pure state* is a function $\mu_{\text{pure}} \in L^2(\Lambda)$ satisfying $\mu_{\text{pure}} \star_{\mathfrak{F}} \mu_{\text{pure}} = \mu_{\text{pure}}$. A general *state* is a function $\mu \in L^2(\Lambda)$ satisfying $\langle \mu, \mu_{\text{pure}}\rangle_{\mathtt{D}} \geqslant 0$ for all pure states and $\int_\Lambda \mathrm{d}\lambda\, \mu(\lambda) = 1$. A *measurement* is represented by a set $\{\xi_k \in L^2(\Lambda)\}$ of *effects* that satisfies $\langle \xi_k, \mu_{\text{pure}}\rangle_{\mathtt{D}} \geqslant 0$ for all pure states and for which $\sum_k \xi_k = \xi_{\mathbb{1}}$, where $\xi_{\mathbb{1}}$ is the identity element in $L^2(\Lambda)$ with respect to the algebra defined by $\star_{\mathfrak{F}}$. That is, $\xi_{\mathbb{1}}$ is the unique element satisfying $\xi_{\mathbb{1}} \star_{\mathfrak{F}} \mu = \mu \star_{\mathfrak{F}} \xi_{\mathbb{1}}$ for all $\mu \in L^2(\Lambda)$.

Now consider the frame representations. Again for this approach, states and measurements in $L^2(\Lambda)$ must meet certain criteria to be valid. The conditions are similar to those in the deformed probability representation. Indeed the pure states and general states are equivalently characterized. However, a measurement is now represented by a set $\{\xi'_k \in L^2(\Lambda)\}$ that satisfies $\langle \xi'_k, \mu_{\text{pure}}\rangle \geqslant 0$ (now the usual pointwise inner product) for all pure states and for which $\sum_k \xi'_k = \xi'_{\mathbb{1}}$, where $\xi'_{\mathbb{1}}$ is the identity element in $L^2(\Lambda)$ 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).

4.4. Transformations

A transformation is a superoperator (an operator acting on operators) $\Phi : \mathbb{D}(\mathcal{H}) \to \mathbb{D}(\mathcal{H})$. Operationally, an experiment consists of preparations followed by transformations and ending in a measurement. Note that, in a purely mathematical sense, the transformations are somewhat redundant as they could be bundled with either the preparations (to make new preparations) or measurements (to make new measurements).

A completely positive (CP) map is a linear superoperator Φ satisfying

$$\mathrm{Tr}[(\Phi \otimes \mathbb{1})\rho] \geqslant 0,$$

for every pure state ρ on an extended system of arbitrary finite dimension. If in addition, the CP map satisfies $\mathrm{Tr}(\Phi(\rho)) = \mathrm{Tr}(\rho)$, it is called a completely positive trace-preserving (CPTP) map. The CPTP maps are transformations that are physically admissible.

In classical theories, transitions in probability are represented by matrices called *stochastic matrices*. It is natural to attempt a similar representation of transitions of quantum states here. Matrix representation are typical in quantum theory. A linear operator A is usually mapped to a matrix with entries a_{ij} given by $a_{ij} = \langle \phi_i, A\phi_j\rangle$, where $\{\phi_i\}$ is an orthonormal basis for $\mathcal{H}$. Then the action of the operator is representation as the usual matrix multiplication. However, a slightly modified approach is required here when using frames (which reduces to usual matrix representations when the frame and an orthonormal basis coincide).

Let $\mu_\rho(\lambda)$ be a frame representation of a density operator ρ for a frame $\mathcal{F}$. Let $\mathcal{D}$ be a dual frame of $\mathcal{F}$ and consider the action of a superoperator

$$\Phi\rho = \Phi \int_\Lambda \mathrm{d}\lambda\ \mu_\rho(\lambda) D(\lambda). \tag{34}$$

The frame representation of $\Phi\rho$ is $\mu_{\Phi\rho}(\gamma) = \langle F(\gamma), \Phi\rho\rangle$. As was the case for including measurements into a frame representation, two approaches can be identified for including the transformations into the frame representation formalism.

