

Phase-space descriptions of operators and the Wigner distribution in quantum mechanics II. The finite dimensional case

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Abstract.

A complete solution to the problem of setting up Wigner distribution for N -level quantum systems is presented. The scheme makes use of some of the ideas introduced by Dirac in the course of defining functions of noncommuting observables and works uniformly for all N . Further, the construction developed here has the virtue of being essentially input-free in that it merely requires finding a square root of a certain $N^2 \times N^2$ complex symmetric matrix, a task which, as is shown, can always be accomplished analytically. As an illustration, the case of a single qubit is considered in some detail and it is shown that one recovers the result of Feynman and Wootters for this case without recourse to any auxiliary constructs.

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1. Introduction

There has been considerable interest for some time in extending the method of Wigner distributions to describe states of quantum systems, originally developed for the case of continuous Cartesian coordinates and momenta [1]-[3], to the case of finite-dimensional quantum systems [4]-[11].

In its original version, the Wigner distribution is a function on the classical phase space, real but not necessarily pointwise nonnegative, which describes completely any pure or mixed quantum state. Even though it cannot be interpreted as a probability distribution on phase space, it does lead to the correct marginal position and momentum probability distributions as determined by quantum mechanics.

Among the early efforts to set up Wigner distribution for states of quantum systems with a finite-dimensional state space, one may mention the work of Feynman and of Wootters [4]. In the former, attention was devoted to the two-dimensional case, drawing on the treatment of spin in quantum mechanics. In the latter it was shown that one has to treat separately the cases where the dimension of the state space is a power of two, and those where it is odd. In the odd case one has to handle first the case of odd prime dimension, and then pass to the general odd situation by forming a Cartesian product of the prime cases.

The approach of Jagannathan [4] on the other hand is based on the Weyl-ordered unitary operators for translations on a phase-space lattice, leading to the discrete Wigner distribution through the associated characteristic function. The more recent independent work of Luis and Peřina [10] uses a similar approach, but presents a thorough analysis of the problem.

In a previous paper [12] it has been shown that one can arrive at the Wigner distribution concept, in the case of continuous variables, by a novel route starting from an idea of Dirac [13] to describe a general quantum-mechanical operator by a collection of mixed matrix elements, using vectors chosen from two different orthonormal bases in Hilbert space. The steps that lead from Dirac's starting point to the expression for the Wigner distribution, indeed even the introduction of classical phase space ideas to describe operators, are particularly transparent and elementary, and they automatically ensure the property of correctly reproducing the quantum-mechanical probability distributions as marginals.

The purpose of the present paper is to show that the same approach based on Dirac's method can be used in the finite-dimensional case as well to set up the Wigner distribution formalism, incorporating all the desirable features including the reproduction of the marginals. It is worth particularly emphasizing that, denoting the dimensionality of the state space by N , the present approach works uniformly for all N ; there is no need to treat separately the cases of N a power of two, N an odd prime and N an odd number. In the case $N = 2$, the earlier results of Feynman and Wootters are immediately recovered, without having to call upon the specific properties of spin-1/2 systems.

The construction presented here assumes particular significance in the light of the intimate connection between Wigner distributions and mutually unbiased bases [14] as was brought out by Wootters and coworkers in a series of insightful papers [15]. Mutually unbiased bases, in turn, are known to be related to questions pertaining to affine planes in finite geometries, mutually orthogonal arrays, complex polytopes and finite designs [16] and one expects that the work presented here would provide a new mathematical perspective to some of these questions and their interrelations.

A brief summary of the present work is as follows. In Section 2 we discuss the kinematics of N -level quantum systems. In particular we examine the trace of product of two operators \hat{A} and \hat{B} and show how this can be expressed as a phase space sum of products of mixed matrix elements of the operators involved such that it manifestly reflects the symmetry under interchange of \hat{A} and \hat{B} . This entails introducing a kernel whose properties are investigated in Section 3. In Section 4, we show how, by taking the ‘square root’ of this kernel in a certain fashion, one is directly led to the concept of a Wigner distribution associated with operators on a N -dimensional Hilbert space for any N . In Section 5, by way of illustration, we consider the case of a single qubit and recover known results with economy. Section 6 contains concluding remarks and further outlook.

