Some nonclassical features of phase-space representations of quantum mechanics*

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It is shown that phase-space distribution functions that characterize a single-particle quantum system obey a certain "generalized non-negativity condition," which reflects the fact that the density operator is a positive operator. A corresponding criterion is obtained for the associated characteristic functions and is found to resemble, to some extent, Bochner's theorem of classical probability theory. Necessary and sufficient conditions on a phase-space representation of quantum mechanics are also derived, which ensure that all the possible distribution functions in that representation are non-negative; but it is also shown that such distribution functions are not joint probabilities for position and momentum. In fact, our results readily provide a new proof of theorems of Wigner, and of Cohen and Margenau, which imply that quantum mechanics cannot be formulated as a stochastic theory in phase space.

I. INTRODUCTION

The possibility of expressing the quantum mechanical expectation values as averages over phase-space distribution functions has been widely discussed (see, for example, Refs. 1–7). It is well known that a correspondence between quantum states and phase-space distributions is generated by a rule of association between operators and c-number functions. These distribution functions are often called "quasiprobabilities," as they do not possess all the attributes of ordinary probabilities. In particular, they are not non-negative in general. The fact that they may become negative has been taken as the distinguishing feature of such quantum distribution functions. However, non-negative distribution functions have also been discussed in the literature,[8-11] for example in the so-called "antinormal correspondence" between operators and c numbers.[10] But they too are not true joint probability distributions for position and momentum. This is clear from a result due to Wigner[1,12] that "if one imposes the condition that the distribution function yields the usual marginal probabilities, in addition to the requirements such as reality, and linear association, then one cannot avoid negative probabilities, in general."

In this investigation we first analyze the role of a non-negativity requirement on the distribution functions, in a general phase-space formulation of quantum mechanics. In such a formulation, the non-negativity requirement that is imposed on the classical distribution function is shown to be replaced by a "generalized non-negativity requirement" which reflects the fact that the density operator is a positive operator. Using this generalized non-negativity requirement we will elucidate the general conditions that completely characterize a quantum distribution function in phase space. The corresponding result for the characteristic function is similar to Bochner's theorem in classical probability theory.[13] Then the necessary and sufficient condition on a phase-space representation of quantum mechanics is obtained, which ensures that all the possible distribution functions in this representation are non-negative. We will see that there is a large class of such phase-space representations. Using the condition for non-negative distribution functions, we will also give an alternative proof of Wigner's theorem, to which we referred earlier.

In the last section of this paper, we discuss briefly the connection between our results and results of Wigner,[1,12] Cohen,[14,15] and Margenau and Cohen,[16] which demonstrate that quantum mechanics cannot be formulated as a classical stochastic theory in phase space.

II. PHASE-SPACE REPRESENTATIONS OF QUANTUM MECHANICS

We begin with a brief review of the phase-space representations of quantum mechanics as formulated by Agarwal and Wolf[7] and indicate a certain generalization of it.

A natural requirement on any phase-space representation of quantum mechanics is that it be a linear one-to-one mapping of operators on a Hilbert space into c-number functions. We will restrict our considerations to the single-particle case, and hence our observables will be functions of the usual position and momentum operators, acting on the space of square-integrable functions. Because of the one-to-one nature of the representative mapping, we may characterize it by the inverse correspondence which associates operators with c-number functions in phase space. Now any square-integrable function $g(q, p)$ can be represented by a Fourier integral:

$$g(q,p)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\gamma(\xi,\eta)\,e^{i(\xi q+\eta p)}\,d\xi\,d\eta\ . \tag{2.1}$$

Because of the linearity of the correspondence, the phase-space representation can be completely specified by the operator associated with the exponential function $\exp[i(\xi q+\eta p)]$. All the well-known correspondences are particular cases of what might be called the Ω rules of association. These are associations of the form [a caret (^) denotes an operator]

$$e^{i(\xi q+\eta p)}\rightarrow\Omega(\xi,\eta)\,e^{i(\xi\hat{q}+\eta\hat{p})}\ . \tag{2.2}$$

Thus, the operator $\hat{g}(\hat{q},\hat{p})$ corresponding to the function $g(q,p)$ is given by

$$\hat{g}(\hat{q},\hat{p})=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\gamma(\xi,\eta)\,\Omega(\xi,\eta)\,e^{i(\xi\hat{q}+\eta\hat{p})}\,d\xi\,d\eta\ . \tag{2.3}$$

We have the inverse mapping

$$g(q,p)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathrm{Tr}(\hat{g}\,e^{-i(\xi\hat{q}+\eta\hat{p})})\times[\Omega(\xi,\eta)]^{-1}\,e^{i(\xi q+\eta p)}\,d\xi\,d\eta\ . \tag{2.4}$$

Usually it is assumed that $\Omega(\xi,\eta)$ is the boundary value of an entire analytic function in two complex variables, and has no zeros for real values ξ,η. Other conditions imposed on $\Omega(\xi,\eta)$ are

$$\Omega(0,0)=1\ , \tag{2.5}$$

and

$$\Omega^*(\xi,\eta)=\Omega(-\xi,-\eta)\ , \tag{2.6}$$

where the asterisk denotes the complex conjugate. Equation (2.5) ensures that unity is mapped onto the unit operator. Equation (2.6) is the "reality condition" ensuring that real functions are mapped onto self-adjoint operators and vice versa. In Table I we list the explicit form of the function $\Omega(\xi,\eta)$ for some of the well-known rules of association.

