Optimum Phase Space Probabilities From Quantum Tomography

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We determine a positive normalised phase space probability distribution $P$ with minimum mean square fractional deviation from the Wigner distribution $W$. The minimum deviation, an invariant under phase space rotations, is a quantitative measure of the quantumness of the state. The positive distribution closest to $W$ will be useful in quantum mechanics and in time frequency analysis.

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1. Quasi-probability distributions in Quantum Mechanics and Time Frequency Analysis. The Wigner quasi-probability distribution $W$ \cite{Braunstein2005}, first proposed to calculate quantum corrections to thermodynamic equilibrium, is now widely used in quantum mechanics, statistical mechanics, and technological areas such as time-frequency analysis of signals in electrical engineering and seismology \cite{Braunstein1984}. The $W$ distribution and other quasi-probability distributions such as the Husimi $Q$ function \cite{Husimi1940}, the Glauber-Sudarshan $P$ function and their $s$-parametrized generalizations \cite{Glauber1963} can be obtained in quantum optics by measuring probability distributions of quadrature phases and making an inverse Radon transform, i.e. quantum tomography \cite{Braunstein2005}.

The Wigner function has the unique distinction of being the quantum analogue of the classical Liouville phase space distribution since its marginals reproduce quantum probability densities of position coordinates $q_i$, momentum coordinates $p_i$ and indeed of quadrature phases $q_i \cos \theta_i + p_i \sin \theta_i$ for all $\theta_i$ with $i$ taking $N$ values for a $2N$-dimensional phase space. In time frequency analysis too $W$ has the correct marginals reproducing energy densities in time or frequency. Unlike the classical Liouville density, $W$ cannot be interpreted as a joint probability density, because there are quantum states for which $W$ is not positive definite. Similarly in time-frequency analysis, $W$ has marginals reproducing the energy densities in time or frequency but cannot be interpreted as their joint density; for that one uses the positive definite ‘Spectrogram’ even though it does not have the correct marginals. In quantum mechanics, the main reason for the importance of the Husimi function $Q$ (a smeared $W$ function) is that it is positive definite; secondly, as shown by Braunstein, Caves and Milburn, it is the optimum of the distributions obtained in the Von-Neumann-Arthurson-Kelly model for joint measurement of position and momentum \cite{Braunstein1984}.

In 2-dimensional phase space, the Husimi function for a quantum state $\psi$ is a particular smearing of the Wigner function $W_\psi(q', p')$ which is explicitly positive definite,

$$ P_H(q,p) = \frac{1}{2\pi} |\langle \psi_{b,q,p}, \psi \rangle|^2 = \int dq' dp' W_\psi(q',p') W_{\psi_{b,q,p}}(q',p'), \quad (1) $$

where,

$$ W_{\psi_{b,q,p}}(q',p') = \frac{1}{\pi} \exp \left(-\frac{(q-q')^2}{2b^2} - 2i\theta(p-p') \right) \quad (2) $$

is the Wigner function for the minimum uncertainty state centered at position $q$, momentum $p$.

$$ \psi_{b,q,p}(q') = \frac{\exp \left(-\frac{(q-q')^2}{2b^2} + ipq' \right)}{(2\pi)^{1/4} b}. \quad (3) $$

The Husimi $Q$ function is obtained from $P_H(q,p)$ if we choose $b^2 = 1/2$. The variances differ from the true quantum values $(\Delta q)^2$, $(\Delta p)^2$,

$$ (\Delta q)_H^2 = (\Delta q)^2 + b^2, \quad (\Delta p)_H^2 = (\Delta p)^2 + \frac{1}{4b^2}. \quad (4) $$

Hence, marginals of the Husimi function differ from the corresponding quantum probability densities, even when the Wigner function (which has the correct marginals) is positive definite. This suggests that a positive distribution closer to the Wigner function may exist also in cases where the Wigner function is not positive definite. The acute need for the best such distribution can be illustrated in a practical context.

Need for an optimum positive joint density function. We give one example in time frequency analysis, where there is a practical need for such a positive distribution in order to define the bandwidth at a given time. We need to define the expectation values of frequency $\omega$ and its square $\omega^2$ at time $t$; this is done easily if there is a positive density function $P$ (e.g. see Cohen \cite{Cohen1966}),

$$ \langle \omega \rangle_t = \frac{\int d\omega \omega P(t, \omega)}{\int d\omega P(t, \omega)}, \quad \langle \omega^2 \rangle_t = \frac{\int d\omega \omega^2 P(t, \omega)}{\int d\omega P(t, \omega)}. \quad (5) $$
However if we substitute the Wigner function \( W(t, \omega) \) in place of \( P(t, \omega) \) we obtain an expression for the square of the bandwidth at time \( t \), in terms of the amplitude \( A(t) \) of the signal,