2. Kinematics of an N -level quantum system

We consider a quantum system possessing N independent states, so that its state space is a complex (finite-dimensional) Hilbert space $\mathcal{H}^{(N)}$ of (complex) dimension N . We select a particular orthonormal basis for $\mathcal{H}^{(N)}$, written as $|q\rangle$, with $q = 0, 1, \dots, N - 1$, to be called the set of “position eigenstates” of the system. Then:

$$\begin{aligned} \langle q|q'\rangle &= \delta_{q,q'}, \quad q, q' = 0, 1, \dots, N - 1; \\ \sum_{q=0}^{N-1} |q\rangle\langle q| &= \mathbb{I}. \end{aligned} \tag{1}$$

A general vector $|\psi\rangle \in \mathcal{H}^{(N)}$ is described in this basis by a corresponding wave function which is an N -component complex column vector:

$$\begin{aligned} \psi(q) &= \langle q|\psi\rangle, \\ \langle\psi|\psi\rangle &= \|\psi\|^2 = \sum_{q=0}^{N-1} \langle\psi|q\rangle\langle q|\psi\rangle = \sum_{q=0}^{N-1} |\psi(q)|^2. \end{aligned} \tag{2}$$

By means of an N -point Fourier series transformation we arrive at a complementary orthonormal basis of “momentum eigenstates” $|p\rangle$ with $p = 0, 1, \dots, N - 1$. The principal

equations are:

$$\begin{aligned}
|p\rangle &= \frac{1}{\sqrt{N}} \sum_{q=0}^{N-1} e^{2\pi i q p / N} |q\rangle, \\
\langle p|p'\rangle &= \delta_{p,p'}, \quad p, p' = 0, 1, \dots, N-1, \\
\sum_{p=0}^{N-1} |p\rangle\langle p| &= \mathbb{I}, \\
\langle q|p\rangle &= \frac{1}{\sqrt{N}} e^{2\pi i q p / N}.
\end{aligned} \tag{3}$$

Now consider a general operator \hat{A} on $\mathcal{H}^{(N)}$. Using either the basis $\{|q\rangle\}$ or the basis $\{|p\rangle\}$ for $\mathcal{H}^{(N)}$, it can be completely described by the corresponding $N \times N$ square complex matrices $\langle q'|\hat{A}|q\rangle$ or $\langle p'|\hat{A}|p\rangle$. Following the method of Dirac, however, we can equally well describe \hat{A} completely by the collection of “mixed matrix elements” $\langle q|\hat{A}|p\rangle$; we call this an $N \times N$ “array” rather than a matrix since operator multiplication is not simply the multiplication of these arrays thought of as matrices. We also notice that with the introduction of such arrays the step to a “phase-space” description of \hat{A} has been taken. More precisely, we define the (left) phase-space representative of \hat{A} by:

$$A_l(q, p) = \langle q|\hat{A}|p\rangle\langle p|q\rangle = \text{Tr} \left\{ \hat{A}|p\rangle\langle p|q\rangle\langle q| \right\} = \frac{1}{\sqrt{N}} \langle q|\hat{A}|p\rangle \exp \{-2\pi i p q / N\}. \tag{4}$$

(By interchanging the rôles of q and p we can equally well define an expression $A_r(q, p) = \langle p|\hat{A}|q\rangle\langle q|p\rangle$, however we will work with the quantities $A_l(q, p)$). The following are immediate consequences of this definition:

$$\begin{aligned}
\sum_p A_l(q, p) &= \langle q|\hat{A}|q\rangle, \\
\sum_q A_l(q, p) &= \langle p|\hat{A}|p\rangle, \\
\sum_{q,p} A_l(q, p) &= \text{Tr} \left\{ \hat{A} \right\}.
\end{aligned} \tag{5}$$

We may notice at this point that even for hermitian \hat{A} , $A_l(q, p)$ is in general complex.

Now take two operators \hat{A} and \hat{B} and the trace of their product. We can express this in terms of their (left) phase-space representatives as follows:

$$\begin{aligned}
\text{Tr} \left\{ \hat{A}\hat{B} \right\} &= N \sum_{q,p} A_l(q, p) B_r(q, p) = \sum_{q,p} \sum_{q',p'} \langle q|\hat{A}|p\rangle\langle p|q'\rangle\langle q'|\hat{B}|p'\rangle\langle p'|q\rangle \\
&= \sum_{q,p} \sum_{q',p'} A_l(q, p) K_l(q, p; q', p') B_l(q', p'),
\end{aligned} \tag{6}$$

where:

$$K_l(q, p; q', p') = N^2 \langle q|p\rangle\langle p|q'\rangle\langle q'|p'\rangle\langle p'|q\rangle = \exp \{2\pi i (q - q')(p - p') / N\}. \tag{7}$$

Thus an important phase-space kernel K_l has been introduced. We note in passing that (apart from the N^2 factor) it is a four-vertex Bargmann invariant, so its phase is an instance of the kinematic geometric phase [17].

