Wigner distributions for \( n \) arbitrary operators

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We show that for any collection of hermitian operators \( A_1, \ldots, A_n \), and any quantum state there is a unique joint distribution on \( \mathbb{R}^n \), with the property that the marginals of all linear combinations of the \( A_k \) coincide with their quantum counterpart. We call it the Wigner distribution, because for position and momentum this property defines the standard Wigner function. In this note we discuss the application to finite dimensional systems, establish many basic properties and illustrate these by examples. The properties include the support, the location of singularities, positivity, the behaviour under symmetry groups, and informational completeness.

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Wigner functions, introduced in 1932 [1] for treating the classical limit, have become a key tool for understanding systems with canonical degrees of freedom like position/momentum, or field quadratures in quantum optics. They have been particularly helpful in providing a visualisation of quantum states. While listing all the matrix elements of the density matrix is a correct way to completely characterize a state, it is hard to present this information in a way that would help to gain a useful insight. The Wigner function of a state contains the same information, but combines it with a localization in phase space, so that some properties, like negativity of the Wigner function, can be associated with particular regions of phase space, carrying direct suggestions as to what experiments might see these effects. Accordingly, there is a rich literature on Wigner functions [2–12]. There are various generalizations focusing on the group theoretical structure [13–18] for which the Wigner function typically is a function on the group. The aim of this note is to explore another generalization, which is directly based on the well-known fact, that the Wigner function not only gives correct marginals for canonical momentum \( P \) and position \( Q \), but also for all real linear combinations of these operators. Replacing here the pair \( (P, Q) \) by \( n \) arbitrary hermitian operators \( (A_1, \ldots, A_n) \) singles out a unique distribution of \( n \) variables, which we call the Wigner distribution. Apart from the operators \( A_k \) and the state there are no arbitrary choices or parameters in this definition. To our knowledge it has first been suggested in the in the 80s [19] (see also [20], [5, Ch. 17]), although worked out only in a very limited context. We will extend this by general results, a numerical method for obtaining graphs at any desired resolution, and further examples. We hope to thereby convey an impression of the kind of quantum structures that can be seen in this representation, and what intuitions might be based on it. Detailed proofs, more background, and further examples are provided in a companion paper [21]. A basic example, demonstrating that even in simple cases the Wigner function may display a lot of structure, is shown in Fig. 1.

When setting up a generalization of Wigner functions it is clear from the outset that the case of two canonical observables is special due to its high symmetry: phase space translations make every pair of values \((q,p)\) essentially the same. If we take two arbitrary observables \( A_1, A_2 \), even before selecting a particular state, we expect to see structures expressing the non-commutativity of the observables in a non-homogeneous way, so that certain value pairs \((a_1,a_2)\) may play a special role. Therefore,
definitions of the Wigner functions in terms of the phase space translations [22], or as the expectation of phase space reflections [7] do not generalize. The property that does generalize is the marginal property. We get the correct quantum mechanical probability distribution of any linear combination of the given operators by integrating the corresponding classical function against the Wigner function. Indeed, this completely fixes the Wigner distribution. No group, and no commutation relations, are needed for our generalization so that it applies also to finite dimensional systems. In this case all eigenvalues are discrete, so the marginal distributions to be considered will be sums of δ-functions. Necessarily, this will also make the Wigner function singular, so it will be a proper distribution (in the sense of “generalized function”) on \( \mathbb{R}^n \).

The marginal property for linear combinations of the \( A_k \) indicates that our definition might be especially helpful in contexts where all these linear combinations have an equally good physical interpretation. Apart from canonical observables this points to the case for angular momenta, where we get in this way the angular momentum components in arbitrary spatial directions (see Fig. 5). More generally, this points to Lie group representations, where the linear space of observables consists of the generators of all one-dimensional subgroups. However, the definition is not limited to these cases, and neither are the general properties.

**Definition.** Let \( A_1, \ldots, A_n \) be self-adjoint operators, which we assume to be bounded for simplicity of presentation[23]. Linear combinations with real coefficients \( \xi = (\xi_1, \ldots, \xi_n) \) are written as \( \xi \cdot A = \sum_k \xi_k A_k \).