We can discuss more general representations by considering the set of representation operators $\Delta(\hat{q},\hat{p};q,p)$ onto which the Dirac δ function is mapped:

$$\delta(q-q')\,\delta(p-p')\rightarrow\Delta(\hat{q},\hat{p};q',p')\ , \tag{2.7}$$

for all q',p'. Then (retaining the assumption of linear mapping), the operator $\hat{g}$ corresponding to the function $g(q,p)$ will be given by

$$\hat{g}(\hat{q},\hat{p})=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}g(q',p')\,\Delta(\hat{q},\hat{p};q',p')\,dq'\,dp'\ . \tag{2.8}$$

The one-to-one nature of a representation mapping demands the existence of a family of operators $\overline{\Delta}(\hat{q},\hat{p};q,p)$ orthogonal to $\Delta(\hat{q},\hat{p};q',p')$, i.e., such that

$$\mathrm{Tr}[\overline{\Delta}(\hat{q},\hat{p};q,p)\,\Delta(\hat{q},\hat{p};q',p')]=\delta(q-q')\,\delta(p-p')\ . \tag{2.9}$$

From (2.8) and (2.9), we deduce that

$$g(q,p)=\mathrm{Tr}[\hat{g}(\hat{q},\hat{p})\,\overline{\Delta}(\hat{q},\hat{p};q,p)]\ . \tag{2.10}$$

The requirement that the "identity function," $g(q,p)\equiv1$, is mapped onto the unit operator implies that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Delta(\hat{q},\hat{p};q,p)\,dq\,dp=\hat{1}\ , \tag{2.11}$$

and the "reality condition" implies that the operator Δ is self-adjoint, i.e.,

$$\Delta^{\dagger}(\hat{q},\hat{p};q,p)=\Delta(\hat{q},\hat{p};q,p)\ . \tag{2.12}$$

It should be clear that a general representation in phase space is completely characterized by the two-parameter family of representation operators $\Delta(\hat{q},\hat{p};q,p)$ which satisfy Eqs. (2.7), (2.9), (2.11), and (2.12). The operator $\overline{\Delta}(\hat{q},\hat{p};q,p)$ orthogonal to $\Delta(\hat{q},\hat{p};q',p')$ can also be shown to be Hermitian and satisfies the relation

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\overline{\Delta}(\hat{q},\hat{p};q,p)\,dq\,dp=\{\mathrm{Tr}[\Delta(\hat{q},\hat{p};q,p)]\}^{-1}=1/C\ , \tag{2.13}$$

where C is a constant. Thus, one can define a representation "conjugate" to the original representation, via the correspondence

$$\delta(q-q')\,\delta(p-p')\rightarrow\tilde{\Delta}(\hat{q},\hat{p};q',p')\ , \tag{2.14}$$

where

$$\tilde{\Delta}(\hat{q},\hat{p};q',p')=C\,\overline{\Delta}(\hat{q},\hat{p};q',p')\ .$$

It is clear that $\tilde{\Delta}(\hat{q},\hat{p};q',p')$ satisfies Eqs. (2.7), (2.9), (2.11), and (2.12) and thus defines a representation.

The orthogonality relation (2.9) leads to the general result that for any two operators $\hat{A}$ and $\hat{B}$

TABLE I. The explicit form of the function $\Omega(\xi,\eta)$ for some of the well-known rules of association. In the table $z=(q+ip)/\sqrt{2}$, $z^*=(q-ip)/\sqrt{2}$, $\hat{a}=(\hat{q}+i\hat{p})/\sqrt{2}$, and $\hat{a}^{\dagger}=(\hat{q}-i\hat{p})/\sqrt{2}$.

$\Omega(\xi,\eta)$	Rule of association	Example
1	Wigner-Weyl	$p^2q\longleftrightarrow\frac{1}{3}(\hat{p}^2\hat{q}+\hat{p}\hat{q}\hat{p}+\hat{q}\hat{p}^2)$
$\cos[\xi\eta/2]$	Symmetric	$p^2q\longleftrightarrow\frac{1}{2}(\hat{p}^2\hat{q}+\hat{q}\hat{p}^2)$
$\exp[(\xi^2+\eta^2)/4]$	Normal	$z^2z^*\longleftrightarrow\hat{a}^{\dagger}\hat{a}^2$
$\exp[-(\xi^2+\eta^2)/4]$	Antinormal	$z^2z^*\longleftrightarrow\hat{a}^2\hat{a}^{\dagger}$

$$\mathrm{Tr}(\hat{A}\hat{B}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{Tr}[\hat{A}\,\Delta(\hat{q},\hat{p};q,p)] \times \mathrm{Tr}[\hat{B}\,\bar{\Delta}(\hat{q},\hat{p};q,p)]\,dq\,dp\ . \quad (2.15)$$