The study of the detailed properties of K_l will lead us to the solution of setting up a physically reasonable Wigner distribution, *for any value of the dimension N* .

3. Properties of the Kernel K_l

We can regard $K_l(q, p; q', p')$ as defined in Eq. (7) as constituting a complex square matrix of dimension N^2 , with the first pair of arguments (q, p) being row index and the second pair (q', p') column index \S . We denote by $\mathcal{K}^{(N^2)}$ a complex linear space of dimension N^2 , made up of vectors f with components $f(q, p)$:

$$f \in \mathcal{K}^{(N^2)} \rightarrow f(q, p), q, p = 0, 1, 2, \dots, N-1. \quad (8)$$

It is to be understood that these vectors are “periodic” in the sense that

$$f(q + nN, p + n'N) = f(q, p), n, n' = 0, \pm 1, \pm 2, \dots \quad (9)$$

The norm is defined in the natural way by

$$\|f\|^2 = (f, f) = \sum_{q,p=0,1,\dots}^{N-1} |f(q, p)|^2. \quad (10)$$

Then K_l acts on such vectors according to

$$(K_l f)(q, p) = \sum_{q', p'} K_l(q, p; q', p') f(q', p'). \quad (11)$$

The following properties are immediately evident:

- Symmetry:

$$K_l(q, p; q', p') = K_l(q', p'; q, p); \quad (12)$$

- Essential unitarity:

$$\sum_{q', p'} K_l(q, p; q', p') K_l(q'', p''; q', p')^* = N^2 \delta_{qq''} \delta_{pp''}; \quad (13)$$

- Translation invariance:

$$K_l(q + q_0, p + p_0; q' + q_0, p' + p_0) = K_l(q, p; q', p'), \quad (14)$$

$$q_0, p_0 = 0, 1, 2, \dots, N-1.$$

Here and in the following we interpret translated arguments $q + q_0, p + p_0, \dots$ as always taken modulo N , so that they always lie in the range $0, 1, \dots, N-1$. Property (13)

\S We introduce below a more compact efficient notation to express this.

means that any eigenvalue of K_l is of the form $Ne^{i\varphi}$ for some phase φ . In addition to the above, the following ‘marginals’ properties are also evident from the definition (7):

$$\sum_{p'} K_l(q, p; q', p') = N\delta_{qq'}, \text{ independent of } p, \quad (15a)$$

$$\sum_{q'} K_l(q, p; q', p') = N\delta_{pp'}, \text{ independent of } q. \quad (15b)$$

These are particularly important for the Wigner distribution problem, so we explore them in some detail and relate them to the eigenvalue and eigenvector properties of K_l . From either one of Eqs.(15a,15b) we get the (weaker) relations:

$$\sum_{q'p'} K_l(q, p; q', p') = N, \text{ independent of } q, p. \quad (16)$$

Let us introduce a single symbol σ to denote the pair (q, p) by the definition:

$$\sigma = qN + p + 1. \quad (17)$$

Thus σ runs from 1 to N^2 : for $q = 0, p = 0, 1, \dots, N - 1$ we have $\sigma = 1, 2, \dots, N$; for $q = 1, p = 0, 1, \dots, N - 1$ we have $\sigma = N + 1, N + 2, \dots, 2N$; and so on. For summations and Kronecker symbols we have the rules:

$$\begin{aligned} \sum_{\substack{p \\ q \text{ fixed}}} \dots &= \sum_{\sigma=qN+1, qN+2, \dots, (q+1)N} \dots, \\ \sum_{\substack{q \\ p \text{ fixed}}} \dots &= \sum_{\sigma=p+1, N+p+1, 2N+p+1, \dots, (N-1)N+p+1} \dots, \\ \sum_{qp} \dots &= \sum_{\sigma=1}^{N^2} \dots, \\ \delta_{\sigma\sigma'} &= \delta_{qq'}\delta_{pp'}. \end{aligned} \quad (18)$$