\[
\langle \omega^2 \rangle_t - (\langle \omega \rangle_t)^2 = (1/2) \left( (\dot{A}(t)/A(t))^2 - \ddot{A}(t)/A(t) \right),
\]

which is not positive definite since the second term on the right-hand side can be negative. Thus the Wigner function does not yield a reasonable definition of the instantaneous band-width. The Husimi function will give a positive definite answer; but that answer may not be reliable since its marginals differ from those of \( W \) even when \( W \) is positive definite. In quantum mechanics, exactly the same mathematics demonstrates the difficulty of defining the conditional dispersion in momentum for a given position using the Wigner function. The basic need for a probability density ‘closest’ to the \( W \) is positive definite. In quantum mechanics, exactly the Wigner function is given in terms of the density operator \( \rho \),

\[
W(q, p) = \frac{1}{(2\pi)^N} \int d\tilde{\eta} \exp(i\tilde{\eta}(\tilde{q} - \tilde{p})/2\sqrt{\tilde{\eta}}) W(q, p)^2.
\]

In Sec. 2 we derive our basic result on the best possible positive normalized probability distribution closest to \( W \). In Sec. 3 we solve the corresponding variational problem when additional rotationally invariant constraints in phase space are added. In the particular examples considered in this paper these additional constraints enable reproducing the correct uncertainty product for position and momentum. In Sec. 4 we calculate the two optimal distributions explicitly in the case of the generalized coherent states of quantum optics and compare them numerically with the Wigner and Husimi distributions in Table I and Figs. 1 to 4. The results bring out not only that the optimal distributions are much closer to the Wigner distribution than the Husimi \( Q \) function but also that the marginals of the optimal distributions are much closer to the true position probability density than those of the Husimi function. In Sec. 5 we outline a more ambitious problem of finding the positive normalized distribution closest to the Wigner function which reproduces both the position and momentum probabilities of quantum mechanics exactly. In Sec. 6 we summarise our conclusions.

2. Positive joint probability distribution closest to the Wigner distribution and a measure of quantumness. Suppose we know \( W \) through quantum tomography. We seek a criterion invariant under phase space rotations to define the positive definite phase space probability density ‘closest’ to the \( W \) function and with total phase space integral unity, as necessary for a probability interpretation. The criterion of ‘closeness’ must be such that it gives back the \( W \) function when that is positive definite. In \( 2N \) dimensional phase space, with units \( \hbar = c = 1 \), the Wigner function is given in terms of
where $\theta(x)$ is the Heaviside $\theta$ function, being unity when the argument is positive and zero otherwise, and

$$P_0(\vec{q}, \vec{p}) = W(\vec{q}, \vec{p}) - c. \quad (15)$$

Denoting by $L$ and $L_{\text{min}}$ respectively the values of the Lagrangian for an arbitrary $P(\vec{q}, \vec{p})$ satisfying the constraints, and by $P_{\text{min}}(\vec{q}, \vec{p})$, we obtain,

$$L - L_{\text{min}} = \int_{P_0 \geq 0} (P - P_0) d\vec{q} d\vec{p} + \int_{P_0 < 0} (P^2 - 2PP_0) d\vec{q} d\vec{p} \geq 0, \quad (16)$$

since each of the two integrands is non-negative. We complete the proof by showing the existence and uniqueness of a constant $c$ satisfying the normalization constraint,

$$\int_{W(\vec{q}, \vec{p}) - c \geq 0} (W(\vec{q}, \vec{p}) - c) d\vec{q} d\vec{p} = 1. \quad (17)$$

First, if $W$ is non-negative, $c = 0$ is the unique solution, and gives $\sigma^2 = 0$. Suppose now that $W$ is negative in some regions of phase space. The left-hand side integral is then $\geq 1$ for $c \leq 0$, decreases monotonically as $c$ increases to positive values until it equals $0$ when $c = max_{\vec{q}, \vec{p}} W(\vec{q}, \vec{p})$. Hence there is a unique solution for $c$ in the interval $[0, max_{\vec{q}, \vec{p}} W(\vec{q}, \vec{p})]$. Using this value of $c$ we compute the optimum phase space probability distribution as well as the minimum value of $\sigma^2$, an index of quantumness of the state.