The result expressed by Eq. (2.15) forms the basis for the representation of quantum-mechanical expectation values as averages with respect to a phase-space distribution function. For example, the expectation value of any operator $\hat{A}$ may be expressed as

$$\langle \hat{A}\rangle = \mathrm{Tr}(\hat{\rho}\hat{A}) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(q,p)A(q,p)\,dq\,dp\ , \quad (2.16)$$

where

$$A(q,p) = \mathrm{Tr}[\hat{A}\,\bar{\Delta}(\hat{q},\hat{p};q,p)]$$

is the phase-space representative of operator $\hat{A}$ in the "Δ representation" and the corresponding phase-space distribution function $f(q,p)$ is given by

$$f(q,p) = \mathrm{Tr}[\hat{\rho}\,\Delta(\hat{q},\hat{p};q,p)]\ . \quad (2.17)$$

Thus, every representation associates a phase-space distribution function with each density operator. The reality of the distribution function, viz.,

$$f^*(q,p) = f(q,p)\ , \quad (2.18)$$

and the normalization

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(q,p)\,dq\,dp = 1 \quad (2.19)$$

follow directly from Eqs. (2.12) and (2.11) and the corresponding properties of the density operator:

$$\hat{\rho}^\dagger = \hat{\rho}\ , \quad (2.20)$$

$$\mathrm{Tr}\hat{\rho} = 1\ . \quad (2.21)$$

However, these quantum distribution functions need not obey the non-negativity condition $f(q,p) \geq 0$, as do the distributions of classical statistical mechanics. We can derive a "generalized non-negativity" requirement, using the fact that the density operator $\hat{\rho}$ must be a positive operator, i.e., that

$$\langle\psi|\hat{\rho}|\psi\rangle \geq 0\ , \quad (2.22)$$

for any state vector $|\psi\rangle$. This requirement is equivalent to the condition that

$$\langle \hat{A}^\dagger\hat{A}\rangle = \mathrm{Tr}(\hat{\rho}\hat{A}^\dagger\hat{A}) \geq 0\ , \quad (2.23)$$

where $\hat{A}$ is any operator of the Hilbert-Schmidt class. We will show in the next section that Eq. (2.23) leads to a "generalized non-negativity" requirement on $f(q,p)$ and also on the quantum characteristic function.

III. "GENERALIZED NON-NEGATIVITY REQUIREMENT" ON QUANTUM DISTRIBUTION FUNCTIONS AND THE ASSOCIATED CHARACTERISTIC FUNCTIONS

In this section we will restrict ourselves mainly to representations generated by the Ω rules of association, defined at the beginning of Sec. II. For the Ω rules of association, the representation operators $\Delta_\Omega(\hat{q},\hat{p};q,p)$ are given by[7(a)]

$$\Delta_\Omega(\hat{q},\hat{p};q,p) = (1/2\pi)^2 \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i[\xi(\hat{q}-q)+\eta(\hat{p}-p)]} \times \Omega(\xi,\eta)\,d\xi\,d\eta\ , \quad (3.1a)$$

and

$$\bar{\Delta}_\Omega(\hat{q},\hat{p};q,p) = 2\pi\,\Delta_{\tilde{\Omega}}(\hat{q},\hat{p};q,p)\ , \quad (3.1b)$$

where

$$\tilde{\Omega}(\xi,\eta) = [\Omega(-\xi,-\eta)]^{-1}\ .$$

From (3.1a) we note, on taking the trace, that

$$\mathrm{Tr}[\Delta_\Omega(\hat{q},\hat{p};q,p)] = 1/2\pi\ . \quad (3.2)$$

In classical probability theory, the characteristic function, associated with a joint probability distribution of two random variables p, q, is defined as the expectation value of $e^{i(\xi q+\eta p)}$. Recalling the correspondence (2.2) we may define the characteristic function in the Ω rule of correspondence, for a single-particle quantum system, as

$$M_\Omega(\xi,\eta) = \Omega(\xi,\eta)\,M(\xi,\eta)\ , \quad (3.3a)$$

where

$$M(\xi,\eta) = \langle e^{i(\xi\hat{q}+\eta\hat{p})}\rangle\ . \quad (3.3b)$$

Since $M_\Omega(\xi,\eta) = M(\xi,\eta)$ when $\Omega(\xi,\eta) \equiv 1$, $M(\xi,\eta)$ is the characteristic function in the Wigner-Weyl correspondence (see Table I).

The following properties of the characteristic function may readily be established:

(i) $M_\Omega(0,0) = 1\ ,$ (3.4)

(ii) $M_\Omega^*(\xi,\eta) = M_\Omega(-\xi,-\eta)\ .$ (3.5)

Moreover,

(iii) $M_\Omega(\xi,\eta)$ is continuous.

The property (iii) follows from (3.3a) if we use the fact that the Wigner-Weyl characteristic function $M(\xi,\eta)$ itself is continuous,[17,18] and recall that $\Omega(\xi,\eta)$ is the boundary value of an entire analytic function in two complex variables.