We hereafter use σ or q, p interchangeably as convenient. The kernel $K_l(q, p; q', p')$ can now be written as $K_l(\sigma; \sigma')$, while vectors $f \in \mathcal{K}^{(N^2)}$ have components $f(\sigma)$. In addition to the properties (12),(13),(15a,15b),(16) we have the trace property following from (7):

$$\text{Tr}K_l = \sum_{\sigma} K_l(\sigma, \sigma) = N^2. \quad (19)$$

With this notation one can now see that the marginals properties (15a,15b) can be expressed as follows. For each $q' = 0, 1, \dots, N - 1$ we define a vector $U_{q'}$ in $\mathcal{K}^{(N^2)}$, forming altogether a set of N real orthonormal vectors (not a basis!) by:

$$\begin{aligned} U_{q'}(\sigma) &= \frac{1}{\sqrt{N}}\delta_{qq'}, \text{ independent of } p, \\ (U_{q'}, U_q) &= \delta_{q'q}. \end{aligned} \quad (20)$$

Then Eq. (15a) translates exactly into the statement:

$$K_l U_q = N U_q, \quad q = 0, 1, \dots, N - 1. \quad (21)$$

Similarly, for each $p' = 0, 1, \dots, N-1$ we define a vector $V_{p'}$ in $\mathcal{K}^{(N^2)}$ forming altogether a set of N real orthonormal vectors (again, not a basis!) by:

$$\begin{aligned} V_{p'}(\sigma) &= \frac{1}{\sqrt{N}} \delta_{pp'}, \text{ independent of } q, \\ (V_{p'}, V_p) &= \delta_{p'p}. \end{aligned} \quad (22)$$

Then Eq. (15b) translates into:

$$K_l V_p = N V_p, \quad p = 0, 1, \dots, N-1. \quad (23)$$

These real eigenvectors U_q and V_p are mutually nonorthogonal:

$$(V_p, U_q) = \sum_{\sigma'} V_p(\sigma') U_q(\sigma') = \frac{1}{N}. \quad (24)$$

This leads to the single linear dependence relation among the $2N$ (real) vectors U_q, V_p :

$$\sum_q U_q = \sum_p V_p, \quad (25)$$

which can also be read off from Eqs. (20) and (22). Therefore, the U_q 's and V_p 's together span an $(2N-1)$ -dimensional subspace $\mathcal{K}^{(2N-1)}$ in $\mathcal{K}^{(N^2)}$, over which K_l reduces to N times the identity. We can construct an orthonormal basis of $(2N-1)$ real vectors for $\mathcal{K}^{(2N-1)}$ for instance by the following recipe:

$$\begin{aligned} \Psi_0 &= \frac{1}{\sqrt{N}} \sum_q U_q = \frac{1}{\sqrt{N}} \sum_p V_p, \\ \tilde{U}_j &= \frac{1}{\sqrt{j(j+1)}} (U_0 + U_1 + \dots + U_{j-1} - j U_j), \quad j = 1, 2, \dots, N-1, \\ \tilde{V}_j &= \frac{1}{\sqrt{j(j+1)}} (V_0 + V_1 + \dots + V_{j-1} - j V_j), \quad j = 1, 2, \dots, N-1, \\ (\tilde{U}_{j'}, \tilde{U}_j) &= (\tilde{V}_{j'}, \tilde{V}_j) = \delta_{j'j}, \quad (\Psi_0, \Psi_0) = 1, \\ (\tilde{U}_{j'}, \Psi_0) &= (\tilde{V}_{j'}, \Psi_0) = (\tilde{U}_{j'}, \tilde{V}_j) = 0. \end{aligned} \quad (26)$$

If the orthogonal complement of $\mathcal{K}^{(2N-1)}$ in $\mathcal{K}^{(N^2)}$, of dimension $(N-1)^2$, is written as $\mathcal{K}^{(N-1)^2}$, i.e.:

$$\mathcal{K}^{(N^2)} = \mathcal{K}^{(2N-1)} \oplus \mathcal{K}^{(N-1)^2}, \quad (27)$$

then we can supplement the basis (26) for $\mathcal{K}^{(2N-1)}$ by (any) additional real orthonormal vectors to span $\mathcal{K}^{(N-1)^2}$. The essential unitarity of K_l means that it leaves $\mathcal{K}^{(N-1)^2}$ also invariant; the transition from the original (standard) basis of $\mathcal{K}^{(N^2)}$ to the present one can be accomplished by an element of the real orthogonal rotation group $SO(N^2)$, thus preserving the symmetry (12) of K_l . Therefore the matrix K_l has the following structure in a (real) basis adapted to the decomposition (27):

$$K_l \rightarrow \begin{pmatrix} \mathbf{N} \cdot \mathbb{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{A} + i\mathbf{B} \end{pmatrix}. \quad (28)$$

