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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. The position-momentum correlations given by the distribution can be tested experimentally in quantum optics. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4854035]

I. QUASI-PROBABILITY DISTRIBUTIONS IN QUANTUM MECHANICS AND TIME FREQUENCY ANALYSIS

The Wigner quasi-probability distribution W,[1] 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.[2] The W distribution and other quasi-probability distributions such as the Husimi Q function,[3] the Glauber-Sudarshan P function and their s-parametrized generalizations[4] can be obtained in quantum optics by measuring probability distributions of quadrature phases and making an inverse Radon transform, i.e., quantum tomography.[5]

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 θ_i with i taking N values for a $2N$-dimensional phase space. In addition, as proved first by Moyal and reviewed by Hillery, O'Connell, Scully, and Wigner,[1] expectation values of c-number phase space functions calculated from this distribution agree exactly with quantum expectation values of the corresponding Weyl ordered function of the position and momentum operators. 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; second, as shown by Braunstein, Caves, and Milburn,[3] it is the optimum of the distributions obtained in the Von-Neumann-Arthurs-Kelly model for joint measurement of position and momentum.[3]

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

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

where

$$W_{\psi_{b,q,p}}(q', p') = \frac{1}{\pi}\exp\big(-\frac{(q-q')^2}{2b^2} - 2b^2(p-p')^2\big) \tag{2}$$

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

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

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 $(\Delta q)^2$, $(\Delta p)^2$,

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

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 some practical contexts.

A. Need for an optimum positive joint density function

(i) *Position-momentum correlations in quantum mechanics*: Phase space distributions enable a semi-classical understanding of quantum mechanics. For example, even for non-commuting observables such as position $\hat{q}$ and momentum $\hat{p}$, if there is a suitable positive density $P(q, p)$, we can define the conditional probability $dP(q)$ for p to belong to the interval dp for a given value of q, and hence conditional expectation value of any function $f(p)$ for a given q,

$$dP(q) = \frac{P(q, p)dp}{\int P(q, p')dp'},\ \langle f(p)\rangle(q) = \frac{\int f(p)P(q, p)dp}{\int P(q, p')dp'}.$$

These can be tested against expectation values of quantum observables which can be measured experimentally in quantum mechanics. For example, it has recently been shown by one of us[6] that the quantum expectation value,

$$\langle \hat{p}\rangle(q) \equiv \frac{\langle \Lambda(q)\hat{p} + \hat{p}\Lambda(q)\rangle}{2\langle\Lambda(q)\rangle};\ for\ \Lambda(q) \equiv |q\rangle\langle q|,$$

can be measured exactly by von Neumann-Arthurs-Kelly type joint measurements[3] in quantum optics. This can be tested against $\langle p\rangle(q)$ derived from a positive definite phase space density.

(ii) 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 ω and its square ω^2 at time t; this is done easily if there is a positive density function P (e.g., see Cohen[2]),

$$\langle\omega\rangle_t = \frac{\int d\omega\omega P(t, \omega)}{\int d\omega P(t, \omega)},\ \langle\omega^2\rangle_t = \frac{\int d\omega\omega^2 P(t, \omega)}{\int d\omega P(t, \omega)}. \tag{5}$$

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,

$$\langle\omega^2\rangle_t - (\langle\omega\rangle_t)^2 = (1/2)\big((\dot{A}(t)/A(t))^2 - \ddot{A}(t)/A(t)\big), \tag{6}$$

TABLE I. Husimi function versus optimum probability distributions; σ^2 is the mean square fractional deviation from the Wigner distribution.

State	Husimi function σ^2	Optimum probability density σ^2	c	d	x_{max}	$\Delta q\Delta p$
n = 1	0.5093	0.2770	0.01053	0	∞	1.108
$\Delta q\Delta p = 3/2$		0.2877	0.01837	− 0.0014	18	3/2
n = 2	0.6443	0.2681	0.01595	0	∞	1.722
$\Delta q\Delta p = 5/2$		0.3223	0.04235	− 0.00408	15	5/2

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 interpretation in quantum mechanics, and an energy density interpretation in time-frequency analysis motivates the variational problem seeking the best possible positive distribution. The positive joint probability we find has immediate utility for quantum mechanics (especially quantum optics) and in time-frequency analysis (with obvious transcriptions of the variables q, p going to t, ω) as improvement over the Husimi Q function and the Spectrogram $P_{SP}(t, \omega)$, respectively.