The first approach follows directly from equation (34)

$$\mu_{\Phi\rho}(\gamma) = \int_\Lambda \mathrm{d}\lambda\; \Phi^{\mathrm{qp}}(\gamma, \lambda)\mu_\rho(\lambda), \tag{35}$$

where $\Phi^{\mathrm{qp}}(\gamma, \lambda) = \langle F(\gamma), \Phi D(\lambda)\rangle$ ('qp' is a label meant to abbreviate 'quasi-probability'). Note that equation (35) is just the usual (perhaps infinite-dimensional) matrix multiplication rule. It is the same rule for transitioning probability distributions via stochastic matrices in classical theories. However, as opposed to stochastic matrices, Φ^{qp} could have negative entries.

Alternatively, consider the intermediate step

$$D(\lambda) = \int_\Lambda \mathrm{d}\lambda\; \langle D(\eta), D(\lambda)\rangle F(\eta). \tag{36}$$

Then equation (34) becomes

$$\mu_\rho^\Phi(\gamma) = \int_{\Lambda^2} \mathrm{d}\gamma\; \mathrm{d}\eta\; \Phi^{\mathrm{def}}(\gamma, \eta)\mathtt{D}(\eta, \lambda)\mu_\rho(\lambda), \tag{37}$$

where $\Phi^{\mathrm{def}}(\gamma, \eta) = \langle F(\gamma), \Phi F(\eta)\rangle$ ('def' is a label meant to abbreviate 'deformed probability'). This second approach is analogous to the deformed probability representation of section 4.1.

4.5. Example: symmetric informationally complete POVM (SIC-POVM) representation

In [29], the authors conjecture[8] that the set $\{\phi_\alpha \in \mathcal{H} : \alpha \in \mathbb{Z}_d \times \mathbb{Z}_d\} = \{U_{(p,q)}\phi : (p, q) \in \mathbb{Z}_d \times \mathbb{Z}_d\}$ for some $\phi \in \mathcal{H}$ and

$$U_{(p,q)} = \omega^{pq/2} X^p Z^q \tag{38}$$

forms a SIC-POVM. The defining condition of an SIC-POVM is

$$|\langle\phi_\alpha, \phi_\beta\rangle|^2 = \frac{\delta_{\alpha\beta} d + 1}{d + 1}. \tag{39}$$

The set is called symmetric since the vectors have equal overlap. The POVM is formed by taking the projectors onto the one-dimensional subspaces spanned by the vectors. It is informationally complete since these d^2 projectors span $\mathbb{H}(\mathcal{H})$.

As of writing, it is an open question whether SIC-POVMs exist in every dimension. However, there is numerical evidence for there existence for every dimension up to $d = 45$ [29] and analytic construction for a small number of dimensions.

Suppose then that for any dimension d, a SIC-POVM exists. Note that a SIC-POVM forms a frame. Explicitly, let

$$\mathcal{F} = \left\{ F_\alpha := \frac{1}{d}\phi_\alpha\phi_\alpha^* : \alpha \in \mathbb{Z}_d \times \mathbb{Z}_d \right\}$$

[8] Apparently this was conjectured earlier by Zauner in a PhD thesis not available in English. See http://www.imaph.tu-bs.de/qi/problems/23.html.

denote this frame. From the definition of the SIC-POVM, equation (39),

$$\mathtt{F}_{\alpha\beta} := \langle F_\alpha, F_\beta \rangle = \frac{\delta_{\alpha\beta} d + 1}{d^2(d+1)}.$$

Since the frame forms a basis, the dual frame is unique and thus the inverse frame operator must satisfy

$$\langle F_\alpha, S^{-1} F_\beta \rangle = \delta_{\alpha\beta}.$$

By inspection

$$D_\beta = S^{-1} F_\beta = d(d+1) F_\beta - \mathbb{1}.$$

Representing a quantum state via the frame or canonical dual yields the neat reconstruction formulae

$$\rho = \sum_\alpha (d(d+1)\mu_\rho(\alpha) - 1) F_\alpha, \tag{40}$$

$$\rho = \sum_\alpha \mu_\rho(\alpha)(d(d+1)F_\alpha - \mathbb{1}), \tag{41}$$

where $\mu_\rho(\alpha) := \langle F_\alpha, \rho \rangle$ is the frame representation of ρ.