When \( \rho \) is any density operator, we define the **Wigner distribution** by the equation

\[
\int da \, W_\rho(a_1, \ldots, a_n) \, f(\xi \cdot a) = \text{tr} \rho f(\xi \cdot A),
\]

for every bounded infinitely differentiable function \( f: \mathbb{R} \to \mathbb{C} \). If \( W_\rho \) were a probability density this would just equate the classical expectation of some function of the random variable \( \xi \cdot a \) with the quantum expectation of the same function, applied to the operator \( \xi \cdot A \). However, \( W_\rho \) is usually not a probability density, not just because it may be negative, but because it may be a generalized function/distribution. When we take \( f(t) = \exp(it) \) in (1) we directly get an expression for the Fourier transform \( \widehat{W}_\rho \) of \( W_\rho \), namely

\[
\widehat{W}_\rho(\xi) = \text{tr} pe^{i \xi \cdot A}.
\]

This fixes \( W_\rho \) uniquely as a tempered distribution. An alternative and equivalent definition [24] is in terms of operator ordering: The moments of \( W_\rho \) are equal to the **Weyl-ordered** moments of the operators \( A_k \), which are defined by averaging every product of the \( A_k \) over all possible orderings of the factors, and taking the expectation with respect to \( \rho \).

**Basic properties.** We note the following properties in addition to the marginal property (1). Proofs are given in [21].

1. \( W_\rho \) is real, i.e., equal to its complex conjugate distribution.

2. \( W_\rho \) has support in a compact convex set, the **joint numerical range** of the given operators:

\[
\mathcal{R} = \{ a \in \mathbb{R}^n \mid a_k = \text{tr} \rho A_k \},
\]

where \( \rho \) now runs over all density operators. That is, for all \( \rho \), \( W_\rho = 0 \) outside of \( \mathcal{R} \).

3. The singularities of \( W_\rho \) lie on the closure of the set

\[
\mathcal{S} = \{ a \in \mathbb{R}^n \mid a_k = \langle \psi | A_k | \psi \rangle ; \| \psi \| = 1, \xi \cdot A \psi = \lambda \psi \},
\]

where \( \lambda \) is a non-degenerate eigenvalue of some \( \xi \cdot A \). Outside \( \mathcal{S} \), \( W_\rho \) is given by an ordinary function, and \( W_\rho(a) \) for \( a \notin \mathcal{S} \) is given by the \( \rho \) expectation of a bounded operator. The convex hull of \( \mathcal{S} \) is \( \mathcal{R} \). For \( n = 2 \), \( \mathcal{S} \) is an algebraic curve known as Kippenhahn’s boundary generating curve [25–27].

4. When the \( A_k \) are **reducible**, i.e., commute with some hermitian \( B \neq \lambda I \), \( W_\rho \) is the sum of the Wigner distributions computed by projecting \( \rho \) to the eigenspaces of \( B \).
5. When the $A_k$ are finite dimensional matrices, and $ho$ has full rank, then $W_\rho$ is positive if and only if the $A_k$ commute, in which case $W_\rho$ is a sum of $\delta$-functions with $\rho$-dependent weights.

6. When $n = 2$ and $A_1$ and $A_2$ nearly commute, i.e., are small perturbations of a commuting pair, the $\delta$-peaks of the previous item become approximate, and are connected by singular ellipses. These can be computed to first order by restricting all operators to the two-dimensional eigenspace spanned by the eigenvectors of the commuting pair belonging to the two points. This is illustrated in Fig. 4.

7. $W$ is covariant for any symmetry acting on the $A_k$. That is, if $U$ is unitary such that $U^* A_k U = \sum_R R_{k\ell} A_\ell$ for some real coefficients $R_{k\ell}$, then $W_{U A_\ell'}(a) = W_\rho(R a)$. This is illustrated in Fig. 3.

8. For $n \geq 3$ the Wigner distribution is generically informationally complete, i.e., one can reconstruct $\rho$ uniquely from $W_\rho$. This also holds when the $A_k$ span the Lie algebra of an irreducible representation (like the angular momentum operators). However, it always fails in finite dimension for $n = 2$, because density operators $\rho, \rho'$ with $\rho - \rho' = i\lambda [A_1, A_2^\sigma]$ have the same Wigner distribution.

Computation and Visualization.— It may seem that a proper distribution is not suitable for visualization, because $W_\rho(a)$ is not even defined pointwise for every $a$. However, as for all function plots, one needs to specify a resolution $\varepsilon$ for the independent variable. If we take the convolution of $W_\rho$ with a Gaussian $G_\varepsilon$ peaked at the origin with small covariance $\varepsilon$, we still get a good qualitative picture. The resulting density $W_\rho * G_\varepsilon$ will not have exactly the correct marginal distributions, but instead each marginal will appear convolved with a peaked Gaussian as well (see Fig. 1). The regularized Wigner function $W_\rho * G_\varepsilon$ is readily computed by multiplying (2) with a slowly decaying Gaussian $G_\varepsilon$ before taking the inverse Fourier transform, which then converges reasonably well. All pictures in this paper were generated in this way.