The unit matrix is of dimension $(2N - 1)$, while the two real $(N - 1)^2$ -dimensional matrices \mathbf{A} and \mathbf{B} obey:

$$\begin{aligned}\mathbf{A}^T &= \mathbf{A}, \mathbf{B}^T = \mathbf{B}, \mathbf{AB} = \mathbf{BA}, \\ \mathbf{A}^2 + \mathbf{B}^2 &= N^2 \cdot \mathbb{I}_{(N-1)^2 \times (N-1)^2}, \\ Tr\{\mathbf{A}\} &= -N(N - 1), Tr\{\mathbf{B}\} = 0.\end{aligned}\tag{29}$$

Thus the matrix $\mathbf{A} + i\mathbf{B}$ can definitely be diagonalized by a real rotation in $(N - 1)^2$ dimensions, i.e., by an element of $SO((N - 1)^2)$, and each eigenvalue of $\mathbf{A} + i\mathbf{B}$ is of the form $Ne^{i\varphi}$ for some angle φ .

It now turns out that we can carry through this diagonalisation process explicitly. The translation invariance (14) of K_l means that the eigenvectors of K_l can be constructed as ‘‘plane waves’’ in phase space. We can obtain a complete real orthonormal set of vectors of K_l in $\mathcal{K}^{(N^2)}$ by this route, recovering the subset of eigenvectors (26) as part of a complete set.

For each point $\sigma_0 = (q_0, p_0)$ we define a unit vector χ_{σ_0} with components

$$\chi_{\sigma_0}(\sigma) = \frac{1}{N} \exp(2\pi i(q_0 p + p_0 q)/N)\tag{30}$$

(we see that condition (9) is indeed obeyed). Thus we have exactly N^2 vectors χ_{σ_0} . Using the modulo N rule for phase space arguments we then easily obtain the following:

$$K_l \chi_{\sigma_0} = N e^{-2\pi i q_0 p_0 / N} \chi_{\sigma_0},\tag{31a}$$

$$(\chi_{\sigma'_0}, \chi_{\sigma_0}) = \delta_{\sigma'_0 \sigma_0}.\tag{31b}$$

Therefore we have achieved full diagonalisation of K_l , with $\{\chi_{\sigma_0}\}$ forming an orthonormal basis in $\mathcal{K}^{(N^2)}$. The previously found (real) basis for the subspace $\mathcal{K}^{(2N-1)}$, made up exclusively of eigenvectors of K_l with eigenvalues N , is essentially the subset of $(2N - 1)$ vectors $\chi_{q_0,0}$ for $q_0 = 0, 1, \dots, N - 1$ and χ_{0,p_0} for $p_0 = 1, \dots, N - 1$. Indeed we find

$$\begin{aligned}U_q &= \frac{1}{\sqrt{N}} \sum_{p_0=0}^{N-1} e^{-2\pi i q p_0 / N} \chi_{0,p_0}, \\ V_p &= \frac{1}{\sqrt{N}} \sum_{q_0=0}^{N-1} e^{-2\pi i q_0 p / N} \chi_{q_0,0}.\end{aligned}\tag{32}$$

The remaining $(N - 1)^2$ eigenvectors χ_{σ_0} for $q_0, p_0 = 1, 2, \dots, N - 1$ span the orthogonal subspace $\mathcal{K}^{(N-1)^2}$. Here we have in detail the following structure. The two eigenvectors χ_{q_0,p_0} and $\chi_{N-q_0,N-p_0}$ are degenerate, and their components are related by complex conjugation :

$$\begin{aligned}K_l \chi_{q_0,p_0} &= N e^{-2\pi i q_0 p_0 / N} \chi_{q_0,p_0}, \\ K_l \chi_{N-q_0,N-p_0} &= N e^{-2\pi i q_0 p_0 / N} \chi_{N-q_0,N-p_0}; \\ \chi_{N-q_0,N-p_0}(\sigma) &= \chi_{q_0,p_0}(\sigma)^*.\end{aligned}\tag{33}$$

Therefore we have a pattern that depends on the parity of N . For odd N , we have $(N - 1)^2/2$ distinct degenerate pairs of mutually complex conjugate orthogonal

eigenvectors $\{\chi_{q_0,p_0}, \chi_{N-q_0,N-p_0}\}$ for $q_0 = 1, 2, \dots, (N-1)/2$ and $p_0 = 1, 2, \dots, N-1$. For even N we have one real eigenvector $\chi_{N/2,N/2}$ with eigenvalue $N(-1)^{N/2}$ followed by $((N-1)^2 - 1)/2$ distinct degenerate pairs $\{\chi_{q_0,p_0}, \chi_{N-q_0,N-p_0}\}$ where we omit $q_0 = p_0 = N/2$. In either case it is clear that by passing to the real and imaginary parts of χ_{q_0,p_0} , while leaving $\chi_{N/2,N/2}$ unchanged, we get a real orthonormal basis for $\mathcal{K}^{(N-1)^2}$ in which the matrix $\mathbf{A} + i\mathbf{B}$ of Eq. (28) is diagonal.