Equation (40) was given in [30]. This equation fits naturally into the deformed probability representation formalism discussed in section 4.1. Note that the dual frame satisfies

$$\begin{aligned}
\mathtt{D}_{\alpha\beta} &= \langle D_\alpha, D_\beta \rangle \\
&= \langle d(d+1)F_\alpha - \mathbb{1}, d(d+1)F_\beta - \mathbb{1} \rangle \\
&= d^2(d+1)^2 \mathtt{F}_{\alpha\beta} - 2(d+1) + d \\
&= d(d+1)\delta_{\alpha\beta} - 1.
\end{aligned}$$

If an arbitrary measurement $\{E_k\}$ is also represented via the SIC-POVM frame as $\xi_{E_k}(\beta) := \langle F_\beta, E_k \rangle$, then equation (40) is identical to the deformed law of total probability

$$\Pr(k) = \sum_{\alpha\beta} \mu_\rho(\alpha) \xi_{E_k}(\beta) \mathtt{D}_{\alpha\beta}.$$

Equation (41) fits more naturally into the frame representation formalism discussed in section 4.2. If an arbitrary measurement $\{E_k\}$ is represented via the canonical dual to the SIC-POVM frame as $\xi'_{E_k}(\alpha) := \langle D_\alpha, E_k \rangle$, then equation (41) is identical to the usual law of total probability

$$\Pr(k) = \sum_\alpha \mu_\rho(\alpha) \xi'_{E_k}(\alpha).$$

Since the SIC-POVM frame is made of projectors, the frame representation of the density operator is a true probability distribution. However, the dual frame operators are not positive. Thus in a SIC-POVM frame representation, the measurement objects (meant to represent conditional probabilities) contain negative values while the states are represented by true probabilities. The appearance of negativity is a necessary feature of frame representations, as was shown in [12].

5. Non-classicality of quantum theory

In this section, we prove the impossibility of representing quantum theory classically via a mapping from the quantum operators to classical probability functions.

5.1. Classical representations of quantum theory

In classical probability, we postulate that a physical system has a set of properties mathematically represented by a measure space Λ. The ontological states are represented by the Dirac measures that are the extreme points of the set of all probability measures on Λ. The probability measures are the epistemic states representing our ignorance of the ontic state of the system. To measure the properties of the system we partition the space Λ into disjoint subsets $\{\triangle_k\}$. The probability of the system to have properties in $\triangle_k$ (we will call this 'outcome k') is

$$\Pr(k|\mu) = \int_{\triangle_k} \mathrm{d}\lambda\ \mu(\lambda) = \int_{\Lambda} \mathrm{d}\lambda\ \mu(\lambda)\chi_k(\lambda),$$

where $\chi_k(\lambda) \in \{0, 1\}$ is an idempotent indicator function associated with $\triangle_k$. The measurement is equivalently specified by the set $\{\chi_k(\lambda)\}$, which is interpreted as the conditional probability of outcome k given the systems is known to have the properties λ. 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 $\{\xi_k(\lambda) \in [0, 1]\}$. Each of these can be decomposed as a convex combination of idempotent indicator functions. For this reason, idempotent indicator functions are emphasized as being *sharp* within the set of more general measurement functions. Put concisely, the indicator functions form a convex set with the sharp indicator functions as the extreme points.

Consider the problem of proving whether or not it is possible to construct a representation of quantum theory that satisfies these classical postulates. That is, we are interested if there exists a space Λ such that for every density operator there is a unique probability measure and every effect there is a unique indicator function on this space which reproduces the Born rule via the law of total probability. We can formalize this idea into the following definition.

Definition 8. *A classical representation of quantum theory is a pair of mappings μ and ξ whose domains are $\mathbb{D}(\mathcal{H})$ and $\mathbb{E}(\mathcal{H})$, respectively, and whose co-domains are a convex set of probability functions. These mappings satisfy, for all $\rho \in \mathbb{D}(\mathcal{H})$ and all $E \in \mathbb{E}(\mathcal{H})$,*

(a) $\mu_\rho(\lambda) \geqslant 0$ *and* $\xi_E(\lambda) \in [0, 1]$;
(b) $\int_\Lambda \mathrm{d}\lambda\, \mu_\rho(\lambda) = 1$; *and,*
(c) $\mathrm{Tr}(\rho E) = \int_\Lambda \mathrm{d}\lambda\, \mu_\rho(\lambda)\xi_E(\lambda)$.

We submit definition 8 as the most natural set of requirements for what can reasonably be called a 'classical representation' of quantum theory.

5.2. Quasi-probability representations of quantum theory

In light of the above considerations, the most natural approach to obtaining a set of quasi-probability representations is to take the definition of a classical representation and simply relax the requirement of non-negativity. This motivates defining the following set of generalized representations.