In order to transcribe the positivity condition (2.23) as a requirement on the characteristic function, we use the result that any Hilbert-Schmidt operator $\hat{A}$ has a "Fourier" representation[19]

$$\hat{A} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \alpha(\xi,\eta)\,e^{i(\xi\hat{q}+\eta\hat{p})}\,d\xi\,d\eta\ , \quad (3.6)$$

where $\alpha(\xi,\eta)$ is a square-integrable function. Hence, since according to Eq. (2.23), $\langle \hat{A}^\dagger \hat{A}\rangle \geq 0$, it follows that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \alpha^*(\xi_1,\eta_1)\,\alpha(\xi_2,\eta_2)\,e^{-i\hbar(\xi_1\eta_2-\xi_2\eta_1)/2}\langle e^{i[(\xi_2-\xi_1)\hat{q}+(\eta_2-\eta_1)\hat{p}]}\rangle\, d\xi_1\,d\eta_1\,d\xi_2\,d\eta_2 \geq 0. \tag{3.7}$$

Clearly, (3.7) has to be satisfied for all square-integrable functions $\alpha(\xi,\eta)$. This implies the "generalized non-negative–definiteness requirement"

$$\text{(iv)}\ \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \alpha^*(\xi_1,\eta_1)\,\alpha(\xi_2,\eta_2)\,e^{-i\hbar(\xi_1\eta_2-\xi_2\eta_1)/2} \times[\Omega(\xi_2-\xi_1,\eta_2-\eta_1)]^{-1} M_\Omega(\xi_2-\xi_1,\eta_2-\eta_1)\,d\xi_1\,d\eta_1\,d\xi_2\,d\eta_2 \geq 0\ , \tag{3.8}$$

for all square-integrable functions $\alpha(\xi,\eta)$. Thus, we have established the following result:

Theorem 1. A quantum characteristic function in any Ω representation is completely characterized by the conditions[20] (i)–(iv).

The condition (3.8) can be equivalently written in the discrete form as

$$\sum_{j=1}^{N}\sum_{k=1}^{N} z_j^* z_k\, e^{-i\hbar(\xi_j\eta_k-\xi_k\eta_j)/2}[\Omega(\xi_k-\xi_j,\eta_k-\eta_j)]^{-1} \times M_\Omega(\xi_k-\xi_j,\eta_k-\eta_j)\geq 0\ , \tag{3.9}$$

for arbitrary non-negative integer N, arbitrary set of pairs of real numbers $\{(\xi_r,\eta_r)\}$, and any set of complex numbers $\{z_r\}$.

We can contrast this "generalized non-negative–definiteness requirement" with the usual non-negative–definiteness requirement

$$\text{(iv}')\ \sum_{j=1}^{N}\sum_{k=1}^{N} z_j^* z_k\, M(\xi_k-\xi_j,\eta_k-\eta_j)\geq 0 \tag{3.10}$$

on the characteristic functions in classical probability theory,[13] which arises from the non-negativity of the distribution function. That the conditions (i), (ii), (iii), and (iv′) are obeyed by all classical characteristic functions is embodied in a well-known theorem (essentially due to Bochner) in classical probability theory. It is clear now that a similar result holds for the quantum characteristic functions in phase space, provided that the condition (iv′) [Eq. (3.10)] is replaced by the condition (iv) [Eq. (3.9)].

The "generalized non-negative–definiteness requirement" (3.9) on the characteristic function can also be expressed in terms of the quantum phase-space distribution function itself. We will establish this result here for a general Δ representation (as we already noted, Ω representations are special cases of it) using the following "product theorem," established in the Appendix:

Theorem 2 (product theorem). If $g(q,p)$ and $h(q,p)$ are the phase-space functions representing the operators $\hat{g}(\hat{q},\hat{p})$ and $\hat{h}(\hat{q},\hat{p})$, respectively, then the phase-space function that represents the product $\hat{g}(\hat{q},\hat{p})\hat{h}(\hat{q},\hat{p})$, which we denote by $g(q,p)\otimes h(q,p)$, is given by

$$g(q,p)\otimes h(q,p)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} R(q,p;q_1,p_1,q_2,p_2)\,g(q_1,p_1)\,h(q_2,p_2)\,dq_1\,dp_1\,dq_2\,dp_2\ , \tag{3.11}$$

where

$$R(q,p;q_1,p_1,q_2,p_2)=\mathrm{Tr}[\Delta(\hat{q},\hat{p};q_1,p_1)\,\Delta(\hat{q},\hat{p};q_2,p_2)\,\overline{\Delta}(\hat{q},\hat{p};q,p)]\ . \tag{3.12}$$

With the help of this product theorem we may at once transcribe the positivity condition (2.23) into phase space and obtain the following "generalized non-negativity requirement" on the quantum distribution function:

Theorem 3. If $f(q,p)$ is the phase-space distribution function of a single-particle quantum system in a Δ representation, then

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}[A^*(q,p)\otimes A(q,p)]f(q,p)\,dq\,dp\geq 0\ , \tag{3.13}$$

where $A(q,p)$ is an arbitrary function of q and p.

The function $A(q,p)$ in (3.13) is, of course, the phase-space representative of the operator $\hat{A}(\hat{q},\hat{p})$, which enters the positivity condition (2.23) on the density operator.