In Sec. II, we derive our basic result on the best possible positive normalized probability distribution closest to W. In Sec. III, 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. IV, 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. 1–4. The results bring out not only that the

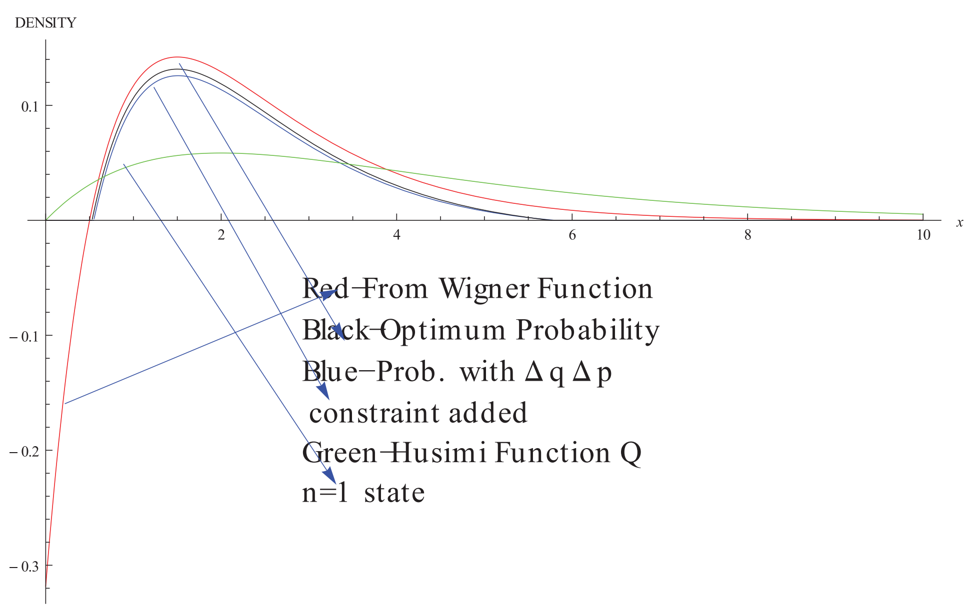

FIG. 1. For the n = 1 coherent state, the optimum phase space probability distributions with only normalization constraint (black), and including additional constraints fixing $\Delta q\Delta p$ (blue) are compared with the Wigner (red) and Husimi (green) distributions as a function of $x = (q - q_{cl})^2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

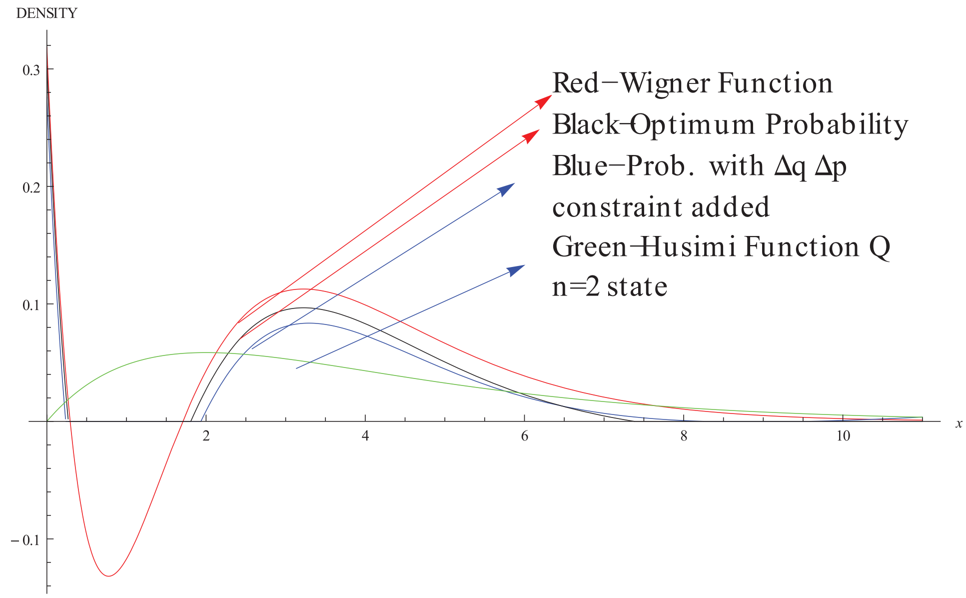

FIG. 2. The same plots as in Fig. 1 for the n = 2 coherent state. The optimum and Husimi distributions have $\sigma^2 = 0.268084$ and 0.64429, respectively.