Equipped with these important properties of K_l we turn to Eq. (6) from where we can find the route to the Wigner distribution.

4. The Kernel ξ and the Wigner Distribution

Motivated by the structure (6) for $Tr \{\widehat{A}\widehat{B}\}$ for two general operators \widehat{A} and \widehat{B} on $\mathcal{H}^{(N)}$, we try to express the kernel $K_l(q, p; q', p')$ in the form:

$$K_l(\sigma, \sigma') = \sum_{\sigma''} \xi(\sigma'', \sigma) \xi(\sigma'', \sigma'), \quad (34)$$

with suitable conditions imposed on ξ . The desirable conditions are, as with K_l itself: symmetry, essential unitarity, translation invariance and marginal conditions similar to Eqs. (15a,15b) for K_l :

$$\xi(\sigma, \sigma') = \xi(\sigma', \sigma), \quad (35a)$$

$$\sum_{\sigma'} \xi(\sigma, \sigma') \xi(\sigma'', \sigma')^* = N \delta_{\sigma\sigma''}, \quad (35b)$$

$$\xi(q + q_0, p + p_0; q' + q_0, p' + p_0) = \xi(q, p; q', p'), \quad (35c)$$

$$\xi U_q = \sqrt{N} U_q, \quad \xi V_p = \sqrt{N} V_p. \quad (35d)$$

Here we have expressed the last marginal conditions already in terms of the eigenvectors (not all independent!) U_q, V_p of K_l lying in $\mathcal{K}^{(2N-1)}$. More explicitly they read

$$\begin{aligned} \sum_{p'} \xi(q, p; q', p') &= \sqrt{N} \delta_{qq'}, \\ \sum_{q'} \xi(q, p; q', p') &= \sqrt{N} \delta_{pp'}. \end{aligned} \quad (36)$$

The detailed analysis of the eigenvectors and eigenvalues of K_l in the previous section immediately leads to solutions for ξ . The translation invariance of (35c) is ensured by arranging that the ‘‘plane waves’’ eigenvectors χ_{q_0,p_0} of K_l are eigenvectors of ξ as well. We take ξ to obey:

$$\xi \chi_{q_0,0} = \sqrt{N} \chi_{q_0,0}, \quad q_0 = 0, 1, \dots, N-1; \quad (37a)$$

$$\xi \chi_{0,p_0} = \sqrt{N} \chi_{0,p_0}, \quad p_0 = 0, 1, \dots, N-1; \quad (37b)$$

$$\xi (\chi_{q_0,p_0} \text{ or } \chi_{N-q_0,N-p_0}) = \pm \sqrt{N} e^{-i\pi q_0 p_0 / N} (\chi_{q_0,p_0} \text{ or } \chi_{N-q_0,N-p_0}), \quad (37c)$$

$$q_0, p_0 = 1, \dots, N-1.$$

In the subspaces $\mathcal{K}^{(2N-1)}$ and $\mathcal{K}^{(N-1)^2}$ we then have:

$$\begin{aligned} \xi &= \sqrt{N} \cdot \mathbb{I} \quad \text{on } \mathcal{K}^{(2N-1)}, \\ \xi &= (\mathbf{A} + i\mathbf{B})^{1/2} \quad \text{on } \mathcal{K}^{(N-1)^2}. \end{aligned} \quad (38)$$

Equations (37a) ensure the validity of the marginals properties (35d) or (36) while Eq. (35b) is obeyed by construction. It is the symmetry requirement (35a) that dictates that in the case of degenerate orthonormal pairs of K_l eigenvectors $\{\chi_{q_0, p_0}, \chi_{N-q_0, N-p_0}\}$ we choose the square root of the eigenvalue $N e^{-2\pi i q_0 p_0 / N}$ of K_l in the same way; this is expressed in Eq. (37c). Thus we see: for odd N there is a $2^{(N-1)^2/2}$ -fold freedom in the choice of ξ ; for N even there is a $2^{((N-1)^2+1)/2}$ -fold freedom. In each case, a particular square root of $\mathbf{A} + i\mathbf{B}$ is involved in (38).