IV. CONDITION FOR NON-NEGATIVE QUANTUM PHASE DISTRIBUTION FUNCTIONS

We have already seen that for a general "Δ representation" the phase-space distribution function corresponding to the density operator $\hat{\rho}$ is given by

$$f(q,p)=\mathrm{Tr}[\hat{\rho}\,\Delta(\hat{q},\hat{p};q,p)] \ . \tag{4.1}$$

We have also seen that one has to impose the conditions

$$\Delta^{\dagger}(\hat{q},\hat{p};q,p)=\Delta(\hat{q},\hat{p};q,p) \ , \tag{4.2}$$

and

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Delta(\hat{q},\hat{p};q,p)\,dq\,dp=1 \ . \tag{4.3}$$

Let us now impose the condition that all the distributions that arise in the representation should be non-negative, i.e., that for all values of q and p

$$f(q,p)\geq 0 \ . \tag{4.4a}$$

Equation (4.4a), implies, according to (4.1), that

$$\langle\,\Delta(\hat{q},\hat{p};q,p)\rangle\geq 0 \ , \tag{4.4b}$$

for all states. Thus, the necessary and sufficient condition for all the distributions to be non-negative is that $\Delta(\hat{q},\hat{p};q,p)$ be a positive operator. But by (2.12) and (2.13), $\Delta(\hat{q},\hat{p};q,p)$ is a self-adjoint operator with constant trace C and hence, $\Delta(\hat{q},\hat{p};q,p)/C$ satisfies, for every q and p, all the properties of a density operator. Thus, we have established the following general result:

Theorem 4. The necessary and sufficient condition that a phase-space representation, characterized by the set of operators $\Delta(\hat{q},\hat{p};q,p)$, induces distribution functions that for any state are non-negative is that for each q and p, the operator $\Delta(\hat{q},\hat{p};q,p)$ be proportional to a density operator, the proportionality constant being independent of q and p.

We will elucidate the above result by simple examples. For the antinormal rule of correspondence, we have[7(a)]

$$\Delta(\hat{q},\hat{p};q,p)=\frac{1}{2\pi}\,|q,p\rangle\langle q,p| \ , \tag{4.5}$$

i.e., $\Delta(\hat{q},\hat{p};q,p)$ is the projection operator onto the coherent state labeled by the complex number $z=(q+ip)/\sqrt{2}$, and thus, for each (q,p), is the density operator of a pure state. It is also clear that we obtain non-negative distribution functions if our representation operator is the projection operator onto the so-called generalized coherent state[21]

$$|q,p\rangle_U=U|q,p\rangle \ , \tag{4.6a}$$

where U is a unitary operator. We define the corresponding representation by the representation operator

$$\Delta(\hat{q},\hat{p};q,p)=\frac{1}{2\pi}\,|q,p\rangle_U\,{}_U\langle q,p| \ , \tag{4.6b}$$

and it is obvious that the condition of Theorem 4 is satisfied in this case, so that the distribution function in such a representation, viz.,

$$f(q,p)=\frac{1}{2\pi}\,{}_U\langle q,p|\rho|q,p\rangle_U \ , \tag{4.7}$$

is necessarily non-negative.

We can now use the general result expressed by Theorem 4 to find all the Ω representations which lead to non-negative distributions.

Let $\Delta_\Omega(\hat{q},\hat{p};q,p)$ denote, as before, the representation operator of an Ω representation. Then it follows at once from Theorem 4 and from Eq. (3.2) that this representation will give rise to non-negative distribution functions, provided that for every q and p, $2\pi\Delta_\Omega(\hat{q},\hat{p};q,p)$ is a density operator. According to (3.1a),

$$\Delta_\Omega(\hat{q},\hat{p};q,p)=\left(\frac{1}{2\pi}\right)^2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{i[\xi(\hat{q}-q)+\eta(\hat{p}-p)]}\times\Omega(\xi,\eta)\,d\xi\,d\eta \ .$$

We have also the identity

$$e^{i[\xi(\hat{q}-q)+\eta(\hat{p}-p)]}=\hat{D}^{\dagger}(q,p)\,e^{i(\xi\hat{q}+\eta\hat{p})}\,\hat{D}(q,p) \ , \tag{4.8}$$

where

$$\hat{D}(q,p)=e^{-i(p\hat{q}-q\hat{p})} \tag{4.9}$$

is the unitary translation operator. The relation (4.8) can readily be established by using the Baker-Hausdorff identity.[22] Using Eqs. (3.1a) and (4.8), we obtain the formula

$$\Delta_\Omega(\hat{q},\hat{p};q,p)=\hat{D}^{\dagger}(q,p)\,\Delta_\Omega(\hat{q},\hat{p};0,0)\,\hat{D}(q,p) \ . \tag{4.10}$$

Since $\hat{D}(q,p)$ is a unitary operator, we conclude that in order that $2\pi\Delta_\Omega(\hat{q},\hat{p};q,p)$ be a density operator for every q and p, it is necessary and sufficient that $2\pi\Delta_\Omega(\hat{q},\hat{p};0,0)$ be a density operator. Hence, for an Ω representation to yield only non-negative distribution functions, it is necessary and sufficient that

$$2\pi\Delta_\Omega(\hat{q},\hat{p};0,0)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Omega(\xi,\eta)\,e^{i(\xi\hat{q}+\eta\hat{p})}\,d\xi\,d\eta$$

be a density operator. It is immediately seen from (3.3b) that the Wigner-Weyl characteristic function of this state coincides with the function $\Omega(\xi,\eta)$. Thus, we have established the following:

Theorem 5. The necessary and sufficient condition for all the distribution functions in an Ω representation to be non-negative is that $\Omega(\xi,\eta)$ be the Wigner-Weyl characteristic function of some quantum state.