3. Incorporating additional rotationally invariant constraints in phase space. The variational method outlined above is invariant under phase space rotations. Can we incorporate other quantum constraints preserving such invariance? In addition to the phase space volume, the surface of the sphere with centre $\vec{q}_{cl}, \vec{p}_{cl}$,

$$(\vec{q} - \vec{q}_{cl})^2 + (\vec{p} - \vec{p}_{cl})^2 = x$$

is an invariant under rotations in phase space, and hence may be used as an additional constraint. With a view towards imposing the correct sum of quantum dispersions $(\Delta q)^2 + (\Delta p)^2$ on the variational phase space density, we choose $\vec{q}_{cl}, \vec{p}_{cl}$ as the quantum expectation values of $\vec{q}_{op}, \vec{p}_{op}$. Further, if $W$ remains positive in the region $x \geq x_{\text{max}}$, we may choose $P(\vec{q}, \vec{p}) = W(\vec{q}, \vec{p})$ in that region, and for sufficiently large $x_{\text{max}}$ still find a solution $P(\vec{q}, \vec{p})$ that minimises $\sigma^2$ under the positivity constraint $P(\vec{q}, \vec{p}) \geq 0$, the normalisation constraint,

$$\int \int_{x \leq x_{\text{max}}} d\vec{q} d\vec{p} (P(\vec{q}, \vec{p}) - W(\vec{q}, \vec{p})) = 0, \quad (18)$$

and the additional constraint,

$$\int \int_{x \leq x_{\text{max}}} d\vec{q} d\vec{p} (P(\vec{q}, \vec{p}) - W(\vec{q}, \vec{p})) x = 0. \quad (19)$$

The last equation imposes the sum of quantum dispersions $(\Delta q)^2 + (\Delta p)^2$ on $P$ since the Wigner function obeys that constraint. We then prove as before that the solution minimising $\sigma^2$ is, for $x \leq x_{\text{max}}$

$$P_{\text{min}}(\vec{q}, \vec{p}) = P_{01}(\vec{q}, \vec{p}) \theta(P_{01}(\vec{q}, \vec{p})), \quad (20)$$

where

$$P_{01}(\vec{q}, \vec{p}) = W(\vec{q}, \vec{p}) - c - xd, \quad (21)$$

provided that constants $c, d$ are found satisfying the two equality constraints given above.

4. Optimum positive joint probability distributions and Husimi distribution for generalized coherent states. The Husimi $Q$ function in $2N$-dimensional phase space is,

$$Q(\vec{q}, \vec{p}) = (2\pi)^{-N} \langle \vec{a}\mid \rho \mid \vec{a} \rangle \quad (22)$$

where $|\alpha\rangle$ are the coherent states.

$$\vec{a}|\alpha\rangle = \vec{a}|\alpha\rangle, \alpha = (\vec{q} + i\vec{p})/\sqrt{2}\iota, \quad (23)$$

Generalized coherent states [2] are displaced excited eigen state solutions of the time dependent Schrödinger equation for the one dimensional oscillator whose probability density packets move classically with shape unchanged, and have uncertainty product $\Delta q \Delta p = n + 1/2$,

$$\langle q | \psi(t) \rangle = (q - q_{cl}(\tau) | n \rangle \exp(-i(n + 1/2)\tau)$$

$$\exp(i\dot{q}_{cl}(\tau)(q - 1/2\dot{q}_{cl}(\tau))), \quad (24)$$

where, $|n\rangle$ is the $n$-th excited state and $q_{cl}$ has classical motion

$$\tau = \omega t, \quad q_{cl}(\tau) = A \cos(\tau + \phi). \quad (25)$$

The quantum expectation values for position and momentum operators are,

$$\langle q_{op} \rangle = q_{cl}(\tau), \quad \langle p_{op} \rangle = \dot{q}_{cl}(\tau) \equiv p_{cl}. \quad (26)$$

Wigner functions and Husimi functions can be seen to depend on $q, p$ only through the combination,

$$x = (q - q_{cl})^2 + (p - p_{cl})^2. \quad (27)$$

For $n = 0$ the optimum phase space probability density is just the Wigner function which is positive definite. For $n = 1, 2$ the $W_n(q, p)$ and $Q_n(q, p)$ functions are given by,

$$W_1 = (2\pi)(x - 1/2) \exp(-x),$$

$$Q_1 = (x/(4\pi)) \exp(-x/2), \quad (28)$$

$$W_2 = (2\pi)((x - 1)^2 - 1/2) \exp(-x),$$

$$Q_2 = (x^2/(16\pi)) \exp(-x/2). \quad (29)$$

We have numerically evaluated the optimum phase space probability distribution $P_{\text{min}}$ of Sec.2 with only
positivity and normalization constraint, and $P_{\text{min1}}$ of Sec.3 with the additional constraint of the correct $\Delta q \Delta p$ for the generalized coherent states with $n = 1$ and $n = 2$.