With any such ξ , we can return to Eq. (6) and write it in a manifestly kernel-independent manner:

$$\text{Tr} \left\{ \widehat{A}\widehat{B} \right\} = N \sum_{q,p} A(q,p) B(q,p), \quad (39)$$

where:

$$\begin{aligned} A(q,p) &= \frac{1}{\sqrt{N}} \sum_{q',p'} \xi(q,p; q', p') A_l(q', p') \\ &= \frac{1}{\sqrt{N}} \sum_{q',p'} \xi(q,p; q', p') \langle q' | \widehat{A} | p' \rangle \langle p' | q' \rangle, \end{aligned} \quad (40)$$

with a similar expression for $B(q,p)$ in terms of \widehat{B} . We will show below that for hermitian \widehat{A} , $A(q,p)$ is real. Combining Eqs.(5) and (35d) we have ensured the marginals properties:

$$\begin{aligned} \sum_p A(q,p) &= \langle q | \widehat{A} | q \rangle, \\ \sum_q A(q,p) &= \langle p | \widehat{A} | p \rangle. \end{aligned} \quad (41)$$

For the density matrix $\widehat{\rho}$ describing some pure or mixed state of the N -level system, we then have the real Wigner distribution:

$$W(q,p) = \frac{1}{\sqrt{N}} \sum_{q',p'} \xi(q,p; q', p') \langle q' | \widehat{\rho} | p' \rangle \langle p' | q' \rangle \quad (42)$$

and by Eqs.(41) the two marginal probability distributions in q and p are immediately recovered. In particular, we find that for position eigenstates and momentum eigenstates the freedom in the choice of ξ (which in any case is limited to its action on $\mathcal{K}^{(N-1)^2}$) does not matter and we get the anticipated results:

$$\begin{aligned} \widehat{\rho} = |q'\rangle\langle q'| &\Rightarrow W(q,p) = \frac{1}{N} \delta_{qq'}, \text{ independent of } p, \\ \widehat{\rho} = |p'\rangle\langle p'| &\Rightarrow W(q,p) = \frac{1}{N} \delta_{pp'}, \text{ independent of } q. \end{aligned} \quad (43)$$

Returning to the Wigner distribution (42) we may rewrite it as

$$W(q,p) = \frac{1}{N} \text{Tr} \{ \rho \widehat{W}(q,p) \} \quad (44)$$

by introducing elements of Wigner basis [18] or phase point operators [19]:

$$\widehat{W}(q,p) = \sqrt{N} \sum_{q',p'} \xi(q,p; q', p') \langle p' | q' \rangle |p'\rangle \langle q'|. \quad (45)$$

It is an interesting exercise to verify, by combining the definition (7) of K_l and (34,35b), that these are hermitian:

$$\widehat{W}(q, p)^\dagger = \widehat{W}(q, p). \quad (46)$$

This proves that $W(q, p)$, and more generally $A(q, p) = \text{Tr}\{\widehat{A}\widehat{W}(q, p)\}$ for hermitian \widehat{A} , are both real. In addition one can check, by virtue of eqs (34,35a-d), they satisfy

$$\begin{aligned} \text{Tr}\{\widehat{W}(\sigma)\} &= 1, \\ \text{Tr}\{\widehat{W}(\sigma)\widehat{W}(\sigma')\} &= N\delta_{\sigma\sigma'}. \end{aligned} \quad (47)$$

5. The case of $N = 2$: the Qubit

This case is particularly interesting in that earlier treatments have had to treat it on its own, in a sense in an ad hoc manner, as distinct from N an odd prime or an odd integer. In the standard basis for the two-dimensional Hilbert space $\mathcal{H}^{(2)}$ made up of $|q\rangle$ for $q = 0, 1$, accompanied by its complementary basis $|p\rangle$, the matrix $K_l(q, p; q', p')$ is the following:

$$K_l = \begin{pmatrix} 1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \end{pmatrix}. \quad (48)$$

The rows and columns are labelled in the sequence: $(q, p) = (0, 0), (0, 1), (1, 0), (1, 1)$, and the matrix elements are read off from Eq. (7). The three orthonormal eigenvectors of K_l with eigenvalue 2, spanning the subspace $\mathcal{K}^{(3)}$ of the general treatment in Section 3 are:

$$\Psi_0 = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \quad \tilde{U}_1 = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}, \quad \tilde{V}_1 = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}. \quad (49)$$