If $\Omega(\xi,\eta)$ is the Wigner-Weyl characteristic function of a pure state, all the operators $2\pi\Delta_\Omega(\hat{q},\hat{p};q,p)$ will be pure-state projection operators. If $\Omega(\xi,\eta)$ is the Wigner-Weyl characteristic function of a mixture, all the operators $2\pi\Delta_\Omega(\hat{q},\hat{p};q,p)$ will be density operators representing mixed states. The usual conditions imposed on $\Omega(\xi,\eta)$, such as those expressed by Eqs. (2.5) and (2.6) and the requirement of analyticity show that $\Omega(\xi,\eta)$ is already chosen to satisfy conditions (i), (ii), and (iii) for a quantum characteristic function. Thus, the condition of Theorem 5 that $\Omega(\xi,\eta)$ be a Wigner-Weyl characteristic is that for arbitrary non-negative integer N, any set of pairs of real numbers $\{(\xi_r,\eta_r)\}$ and any set of complex numbers $\{z_r\}$,

$$\sum_{j=1}^{N}\sum_{k=1}^{N} z_j^* z_k e^{-i\hbar(\xi_j\eta_k-\xi_k\eta_j)/2}\,\Omega(\xi_k-\xi_j,\eta_k-\eta_j)\geq 0 \;. \tag{4.11}$$

This condition is automatically satisfied, for example, for the case of antinormal rule of association, where

$$\Omega(\xi,\eta)=\exp[-\tfrac{1}{4}(\xi^2+\eta^2)] \;.$$

It is also clear that one can construct many other examples of Ω representations with non-negative distribution functions.

V. NONCLASSICAL FEATURES OF PHASE-SPACE REPRESENTATIONS OF QUANTUM MECHANICS

The results of the previous section provide us with a large class of representations which lead to distribution functions that are non-negative. However, as we will now show, these distribution functions cannot be joint probability distributions for the noncommuting observables $\hat{q}$ and $\hat{p}$.

In a search for joint distributions, one may proceed along the lines of classical probability theory, using the relation between the joint probability distribution of the random variables X and Y and the distributions of the linear combination $\lambda X+\mu Y$. Then one could consider the Wigner distribution function, obtained as the Fourier transform of $\langle\exp[i(\xi\hat{q}+\eta\hat{p})]\rangle$. Since the Wigner distribution function will, in general, take on negative values, an attempt can be made to circumvent this by noting that there is an ambiguity in the definition of functions of noncommuting operators $\hat{q}$, $\hat{p}$, and consider differently ordered exponential forms. The existence of different phase-space representations of a quantum system was noted by Wigner already in his basic paper.[1] However, in the same paper he stated and later[12] published the proof of a theorem that shows that it is impossible to obtain proper joint distribution functions by any such generalization. More precisely, Wigner's theorem may be stated (in our notation), essentially as follows:

Theorem 6 (Wigner's theorem[1,12]). There is no phase-space representation of quantum mechanics which satisfies all the following three requirements.

(i) The distribution function $f(q,p)$ is the expectation value of a self-adjoint operator $\Delta(\hat{q},\hat{p};q,p)$, i.e.,

$$f(q,p)=\mathrm{Tr}[\hat{\rho}\Delta(\hat{q},\hat{p};q,p)] \;; \tag{5.1}$$

(ii)

$$f(q,p)\geq 0 \;; \tag{5.2}$$

and

(iii) it gives correct quantum-mechanical marginal probabilities

$$\int_{-\infty}^{\infty} f(q,p)\,dp=\langle q|\hat{\rho}|q\rangle \,,\qquad \int_{-\infty}^{\infty} f(q,p)\,dq=\langle p|\hat{\rho}|p\rangle \,. \tag{5.3}$$

In establishing this theorem, Wigner pointed out that the same result holds if requirement (iii) is replaced by a milder requirement (iii′), namely, the following.

(iii′) The operator that corresponds to a phase-space function of the form $A(q)+B(p)$, where $A(q)$ and $B(p)$ are arbitrary functions of their arguments, is $A(\hat{q})+B(\hat{p})$.

We will now show that Wigner's theorem, in this stronger form, follows readily from our analysis. First we note that requirement (i) is nothing but our representation requirement; it takes care of the linearity and the reality requirements.

Requirement (ii) implies, according to Theorem 4, that for all q and p $\Delta(\hat{q},\hat{p};q,p)/C$ (where C is a constant) is a density operator.