Definition 9. *A quasi-probability representation of quantum theory is a pair of mappings μ and ξ whose domains are $\mathbb{D}(\mathcal{H})$ and $\mathbb{E}(\mathcal{H})$, respectively, and whose co-domains are a convex set of quasi-probability functions (real valued functions). These mappings satisfy, for all $\rho \in \mathbb{D}(\mathcal{H})$ and all $E \in \mathbb{E}(\mathcal{H})$,*

(a) $\mu_\rho(\lambda) \in \mathbb{R}$ *and* $\xi_E(\lambda) \in \mathbb{R}$*;*
(b) $\int_\Lambda \mathrm{d}\lambda\, \mu_\rho(\lambda) = 1$*; and,*
(c) $\mathrm{Tr}(\rho E) = \int_\Lambda \mathrm{d}\lambda\, \mu_\rho(\lambda)\xi_E(\lambda)$*.*

It should be obvious that a non-negative quasi-probability representation is just a classical representation. Now we show that a consequence of these requirements is that a quasi-probability satisfies a very important property that will be used later on.

Lemma 2. *The mappings in a quasi-probability representation of quantum theory are affine*[9].

Proof. First note from property (c) that we have

$$\int_\Lambda \mathrm{d}\lambda\, \mu_\rho(\lambda)\xi_E(\lambda) = \int_\Lambda \mathrm{d}\lambda\, \mu_\sigma(\lambda)\xi_E(\lambda) \Rightarrow \mathrm{Tr}(\rho E) = \mathrm{Tr}(\sigma E) \Rightarrow \rho = \sigma \Rightarrow \mu_\rho(\lambda) = \mu_\sigma(\lambda). \tag{42}$$

Now consider the density operator $\rho = p\sigma_1 + (1-p)\sigma_2$, $0 \leqslant p \leqslant 1$. Multiplying by an arbitrary effect E and taking the trace we have $\mathrm{Tr}(\rho E) = p\mathrm{Tr}(\sigma_1 E) + (1-p)\mathrm{Tr}(\sigma_2 E)$. By property (c) and equation (42) we have

$$\begin{aligned}\int_\Lambda \mathrm{d}\lambda\, \mu_\rho(\lambda)\xi_E(\lambda) = \int_\Lambda \mathrm{d}\lambda\, \left(p\mu_{\sigma_1}(\lambda) + (1-p)\mu_{\sigma_2}(\lambda)\right)\xi_E(\lambda) \Rightarrow \mu_\rho(\lambda)\\ = p\mu_{\sigma_1}(\lambda) + (1-p)\mu_{\sigma_2}(\lambda).\end{aligned}$$

Hence, μ is affine. The proof that ξ is affine is identical. □

Comparing definition 9 to proposition 2 it would seem that a quasi-probability representation is equivalent to a frame representation, and vice versa. It is important to note however, via definition 7, that a frame representation of quantum theory makes explicit reference to frames. Whereas, a quasi-probability representation of quantum theory is defined without any reference to frames. However, we will see in the next section that the two are indeed equivalent.

5.3. Equivalence of frame representations and quasi-probability representations

In [12], it was shown that there does not exist a frame of positive operators that is dual to another frame of positive operators. This establishes that frame representations of quantum theory, as described in section 4.2, must possess negativity. However, this proof does not rule out the possibility of *non-negative* quasi-probability representations (or, equivalently, classical representations) as defined above. We now close this loophole and thereby extend the significance of the no-go theorem in [12] via the following lemma that shows that the set of quasi-probability representations and the set of frame representations are equivalent.

[9] Note that a few authors use the terminology 'convex-linear' to mean affine, the latter being a well understood and precise mathematical term: a mapping that preserves convex combinations.

Lemma 3. *A quasi-probability representation of quantum theory (definition 9) is equivalent to a frame representation of quantum theory (definition 7).*