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. V, 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. VI, we summarise our conclusions.

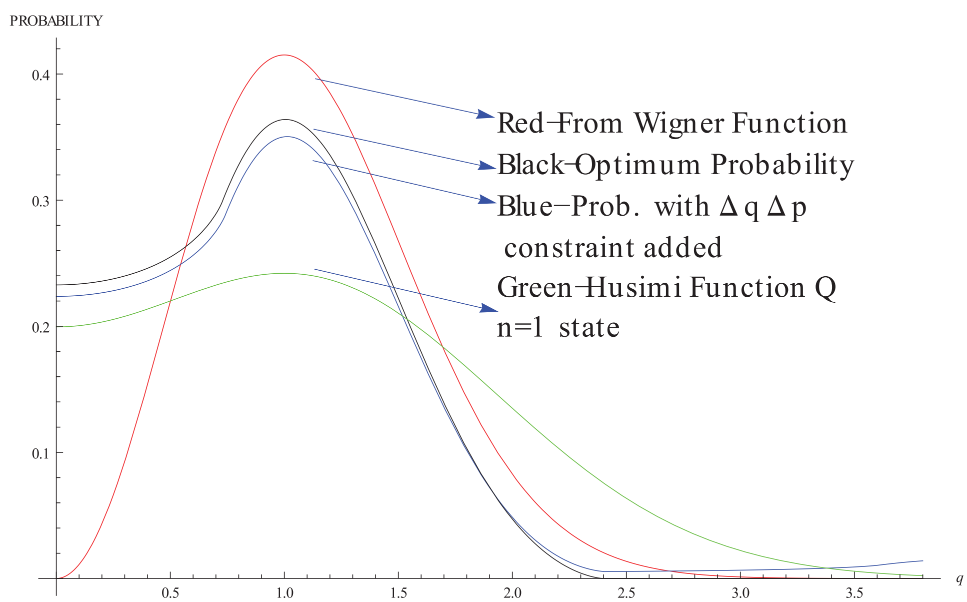

FIG. 3. For the n = 1 coherent state, the position probabilities calculated from the optimum joint probabilities with only normalization constraint (black), and with additional constraints fixing $\Delta q \Delta p$ (blue) are seen to be closer to the true probability (given by the Wigner distribution (red)) than the Husimi distribution result (green).

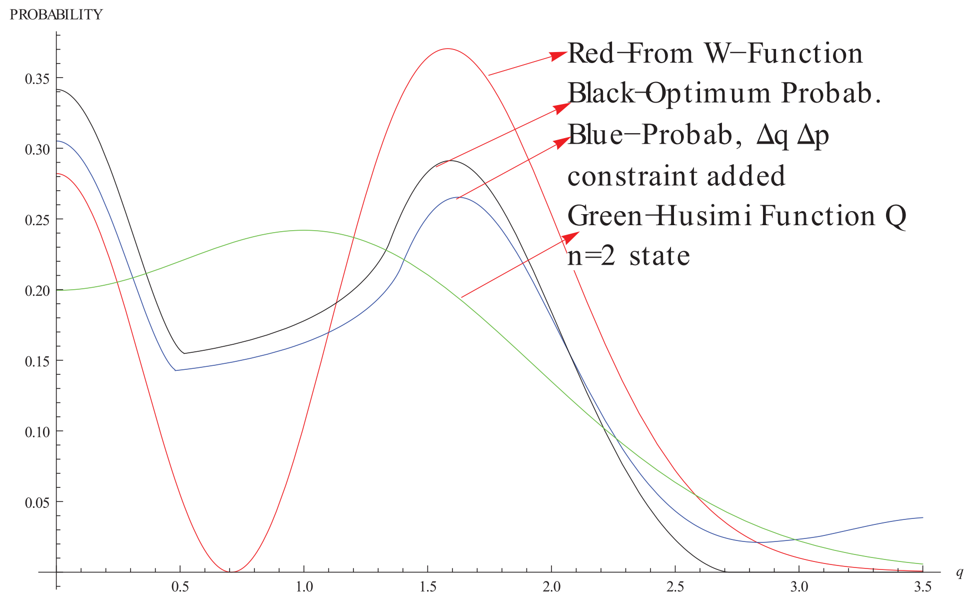

FIG. 4. Same plots as in Fig. 3, for the n = 2 coherent state of the oscillator.