We choose the fourth eigenvector of K_l , with eigenvalue necessarily -2 since $\text{Tr}K_l = 4$, to be:

$$W = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}. \quad (50)$$

Then the kernel ξ can be immediately synthesized from:

$$\xi\Psi_0 = \sqrt{2}\Psi_0, \quad \xi\tilde{U}_1 = \sqrt{2}\tilde{U}_1, \quad \xi\tilde{V}_1 = \sqrt{2}\tilde{V}_1, \quad \xi W = i\sqrt{2}W \quad (51)$$

and in the standard basis turns out to be:

$$\xi = \frac{1}{2\sqrt{2}} \begin{pmatrix} 3+i & 1-i & 1-i & -1+i \\ 1-i & 3+i & -1+i & 1-i \\ 1-i & -1+i & 3+i & 1-i \\ -1+i & 1-i & 1-i & 3+i \end{pmatrix}. \quad (52)$$

Using the above matrix elements of ξ in (45) we obtain, for the phase-point operators:

$$\begin{aligned}\widehat{\mathcal{W}}(0,0) &= \begin{pmatrix} 1 & \frac{1-i}{2} \\ \frac{1+i}{2} & 0 \end{pmatrix}, & \widehat{\mathcal{W}}(0,1) &= \begin{pmatrix} 0 & \frac{1+i}{2} \\ \frac{1-i}{2} & 1 \end{pmatrix}, \\ \widehat{\mathcal{W}}(1,0) &= \begin{pmatrix} 1 & \frac{-1+i}{2} \\ \frac{-1-i}{2} & 0 \end{pmatrix}, & \widehat{\mathcal{W}}(1,1) &= \begin{pmatrix} 0 & \frac{-1-i}{2} \\ \frac{-1+i}{2} & 1 \end{pmatrix}.\end{aligned}\tag{53}$$

and thereby recover the results of Feynman and Wootters [4] and hence also the connection between sums of phase point operators along striations of the qubit phase space [15] and the mutually unbiased bases for $N = 2$.

For the density operator $\widehat{\rho} = \frac{1}{2}(\mathbb{I}_2 + \mathbf{a} \cdot \sigma)$, $\mathbf{a} \cdot \mathbf{a} \leq 1$ describing a general state of a qubit one can easily calculate the corresponding Wigner distribution using (42) or (44). The results arranged in the form of a matrix read:

$$\begin{pmatrix} 1 + a_1 + a_2 + a_3 & 1 + a_1 - a_2 - a_3 \\ 1 - a_1 - a_2 + a_3 & 1 - a_1 + a_2 - a_3 \end{pmatrix}.\tag{54}$$

Using this result it is instructive to verify the validity of (39) for $\widehat{A} = \widehat{\rho}_1 = \frac{1}{2}(\mathbb{I}_2 + \mathbf{a} \cdot \sigma)$, and $\widehat{B} = \widehat{\rho}_2 = \frac{1}{2}(\mathbb{I}_2 + \mathbf{b} \cdot \sigma)$. Further, it is easily seen from (54) that the maximum positive and maximum negative values of the Wigner distribution for a qubit occur when $|a_1| = |a_2| = |a_3| = 1/\sqrt{3}$.

As a final remark, we notice that in calculating the kernel ξ , square root of K_l , we might have chosen W in Eq. (51) to be the eigenvector corresponding to the eigenvalue $-i\sqrt{2}$ instead of $+i\sqrt{2}$. This results in changing $+i(-i)$ with $-i(+i)$ in Eqs. (52,53) and thus in an interchange of the rôle of $\widehat{\mathcal{W}}(0,0)$ and $\widehat{\mathcal{W}}(0,1)$ with $\widehat{\mathcal{W}}(1,0)$ and $\widehat{\mathcal{W}}(1,1)$ respectively. Correspondingly, the coefficient a_2 in Eq. (54) would change sign everywhere. This however can be of no physical consequence as is reflected in the fact that the marginals obtained by summing over q or p are independent of a_2 .

6. Concluding remarks.

To conclude, we have developed a method of constructing Wigner distribution for N -level systems which is remarkable in its directness and economy and works uniformly for all N . The construction is entirely algebraic and solely involves finding a square root of a certain $N^2 \times N^2$ complex symmetric matrix. No other auxiliary inputs are required. As an illustration, we have worked out the qubit case in some detail and obtained results already known in the literature in an extremely economic fashion. The construction presented here provides a fresh perspective to several questions pertaining to quantum tomography in finite state systems and to those associated with finite geometries which are currently being investigated with great vigour owing to their relevance to quantum information theory. We hope to return to some of these elsewhere.

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