Proof. A frame representation clearly satisfies definition 9. Suppose then that μ and ξ form a quasi-probability representations of quantum theory. First consider μ. According to the procedure described in [31], this mapping can be extended to a linear map on $\mathbb{H}(\mathcal{H})$. Then the Riesz representation theorem implies that there exists a unique operator valued function $\mathcal{F} := \{F(\lambda)\}$ such that $\mu_A = \langle A, F\rangle$. To show $\mu_A \in L^2(\Lambda)$ we need to show that $\int_\Lambda \mathrm{d}\lambda\, |\mu_A(\lambda)|^2$ is finite. Note that

$$\int_\Lambda \mathrm{d}\lambda\, |\mu_A(\lambda)|^2 = \int_\Lambda \mathrm{d}\lambda\, |\langle A, F(\lambda)|\rangle^2 = \langle A, SA\rangle,$$

where S is the frame operator of $\mathcal{F}$. Since the range of the frame operator is another Hermitian operator and $\mathbb{H}(\mathcal{H})$ is finite-dimensional, $\langle A, SA\rangle < \infty$. To show that μ is injective we suppose $\mu_A = 0$ and show $A = 0$. From property 9(c)

$$\mathrm{Tr}(AE) = \int_\Lambda \mathrm{d}\lambda\, \mu_A(\lambda)\xi_E(\lambda) = 0.$$

Since E is arbitrary and $\mathbb{E}(\mathcal{H})$ spans $\mathbb{H}(\mathcal{H})$, this immediately implies $A = 0$. Lemma 1 implies $\mathcal{F}$ is a frame. The same logic implies ξ is a frame representation for some unique frame $\mathcal{D} := \{D(\lambda)\}$. To show that together these form an quasi-probability representation, we need only show that $\mathcal{D}$ is dual to $\mathcal{F}$. Property 9(c) implies

$$\mathrm{Tr}(AB) = \int_\Lambda \mathrm{d}\lambda\, \langle F(\lambda), A\rangle\langle D(\lambda), B\rangle,$$

which is true for all $B \in \mathbb{H}(\mathcal{H})$. Thus

$$A = \int_\Lambda \mathrm{d}\lambda\, \langle F(\lambda), A\rangle D(\lambda).$$

By definition 4, $\mathcal{D}$ is dual to $\mathcal{F}$. □

5.4. Non-classicality of quantum theory

Using lemma 3 in combination with the negativity theorem of [12] it is easy to prove the following.

Theorem 1. *A classical representation of quantum theory (definition 8) does not exist. Or, equivalently, a non-negative quasi-probability representation (definition 9) does not exist.*

Proof. Lemma 3 establishes that a classical representation is a quasi-probability representation that requires that the dual of a positive frame be positive. Such a pair of frames does not exist as proven in [12]. For the reader unfamiliar with frames this fact can also be proven directly, without making use of frames, as follows.

It is much easier to see the contradiction when Λ is assumed to be finite. It follows from [31] (see also [32]) that $\mu_\rho(\lambda) = \langle \rho, F(\lambda)\rangle$, where F is some effect-valued function.

Similarly, $\xi_E(\lambda) = \langle E, D(\lambda)\rangle$, where D is state-valued function. That is, each $D(\lambda)$ is a density operator. From property 8(c) it follows that

$$\rho = \sum_{\lambda} \langle \rho, F(\lambda)\rangle D(\lambda). \tag{43}$$

This is true for all ρ including the rank-1 projectors: the extreme points of $\mathbb{D}(\mathcal{H})$. Equation (43) is a convex combination. The fact that extreme point have only the trivial decomposition implies μ maps the extreme of $\mathbb{D}(\mathcal{H})$ to Dirac distributions: the extreme points of probability distributions[10]. There are only finitely many extreme points in the simplex of probability distributions over a finite space. There are infinitely many extreme points in $\mathbb{D}(\mathcal{H})$. Property 8(c) also implies μ must be injective[11]. This is clearly impossible and so all hope of a classical representation must rest on the set Λ having the same cardinality of $\mathbb{D}(\mathcal{H})$[12].

Now assume Λ is infinite. Property 8(c) still requires μ must map the rank-1 projectors to the Dirac measures. Recall for a finite-dimensional simplex that each vector has a unique decomposition into extreme points. The same is true here for the probability measures on Λ; each measure has a unique decomposition into Dirac measures [36]. Since, in general, $\rho \in \mathbb{D}(\mathcal{H})$ has infinitely many non-equivalent decompositions into rank-1 projectors, it is impossible for μ to be injective. □

Theorem 1 establishes the necessity of negativity in quasi-probability representations of quantum theory. In the next section another notion of non-classicality, *contextuality*, will be compared with negativity.

6. Connection with contextuality

Within the quantum formalism there are many notions of non-classicality. In the previous section, negativity was proven to be such a notion. In this section, the idea of *contextuality* is considered as an alternative candidate. In section 6.1, the traditional notion of contextuality is reviewed. A generalization due to Spekkens is presented in section 6.2. In section 6.3, the somewhat misleading claim in [33] that 'negativity and contextuality are equivalent' is clarified. Finally, a more general model of quantum theory that allows both negativity and contextuality is considered in section 6.4.