Considering functions of q alone we have from (2.8) and the requirement (iii′)

$$A(\hat{q})=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}A(q')\Delta(\hat{q},\hat{p};q',p')\,dq'\,dp' \,. \tag{5.4}$$

Taking the expectation value of both the sides of (5.4), in a state $|q\rangle$, we obtain

$$A(q)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}A(q')\langle q|\Delta(\hat{q},\hat{p};q',p')|q\rangle\,dq'\,dp' \,. \tag{5.5}$$

Since (5.5) holds for any arbitrary function $A(q)$, we conclude that

$$\langle q|\Delta(\hat{q},\hat{p};q',p')|q\rangle=\delta(q-q')\alpha(p') \,, \tag{5.6a}$$

where

$$\int_{-\infty}^{\infty} \alpha(p')dp' = 1.$$

Similarly, considering functions $B(p)$ of p alone, and imposing the requirement (iii′), we obtain

$$\langle p|\Delta(\hat{q},\hat{p};q',p')|p\rangle = \delta(p-p')\beta(q'), \tag{5.6b}$$

where

$$\int_{-\infty}^{\infty} \beta(q')dq' = 1.$$

Thus, requirements (i), (ii), and (iii′) together imply that each member of the family of density operators $\Delta(\hat{q},\hat{p};q',p')/C$ has the marginal distributions $[\alpha(p')/C]\delta(q-q')$ in the configuration space, and $[\beta(q')/C]\delta(p-p')$ in the momentum space. However, the existence of a density operator with this property would clearly violate the uncertainty principle, and hence we conclude that there is no phase-space representation that satisfies all the three requirements (i), (ii), and (iii′). Since (iii) implies (iii′), it follows that there is no phase-space representation that satisfies all the requirements (i), (ii), and (iii), in agreement with Wigner's theorem.

Wigner's theorem clearly shows that quantum mechanics cannot be formulated as a classical stochastic theory. The same conclusion was also reached by Cohen[14] (see also Cohen[15] and Margenau and Cohen[16]). They demonstrated that every phase-space representation of quantum mechanics that satisfied the requirements (i) and (iii) of Theorem 6 necessarily violates yet another basic principle of classical stochastic theory that is embodied in the following requirement:

(iv) If $g(q,p)$ is the phase-space representative that is used to calculate the expectation values of an operator $\hat{g}(\hat{q},\hat{p})$, then $K[g(q,p)]$ will be the phase-space representative that gives the expectation values of $K[\hat{g}(\hat{q},\hat{p})]$, where K is an arbitrary function.

We will use our earlier results to provide another proof of Cohen's theorem which can be stated as follows:

Theorem 7 (Cohen[14]). There is no phase-space representation of quantum mechanics that satisfies the three requirements (i), (iii), and (iv). In other words, there is no linear one-to-one representation of quantum mechanics which satisfies the marginal probability condition as well as the requirement (iv).

We will prove Theorem 7 by showing that if all the three requirements (i), (iii), and (iv) were to hold, a contradiction would result.

From Wigner's theorem (Theorem 6), it is clear that if conditions (i) and (iii) are satisfied, then the condition (ii) must be violated; i.e., the phase-space distribution function $f(q,p)$ cannot be non-negative for all states.

Consider now a special case of the requirement expressed by Cohen's condition (iv), with $K[\hat{g}]=\hat{g}^2$, where $\hat{g}$ is a self-adjoint operator, i.e., we require that if the operator $\hat{g}(\hat{q},\hat{p})$ is represented by the c-number function $g(q,p)$, then $[\hat{g}(\hat{q},\hat{p})]^2$ should be represented by $g^2(q,p)$. Since our Theorem 2 implies that the phase-space function corresponding to the operator $[\hat{g}(\hat{q},\hat{p})]^2$ is given by $g(q,p)\otimes g(q,p)$, where $\otimes$ is the nonlocal phase-space product defined by (3.11) and (3.12), condition (iv) demands, in this case, that

$$g(q,p)\otimes g(q,p) = g^2(q,p), \tag{5.7}$$

for any function $g(q,p)$. Now we can use Eq. (5.7) in conjunction with the "generalized positivity condition" on the phase-space distribution function, expressed by Eq. (3.13) (a condition that is valid in any representation, as it just reflects the positivity of the density operator). We then obtain, if we recall that $\hat{g}$ is Hermitian,

$$\begin{aligned}\langle \hat{g}^2\rangle &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}[g(q,p)\otimes g(q,p)]f(q,p)\,dq\,dp\\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}[g(q,p)]^2 f(q,p)\,dq\,dp\\ &\geq 0.\end{aligned} \tag{5.8}$$

Now, since $g(q,p)$ is an arbitrary function, (5.8) implies that $f(q,p)\geq 0$. But this result contradicts our earlier conclusion from Wigner's theorem. Hence, Eq. (5.7) cannot be satisfied, and Theorem 7 is thus established.

The main conclusion of our analysis, then, is that if we restrict ourselves to phase-space representations of quantum mechanics that are linear one-one associations [i.e., which satisfy the requirement (i)] and also give correct marginal probability distributions [i.e., satisfy the requirement (iii)], then the phase-space distributions will necessarily take on negative values for some states, and mappings that involve functions of operators follow rules that are completely foreign to the spirit of the classical theory of stochastic processes [violation of Cohen's requirement (iv)].