II. 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 the density operator ρ,

$$W(\vec{q},\vec{p}) = \frac{1}{(2\pi)^N}\int d\vec{y}\,\exp(i\vec{p}.\vec{y})\langle\vec{q}-\vec{y}/2|\rho|\vec{q}+\vec{y}/2\rangle$$
$$= \frac{1}{(2\pi)^{2N}}\int d\vec{\xi}\int d\vec{\eta}\;Tr\rho\,\exp(i\vec{\xi}.(\vec{q}_{op}-\vec{q}) + i\vec{\eta}.(\vec{p}_{op}-\vec{p})), \tag{7}$$

where time dependence of the density operator and the Wigner function have been suppressed, $\vec{q}_{op}, \vec{p}_{op}$ denote the position and momentum operators and the last equation facilitates discussion of rotation properties in phase space. In quantum optics,

$$\vec{q}_{op} = (\vec{a}+\vec{a}^{\dagger})/\sqrt{2},\;\; \vec{p}_{op} = -i(\vec{a}-\vec{a}^{\dagger})/\sqrt{2}. \tag{8}$$

We vary $P(\vec{q},\vec{p})$ so as to minimise

$$\sigma^2 = \frac{\int d\vec{q}\int d\vec{p}\,(P(\vec{q},\vec{p}) - W(\vec{q},\vec{p}))^2}{\int d\vec{q}\int d\vec{p}\;W(\vec{q},\vec{p})^2} \tag{9}$$

(which is just the mean of the square of the fractional deviation $(P-W)/W$ with the weight function W^2), subject to the constraints

$$\int d\vec{q}\int d\vec{p}\;P(\vec{q},\vec{p}) = 1;\;\; P(\vec{q},\vec{p}) \geq 0. \tag{10}$$

We use Lagrange's method of undetermined multipliers modified to incorporate inequality constraints. The above normalization constraint is equivalent to

$$\int d\vec{q} \int d\vec{p}\,(P(\vec{q},\vec{p}) - W(\vec{q},\vec{p})) = 0, \tag{11}$$

and the expression for σ^2, using Moyal's well known result for phase space integral of W^2[1] simplifies, for pure states, to

$$\sigma^2 = (2\pi)^N \int d\vec{q} \int d\vec{p}\,(P(\vec{q},\vec{p}) - W(\vec{q},\vec{p}))^2. \tag{12}$$

Remark. For impure states, the factor $(2\pi)^N$ on the right-hand side must be replaced by $(2\pi)^N/Tr(\rho^2)$.

This leads to the Lagrangian,

$$L = \int d\vec{q} \int d\vec{p}\,(P(\vec{q},\vec{p}) - W(\vec{q},\vec{p}))^2$$
$$+2c \int d\vec{q} \int d\vec{p}\,(P(\vec{q},\vec{p}) - W(\vec{q},\vec{p})), \tag{13}$$

where c is the Lagrange multiplier. Following a method used widely by Martin[7] to incorporate inequality constraints, we prove by direct subtraction that σ^2 has a global minimum when we choose $P(\vec{q},\vec{p}) = P_{min}(\vec{q},\vec{p})$, where

$$P_{min}(\vec{q},\vec{p}) = P_0(\vec{q},\vec{p})\,\theta(P_0(\vec{q},\vec{p})), \tag{14}$$

where $\theta(x)$ is the Heaviside θ function, being unity when the argument is positive and zero otherwise, and

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

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

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

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,

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

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 ≥ 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 σ^2, an index of quantumness of the state.

III. 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 $(\Delta\vec{q})^2 + (\Delta\vec{p})^2$ 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 $x \geq x_{max}$, we may choose $P(\vec{q}, \vec{p}) = W(\vec{q}, \vec{p})$ in that region, and for sufficiently large x_{max}, still find a solution $P(\vec{q}, \vec{p})$ that minimises σ^2 under the positivity constraint $P(\vec{q}, \vec{p}) \geq 0$, the normalisation constraint,