6.1. Traditional definition of contextuality

The traditional definition of contextuality evolved from a theorem that appears in a paper by Kochen and Specker [37]. The Kochen–Specker theorem concerns the standard quantum formalism: physical systems are assigned states in a complex Hilbert space $\mathcal{H}$ and measurements are made of observables represented by Hermitian operators. The theorem establishes a

[10] Spekkens [33] has also made these observations but follows a different route from here on to obtain a contradiction. See section 6 for details of the connection to [33].
[11] The injectivity of this map can be proven from property 8(c) as in the proof of lemma 3.
[12] Compare this to the 'Ontological excess baggage theorem' of Hardy [34]. Also note that Busch, Hellwig and Stulpe have come to the same conclusion for finite representations: quantum states can be mapped to probability vectors and quantum observables to classical random variables at the expense of quantum effects being mapped to non-classical (i.e. negative valued) objects [35].

contradiction between a set of plausible assumptions which together imply that quantum systems possess a consistent set of pre-measurement values for observable quantities. Let $\mathcal{H}$ be the Hilbert space associated with a quantum system and $A \in \mathbb{H}(\mathcal{H})$ be the operator associated with an observable A. The function $f_\psi(A)$ represents the value of the observable A when the system is in state ψ. One assumption used to derive the contradiction is that for any function F, $f_\psi(F(A)) = F(f_\psi(A))$. This is plausible because, for example, we would expect that the value of A^2 could be obtained in this way from the value of A.

Assuming that physical systems do possess values which can be revealed via measurements, the Kochen–Specker theorem leads to the following counterintuitive example [38]. Suppose three operators A, B and C satisfy $[A, B] = 0 = [A, C]$, but $[B, C] \neq 0$. Then the value of the observable A will depend on whether observable B or C is chosen to be measured as well. That is, the value of A depends on the *context* of the measurement.

What the Kochen–Specker theorem establishes then is the mathematical framework of quantum theory does not allow for a *non-contextual* model for pre-measurement values. This fact is often expressed via the phrase 'quantum theory is contextual'.

6.2. Generalized definition of contextuality

The original notion of contextuality only applies to measurements in standard quantum theory. It does not apply to general operational theories, and, in particular, the mathematical model of open quantum systems (i.e. consisting of mixed states, POVM measurements and completely positive maps). This problem was addressed by Spekkens in [39] as follows.

A general operational model (including classical and quantum theory) specifies the probabilities $\Pr(k|\mathcal{P}, \mathcal{M})$ for the outcomes of a measurement procedure $\mathcal{M}$ given preparation procedure $\mathcal{P}$. Each $\mathcal{P}$ belongs to an equivalence class $e(\mathcal{P})$ in which any two preparations, $\mathcal{P}$ and $\mathcal{P}'$ are equivalent if $\Pr(k|\mathcal{P}, \mathcal{M}) = \Pr(k|\mathcal{P}', \mathcal{M})$ for all $\mathcal{M}$. Each $\mathcal{M}$ defines an equivalence class in a similar manner. The features of an experimental configuration, which are not specified by the equivalence class of the procedure, are called the *context* of the experiment.

One may supplement the operational theory with an ontic state space Λ. Then the preparation procedures become probability densities $\mu_{\mathcal{P}}(\lambda)$, while the measurement procedures become conditional probabilities $\xi_{\mathcal{M},k}(\lambda)$. The probabilities of the outcomes of the measurements is required to satisfy the law of total probability

$$\Pr(k|\mathcal{P}, \mathcal{M}) = \int_\Lambda \mathrm{d}\lambda\, \mu_{\mathcal{P}}(\lambda)\xi_{\mathcal{M},k}(\lambda). \tag{44}$$

Such a supplemented operation model is called an ontological model. The ontological model is *preparation non-contextual* if

$$\mu_{\mathcal{P}}(\lambda) = \mu_{e(\mathcal{P})}(\lambda). \tag{45}$$

That is, the representation of the preparation procedure is independent of context. Similarly the ontological model is *measurement non-contextual* if

$$\xi_{\mathcal{M},k}(\lambda) = \xi_{e(\mathcal{M}),k}(\lambda). \tag{46}$$

The terminology 'contextual' is again shorthand for the inability of an operational theory to admit a (preparation or measurement) non-contextual ontological model. However, the term 'contextual' is also used to describe a specific ontological model that do not satisfy equations (45) and (46) [40]. In [39], it was proven that quantum theory is both preparation and measurement contextual.