APPENDIX: PROOF OF THEOREM 2 (PRODUCT THEOREM)

In this Appendix we will establish Theorem 2 (the product theorem), which gives an expression for the phase-space function [to be denoted by $g(q,p)\otimes h(q,p)$] that represents the product $\hat{g}(\hat{q},\hat{p})\hat{h}(\hat{q},\hat{p})$ of two operators $\hat{g}(\hat{q},\hat{p})$ and $\hat{h}(\hat{q},\hat{p})$.

Since $g(q,p)$ is the phase-space function representing the operator $\hat{g}(\hat{q},\hat{p})$, and $h(q,p)$ is the phase-space function representing the operator $\hat{h}(\hat{q},\hat{p})$, we have from Eq. (2.8)

$$\hat{g}(\hat{q},\hat{p})=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} g(q_1,p_1)\Delta(\hat{q},\hat{p};q_1,p_1)\,dq_1\,dp_1\,, \tag{A1}$$

and

$$\hat{h}(\hat{q},\hat{p})=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} h(q_2,p_2)\Delta(\hat{q},\hat{p};q_2,p_2)\,dq_2\,dp_2\,. \tag{A2}$$

Hence,

$$\hat{g}(\hat{q},\hat{p})\hat{h}(\hat{q},\hat{p})=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} g(q_1,p_1)h(q_2,p_2)\Delta(\hat{q},\hat{p};q_1,p_1)\Delta(\hat{q},\hat{p};q_2,p_2)\,dq_1\,dp_1\,dq_2\,dp_2\,. \tag{A3}$$

According to (2.10), the phase-space function $g(q,p)\otimes h(q,p)$ that represents the operator $\hat{g}(\hat{q},\hat{p})\hat{h}(\hat{q},\hat{p})$ is given by

$$g(q,p)\otimes h(q,p)=\mathrm{Tr}[\hat{g}(\hat{q},\hat{p})\hat{h}(\hat{q},\hat{p})\bar{\Delta}(\hat{q},\hat{p};q,p)]\,. \tag{A4}$$

From Eqs. (A3) and (A4) we immediately find that

$$g(q,p)\otimes h(q,p)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} R(q,p;q_1,p_1,q_2,p_2)g(q_1,p_1)h(q_2,p_2)\,dq_1\,dp_1\,dq_2\,dp_2\,, \tag{A5}$$

where

$$R(q,p;q_1,p_1,q_2,p_2)=\mathrm{Tr}[\,\Delta(\hat{q},\hat{p};q_1,p_1)\,\Delta(\hat{q},\hat{p};q_2,p_2)\bar{\Delta}(\hat{q},\hat{p};q,p)]\,. \tag{A6}$$

Equations (A5) and (A6) constitute the required *product theorem*.

We note that in the special case of the Ω representations, the kernel, given by (A6), becomes

$$R_\Omega(q,p;q_1,p_1,q_2,p_2)=\mathrm{Tr}[\,\Delta_\Omega(\hat{q},\hat{p};q_1,p_1)\Delta_\Omega(\hat{q},\hat{p};q_2,p_2)\bar{\Delta}_\Omega(\hat{q},\hat{p};q,p)]\,. \tag{A7}$$

Using Eqs. (3.1a) and (3.1b), (A7) may be expressed in the form

$$R_\Omega(q,p;q_1,p_1,q_2,p_2)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}[\Omega(\xi_1+\xi_2,\eta_1+\eta_2)]^{-1}\Omega(\xi_1,\eta_1)\Omega(\xi_2,\eta_2)e^{\frac{1}{2}i\hbar(\xi_1\eta_2-\xi_2\eta_1)}$$
$$\times e^{-i(\xi_1q_1+\eta_1p_1+\xi_2q_2+\eta_2p_2)}e^{i[(\xi_1+\xi_2)q+(\eta_1+\eta_2)p]}\,d\xi_1\,d\eta_1\,d\xi_2\,d\eta_2\,. \tag{A8}$$

Equation (A5) together with Eq. (A8) is in agreement with the product theorem for Ω representations, established by Agarwal and Wolf [see Ref. 7(b), Eqs. (3.3)–(3.5)].

In this context, we also note that the relation

$$g(q,p)\otimes h(q,p)=g(q,p)h(q,p) \tag{A9}$$

cannot be satisfied for all functions $g(q,p)$ and $h(q,p)$ in any phase-space representation, for it is clear from Eq. (A5) that Eq. (A9) would hold if and only if

$$R(q,p;q_1,p_1,q_2,p_2)=\delta(q-q_1)\delta(p-p_1)\delta(q-q_2)\delta(p-p_2)\,. \tag{A10}$$

Clearly, (A10) cannot hold in any representation, since the right-hand side is symmetric under the exchange of (q_1,p_1) and (q_2,p_2), whereas the left-hand side is not, as is evident from Eq. (A6) defining the kernel $R(q,p;q_1,p_1,q_2,p_2)$.

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