Qubits.— Not surprisingly, when the Hilbert space is two-dimensional, we can compute the Wigner function explicitly. Taking more than three operators is not interesting, because they would become linearly independent and, by property 2, $W_\rho$ would just live on the corresponding hyperplane. Up to an affine transformation any basis of the hermitian operators will give the same Wigner functions. So we choose $A_k = \sigma_k$, $k = 1, 2, 3$ to be the Pauli matrices. Then the case of general $\rho$ is reduced to the case $\rho = I$ by differentiation, and $W_I$ is easily evaluated because it is radially symmetric. The overall result

\[
W_{\rho}(a) = \left( r_0 + r \cdot a \right) \frac{1}{\pi} \delta'(|a| - 1). \tag{5}
\]

This vanishes exactly in the interior of the Bloch ball. The $\delta'$-singularity produces with Gaussian regularization a sharp positive wall-like peak on the outside and a negative one on the inside of the Bloch sphere. This is also typical for the other graphs shown. The case with just two Pauli matrices $(A_1, A_2) = (\sigma_1, \sigma_2)$ was considered in [19]. It arises from (5) by integrating out the $a_3$-variable. This function does not vanish exactly inside the unit circle. In spite of the expression given in [19] the distribution cannot be split into two terms, of which one is given by an ordinary function inside the unit circle, and the
FIG. 5. Color online. Wigner function of angular momentum components $L_x$ and $L_y$ for spin $s = 4$, depicted for the maximally mixed state, the $j_x = 0$ and the $j_x = 4$ eigenstate. The Wigner function of the maximally mixed state shares the full rotational symmetry. The Wigner function of the $j_x = 0$ state has only reflection symmetries on the $x = 0$ and the $y = 0$ axis. The Wigner function of the $j_x = 4$ state is clearly concentrated in the $\langle L_x \rangle \geq 0$ region and has only a symmetry on the $y = 0$ axis.

other is purely singular on the circle. This is discussed in detail in [21]. From property 8 we see that the vertical coordinate in the Bloch ball cannot be retrieved from the Wigner function, i.e., $W_\rho = W_{\rho'}$ if $\rho' = \rho + \lambda \sigma_3$.

**Spins.**— The angular momentum operators are one of those case in which all linear combinations are equally relevant physical operators. It is this case which originally motivated us [28, Prop. 7]. In the spin-$s$ representation of SU(2), the singular manifold is the collection of concentric spheres of radius $\hbar m$ (see Fig. 5). Moreover, the operators $\exp(\mathbf{i} \mathbf{ξ} \cdot \mathbf{A})$ are just the unitaries of the group representation. Hence their linear span is an algebra, whose closure is dense by irreducibility of the representation. Hence $W_\rho$, and consequently $W_\rho$ determines $\rho$ uniquely. Further properties, including the classical limit, will be analysed in a future publication.

**Outlook.**— The Wigner distributions considered in this paper at first sight look very different from the usual ones (singular distributions vs bounded continuous functions). Since the definition is the same, just applied to different operators, this points to some special features of the case of canonical operators, to which we have become accustomed, and which make the case of canonical pairs special. The high phase space symmetry is certainly a key, but also the fact that all spectra are absolutely continuous, and hence less prone to producing singularities. Of course, in this initial exploration we focused on the singularities as the most conspicuous feature. But it would be interesting to consider intermediate cases.

In this regard it would be interesting to see if some of the group-based distribution functions can be retrieved by integration. For example, for an angle variable $\phi$ one can avoid artificial branch cuts by considering the two hermitian operators $(\cos \phi, \sin \phi)$ (e.g., [17]). The joint distributions of this pair with a momentum or number variable would probably produce some distribution away from the unit circle, but a radial integration in the plane would eliminate that, while retaining the overall symmetry of the problem.

Another question is posed by the simple form in the qubit case: Can $W_\rho$ maybe be written as a non-singular factor times the distribution $W_1$, which depends only on the observables chosen? This separation of a factor coming from the observables and a factor coming from the state, even if the factors were combined in a slightly more complicated way, would be very useful. A related open question is the development of simple inversion formulas, for example in the case of spins.

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