Since the standard quantum formalism is an instance of an operational model, Spekkens' notion of non-contextuality is a generalization of the traditional notion initiated by Kochen and Specker. Moreover, considering only measurements, one can see that Spekkens generalizes the notion of *non-contextuality* from outcomes of individual measurements being independent of the measurement context to *probabilities* from outcomes of measurements being independent of the measurement context.

6.3. On the equivalence of non-negativity and non-contextuality

Recall that, in quantum theory, a preparation is specified by a density operator ρ and a measurement outcome by an effect E. Thus a (preparation and measurement) non-contextual ontological model of quantum theory would require

$$\mu_{\mathcal{P}}(\lambda) = \mu_\rho(\lambda), \qquad \xi_{\mathcal{M}}(\lambda) = \xi_E(\lambda),$$

and the law of total probability

$$\mathrm{Tr}(E\rho) = \int_\Lambda \mathrm{d}\lambda\, \xi_E(\lambda)\mu_\rho(\lambda).$$

Assuming the probabilities satisfy the usual normalization conditions these conditions are equivalent to those proposed in definition 8 identifying a classical representation. Spekkens noticed this equivalence in [33] and has therefore independently obtained a proof of negativity. Similarly, our direct proof of the non-existence of a positive dual frame to a positive frame gives a new independent proof that quantum theory satisfies Spekkens' generalized notion of contextuality.

Note that the terminology 'negativity and contextuality are equivalent' used in [33], is somewhat misleading. A quasi-probability representation that takes on negative values is *not* equivalent to some contextual ontological model. Within the formalism of quasi-probability representations of quantum theory, a classical representation (definition 8) is a special case (a non-negative one). A classical representation of quantum theory is also a special case of a general operational model (a non-contextual ontological model). The key point is that non-negative quasi-probability representations and non-contextual ontological models are the same thing, and one can establish the non-existence of such a classical representation for quantum theory (theorem 1) starting from either formalism. In other words, a classical representation does not exist but one can relax the constraints on definition 8 to achieve a representation, which may contain negativity or contextuality (or both).

6.4. General models for quantum theory

A broader framework is to consider a very general class of models not requiring any classical features. That is, suppose we define a general model as just a pair of *relations* generalizing the (well-defined) *mappings* μ and ξ of definition 9. In that case, quantum states and measurements are represented by functions over an ontic space which allows for negativity, contextuality and a non-canonical (deformed) probability calculus. Within such a framework we can consider the following propositions: the model is non-negative (NN); the model uses the law of total probability to reproduce the Born rule (LTP); and the model is non-contextual (NC). This paper establishes that the logical conjunction

$$\mathrm{NN} \wedge \mathrm{LTP} \wedge \mathrm{NC}$$

is false. We can deny NN to obtain a quasi-probability representation. Alternatively, we can deny LTP to obtain, for example, a deformed probability representation (section 4.1). We have already seen how these two cases are intimately related. Finally, one can instead deny NC while retaining LTP and NN, which explicitly shows that negativity and contextuality are not equivalent. An example of such a contextual model is discussed in [40], section 5.1.

7. Discussion

Although we conjecture that our no-go theorem will hold when $\mathcal{H}$ is infinite-dimensional, it is clear the technique in the proof of lemma 3 will not suffice in that case. The proof makes explicit use of the finite-dimensionality of $\mathcal{H}$. However, the alternate proof of theorem 1 does not make explicit use of this fact. The key fact used in the alternate proof is the non-simplex structure of the quantum state space $\mathbb{D}(\mathcal{H})$. This fact is true regardless of the dimension of $\mathcal{H}$. However, it was also necessary that the quasi-probability representation have the form $\mu_\rho = \langle \rho, F \rangle$. This form is guaranteed for infinite dimensions if we assume that the quasi-probability representation is *bounded*: there exist $b > 0$ such that for all $\rho \in \mathbb{D}(\mathcal{H})$,

$$\int \mathrm{d}\lambda \, |\mu_\rho(\lambda)|^2 \leqslant b \|\rho\|^2. \tag{47}$$

If we demand boundedness on physical grounds, then our proofs hold for physically reasonable quasi-probability representations in infinite-dimensional Hilbert spaces.