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

and the additional constraint,

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

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

$$P_{min1}(\vec{q}, \vec{p}) = P_{01}(\vec{q}, \vec{p})\, \theta(P_{01}(\vec{q}, \vec{p})), \tag{20}$$

where

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

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

IV. OPTIMUM POSITIVE JOINT PROBABILITY DISTRIBUTIONS AND HUSIMI DISTRIBUTION FOR GENERALIZED COHERENT STATES

The Husimi Q function in $2N$-dimensional phase space is

$$Q(\vec{q}, \vec{p}) = (2\pi)^{-N} \langle\vec{\alpha}|\rho|\vec{\alpha}\rangle, \tag{22}$$

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

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

Generalized coherent states[8] are displaced excited eigenstate 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 $\Delta q \Delta p = n + 1/2$,

$$\begin{aligned} \langle q|\psi(t)\rangle = \langle q - q_{cl}(\tau)|n\rangle \exp(-i(n + 1/2)\tau) \\ \exp(i\dot{q}_{cl}(\tau)(q - 1/2\dot{q}_{cl}(\tau))), \end{aligned} \tag{24}$$

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

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

The quantum expectation values for position and momentum operators are

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

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

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

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

$$\begin{aligned} W_1 = (2/\pi)(x - 1/2)\exp(-x), \\ Q_1 = (x/(4\pi))\exp(-x/2), \end{aligned} \tag{28}$$

$$W_2 = (2/\pi)((x-1)^2 - 1/2)\exp(-x),$$
$$Q_2 = (x^2/(16\pi))\exp(-x/2). \tag{29}$$

We have numerically evaluated the optimum phase space probability distribution P_{min} of Sec. II with only positivity and normalization constraint, and P_{min1} of Sec. III 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_{min}, P_{min1} with W, Q distributions in Figs. 1 and 2. We also compared the corresponding position probability densities in Figs. 3 and 4. Both of the optima P_{min}, P_{min1} show a big improvement over the Husimi function, as is obvious qualitatively from the figures, and quantitatively from the σ^2 values listed in the table.

V. OPTIMUM POSITIVE PHASE SPACE DENSITIES REPRODUCING *N* + 1 QUANTUM MARGINALS

Cohen and Zaparovanny[9] 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[10] 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[11] to phase space by Auberson *et al.*,[12] 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 straight forward answer; we give the variational answer explicitly for $N = 2$, and indicates briefly the generalization to $N \geq 2$. Find the phase space density $P(q, p)$ obeying positivity, minimum mean square fractional deviation from the Wigner distribution, reproducing the quantum probability densities of q, and p. Vary $P(q, p)$ to minimise the Lagrangian,

$$L = \int [(P - W)^2 + (2\lambda(q) + 2\mu(p))(P - W)]dq dp, \tag{30}$$

subject to the constraints,

$$\int (P - W)dp = 0, \ \int (P - W)dq = 0, \ P(\vec{q}, \vec{p}) \geq 0. \tag{31}$$

L is minimised if we choose for P, the function P_0 that makes L stationary whenever P_0 is positive, and zero otherwise

$$P_{min} = P_0 \theta(P_0), \ P_0 \equiv W - \lambda(q) - \mu(p), \tag{32}$$

where the multipliers $\lambda(q)$, $\mu(p)$ are determined from the constraints. As in Sec. II, we prove by direct subtraction that $L - L_{min} \geq 0$, the only change being the new choice of $P_0 \equiv W - \lambda(q) - \mu(p)$. The constraints yield a pair of coupled integral equations to determine $\lambda(q)$, $\mu(p)$

$$\int_{P_0 \geq 0} (\lambda(q) + \mu(p))dp = -\int_{P_0 \leq 0} W(q, p)dp,$$
$$\int_{P_0 \geq 0} (\lambda(q) + \mu(p))dq = -\int_{P_0 \leq 0} W(q, p)dq \,, \tag{33}$$

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 coordinate 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.

VI. 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 quantitative measure of quantumness emerges. Qualitative and quantitative improvement with respect to the Husimi function is seen explicitly; e.g., for the generalized coherent states of quantum optics, the optimum and Husimi distributions have, respectively, for $n = 1$, $\sigma^2 = 0.277049$ and 0.509259, for $n = 2$, $\sigma^2 = 0.268084$ and 0.64429. Similar improvements are expected in time frequency analysis. In $2N$-dimensional phase space, the optimum positive density reproducing $N + 1$ marginals can be evaluated. Finally, the conditional expectation values such as the expectation value of momentum for a given position $\langle p\rangle(q)$ derived from the optimum phase space density can be tested against the quantum optical measurement of $\langle \hat{p}\rangle(q)$.[6]

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