We have also evaluated the corresponding Husimi $Q$ distributions. We compared the optimum $P_{\text{min}}, P_{\text{min1}}$ with $W, Q$ distributions in Figs. 1, 2. We also compared the corresponding position probability densities in Figs. 3, 4. Both of the optima $P_{\text{min}}, P_{\text{min1}}$ show a big improvement over the Husimi function, as is obvious qualitatively from the figures, and quantitatively from the $\sigma^2$ values listed in the table.

Red− From Wigner Function
Black− Optimum Probability
Blue− Prob. with $\Delta q \Delta p$ constraint added
Green− Husimi Function $Q$

FIG. 1: For the $n=1$ coherent state, the optimum phase space probability distributions with only normalization constraint (black), and including additional constraints fixing $\Delta q \Delta p$ (blue) are compared with the Wigner (red) and Husimi (green) distributions as a function of $x = (q-q_{cl})^2 + (p-p_{cl})^2$. The optimum and Husimi distributions have $\sigma^2 = 0.277049$, and 0.509259 respectively.

Red− Wigner Function
Black− Optimum Probability
Blue− Prob. with $\Delta q \Delta p$ constraint added
Green− Husimi Function $Q$

FIG. 2: The same plots as in Fig.1 for the $n=2$ coherent state. The optimum and Husimi distributions have $\sigma^2 = 0.268084$, and 0.64429 respectively.

5. Optimum Positive Phase Space Densities Reproducing $N + 1$ Quantum Marginals. Cohen and Zaparovanny [8] constructed the most general positive phase space densities reproducing two marginals of $W$, viz. quantum probability densities of $\vec{q}$ and $\vec{p}$. In $2N$-dimensional phase space, with $N \geq 2$, Roy and Singh [9] noted that in fact $N + 1$ marginals of $W$ (e.g. for $N = 2$, probability densities of $(q_1, q_2), (p_1, q_2), (p_1, p_2)$) can be reproduced with positive densities; they conjectured that no more than $N + 1$ marginals can be so reproduced for arbitrary quantum states, the “$N + 1$” marginal theorem. This was proved later using an extension of Bell inequalities [10] to phase space by Auberson et al [11], who also derived the most general positive phase space density reproducing $N + 1$ marginals; that density is non-unique since it contains an arbitrarily specifiable phase space function. Among the continuous infinity of positive phase space densities reproducing $N + 1$ marginals which one is closest to the Wigner Function? Our method gives a straightforward answer; we give the variational answer
TABLE I: Husimi Function versus Optimum Probability Distributions; \( \sigma^2 \) is the mean square fractional deviation from the Wigner distribution.

| State | Husimi Function | Optimum Probability Density |
|-------|----------------|-----------------------------|
|       | \( \sigma^2 \) | \( \sigma^2 \) | \( c \) | \( d \) | \( x_{\text{max}} \) | \( \Delta q \Delta p \) |
| n=1   | .5093          | .2877                      | .01053 | 0   | \( \infty \)     | 1.108          |
| \( \Delta q \Delta p = 3/2 \) | .3223          | .2877                      | .01837 | - .0014 | 18 | 3/2 |
| n=2   | .6443          | .2877                      | .01595 | 0   | \( \infty \)     | 1.722          |
| \( \Delta q \Delta p = 5/2 \) | .3223          | .2877                      | .04235 | - .00408 | 15 | 5/2 |

which complete evaluation of the optimum phase space density. For \( N \geq 2 \), the positivity constraint is supplemented by \( N + 1 \) marginal constraints, which can, for example, be chosen to be the series of probability densities of \((q_1, q_2, \ldots, q_n), (p_1, q_2, \ldots, q_n), \ldots (p_1, p_2, \ldots, p_n)\), in which each member is obtained by replacing in the previous set one co-ordinate by its conjugate momentum. The optimal phase space density is again constructed by a Lagrange multiplier method which will now involve \( N + 1 \) Lagrange multiplier functions.

6. Conclusion. We have proposed a general method to find the positive phase space distribution closest to the Wigner distribution that can be used in quantum optics as well as in time frequency analysis. A measure of quantumness emerges. Qualitative and quantitative improvement with respect to the Husimi function is seen explicitly; e.g. for the generalized coherent states, the optimum and Husimi distributions have respectively, for \( n = 1 \), \( \sigma^2 = .277049 \), and \( .509259 \), for \( n = 2 \), \( \sigma^2 = .268084 \), and \( .64429 \). Similar improvements are expected in time frequency analysis. In 2N-dimensional phase space the optimum positive density reproducing \( N + 1 \) marginals can be evaluated.

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