Finally, we would like to comment on potential applications of the frame formalism and our analysis of the relationship between non-negativity and non-contextuality. The question of 'What is non-classical about quantum mechanics?' has taken a more practical and well-defined meaning within the context of quantum information theory. On the one hand, the necessary and sufficient conditions on the quantum resources required to outperform classical information are not well understood [41, 42]. On the other hand, the rapid developments in quantum control in various experimental settings, such as trapped ions, superconducting circuits, quantum optics, and both liquid and solid-state NMR, and their application as quantum information processors, has renewed interest in understanding the extent to which specific experimental achievements may be taken as evidence for truly coherent, quantum behaviour [43, 44]. It is our hope that the formalism developed in this work will lead to more systematic and operationally meaningful criteria for characterizing both of these issues.

Acknowledgments

We thank Bernard Bodmann, Matt Leifer, Etera Livine, Ryan Morris and Rob Spekkens for helpful discussions. This work was supported by NSERC and MITACS.

Appendix A. Notation and definitions

Quantum theory makes use of complex Hilbert spaces. If these spaces are finite-dimensional, then they are equivalent to inner product spaces. Unless otherwise noted, a Hilbert space $\mathcal{H}$ will be assumed to have dimension $d < \infty$ and (for $\psi, \phi \in \mathcal{H}$) its inner product will be denoted $\langle \psi, \phi \rangle$. The following list defines some special sets of linear operators acting on $\mathcal{H}$.

1. An operator A satisfying
$$\langle A\psi, \phi \rangle = \langle \psi, A\phi \rangle, \tag{A.1}$$
for all $\psi, \phi \in \mathcal{H}$, is called *Hermitian*. The set of all Hermitian operators is denoted $\mathbb{H}(\mathcal{H})$.
2. An operator E satisfying
$$0 \leqslant \langle \psi, E\psi \rangle \leqslant 1, \tag{A.2}$$
for all $\psi \in \mathcal{H}$, is called an *effect*. The set of all effects is denoted $\mathbb{E}(\mathcal{H})$.
3. An effect ρ satisfying
$$\mathrm{Tr}(\rho) = 1 \tag{A.3}$$
is called a *density operator*. The set of all density operators is denoted $\mathbb{D}(\mathcal{H})$.
4. A set of effects $\{E_k\}$ that satisfy
$$\sum_k E_k = \mathbb{1} \tag{A.4}$$
is called a POVM. The set of all POVMs is denoted POVM$(\mathcal{H})$.
5. An effect P satisfying
$$P^2 = P \tag{A.5}$$
is called a *projector*. The set of all projects is denoted $\mathbb{P}(\mathcal{H})$.
6. A set of projectors $\{P_k\}$, each of rank 1, which satisfy
$$\sum_k P_k = \mathbb{1} \tag{A.6}$$
is called a PVM. The set of all PVMs is denoted PVM$(\mathcal{H})$.

Note that from these definitions we have $\mathbb{P}(\mathcal{H}) \subset \mathbb{D}(\mathcal{H}) \subset \mathbb{E}(\mathcal{H}) \subset \mathbb{H}(\mathcal{H})$ and PVM$(\mathcal{H}) \subset$ POVM$(\mathcal{H})$. The set $\mathbb{H}(\mathcal{H})$ defines its own Hilbert space with inner product (for $A, B \in \mathbb{H}(\mathcal{H})$) $\langle A, B \rangle := \mathrm{Tr}(AB)$. The dimension of $\mathbb{H}(\mathcal{H})$ is d^2. A PVM contains exactly d projectors, which satisfy the *orthogonality condition* $P_k P_j = P_k \delta_{kj}$, for any k and j.

Here are some examples of important Hermitian operators used in this paper. Consider the operator Z whose spectrum is spec$(Z) = \{\omega^k : k \in \mathbb{Z}_d\}$, where $\omega^k = \mathrm{e}^{(2\pi \mathrm{i}/d)k}$. The eigenvectors form a basis for $\mathcal{H}$ and are denoted $\{\phi_k\}$. Consider also the operator defined by $X\phi_k = \phi_{k+1}$, where all arithmetic is modulo d. Define Y implicitly through $[X, Z] = 2iY$. The operators Z, X and Y are often called *generalized Pauli operators* since they are indeed the usual Pauli operators when $d = 2$. The *parity operator* is defined by $P\phi_k = \phi_{-k}$.

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