Bounds on Integrals of the Wigner Function

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The integral of the Wigner function over a subregion of the phase space of a quantum system may be less than zero or greater than one. It is shown that for systems with 1 degree of freedom, the problem of determining the best possible upper and lower bounds on such an integral, over all possible states, reduces to the problem of finding the greatest and least eigenvalues of a Hermitian operator corresponding to the subregion. The problem is solved exactly in the case of an arbitrary elliptical region. These bounds provide checks on experimentally measured quasiprobability distributions.

The Wigner function has been much studied since its introduction [1], not only in the context of quantum physics [2], but also in signal processing [3]. For a quantum system in a pure state, the Wigner function carries the same information as the wave function, up to an unimportant constant phase. In the case of a mixed state, it carries the same information as the density operator.

An important property of the Wigner function, one of several properties which distinguish it from classical probability densities, is that its integral over a given subregion of phase space may be negative or greater than one. Quasiprobability distributions which, according to quantum theory, correspond to Wigner functions, have been measured in recent experiments, for a variety of states of light and matter [4–10], and negative values have indeed been observed. These experiments are probing the basic structure and predictions of quantum mechanics in a new way, and the prospect of increasingly accurate experiments of this type adds greatly to the interest in, and importance of, the theory of the Wigner function.

We consider the problem of determining the best possible bounds on the integral of the Wigner function over a given subregion of the phase plane of any system with 1 degree of freedom. We show for any subregion of a rather general type that this problem reduces to the problem of finding the greatest and least eigenvalues of a Hermitian Fredholm integral operator corresponding to that subregion. The problem is found to be exactly solvable for any elliptical or annular subregion, and the bounds are given explicitly in the case of the ellipse. These best possible bounds provide new information about the structure of the Wigner function, differing from known results such as best possible bounds (7) on the values of the Wigner function itself, bounds on integrals of powers of the function [11], or bounds on various moments of the function [12]. In particular, the new bounds determine the degree to which the integral of any Wigner function over an elliptical subregion of the phase plane can lie outside the interval $[0, 1]$ which applies to classical densities. In principle,

they therefore provide checks on experiments of the type to which we have referred, because they must be respected by any measured quasiprobability distribution consistent with quantum mechanics.

As we shall show, appropriately chosen oscillator stationary states (or single frequency light modes) lead *theoretically* to the exact attainment of these upper and lower bounds. Such states are perhaps the easiest to establish experimentally, and it is just such states for which quasiprobability distributions have been measured in some of the experiments mentioned above [6].

In what follows, we consider systems with 1 degree of freedom, with a Cartesian coordinate q and its conjugate momentum p. Our results refer to the Wigner function considered at a particular instant, and are therefore independent of any particular dynamics. We work in dimensionless variables. Appropriate dimensional factors will appear in what follows if each coordinate q there is replaced by q/L, each momentum p by $Lp/\hbar$, each wave function ψ by $L^{1/2}\psi$, each phase space area A by $A/\hbar$, and each Wigner function W by $\hbar W$, where L is a suitable constant with dimensions of a length.

Given a normalized wave function ψ corresponding to a pure state $|\psi\rangle$, the Wigner function is defined as

$$W_\psi(q, p) = \frac{1}{\pi} \int_{-\infty}^{\infty} \psi^*(q + x)\psi(q - x)e^{i2px} \, dx. \quad (1)$$

Then [1]

$$\int_\Gamma W_\psi \, dq \, dp = 1, \qquad \int_\Gamma [W_\psi]^2 \, dq \, dp = \frac{1}{2\pi}, \quad (2)$$

where Γ denotes the (q, p) phase plane.

For a mixed state, the density operator ρ is positive definite and Hermitian with unit trace, and typically can be resolved in the form

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|, \qquad p_i > 0, \qquad \sum_i p_i = 1,$$
$$(3)$$

where the states $|\psi_i\rangle$ are orthonormal. The corresponding Wigner function has the form

$$W_\rho = \sum_i p_i W_{\psi_i}, \tag{4}$$

where W_{ψ_i} is the Wigner function corresponding to the pure state $|\psi_i\rangle$. More generally, the sum in (3) and (4) could be replaced in part or whole by an integral, but this does not significantly affect the argument of the next paragraph.

It follows from (3) and (4) that any bound on the Wigner function, or on its integral over a given subregion S of Γ, must hold for all possible mixed states if it holds for all possible pure states. For example, if

$$\int_S W_\psi(q, p)\, dq\, dp > L \quad \text{for all } \psi, \tag{5}$$

then for any ρ as in (3),

$$\int_S W_\rho(q, p)\, dq\, dp = \sum_i p_i \int_S W_{\psi_i}(q, p)\, dq\, dp$$
$$> \sum_i p_i L = L. \tag{6}$$

Since a pure state can be regarded as a limiting case of a mixed state, it then follows that *best possible* upper and lower bounds on the Wigner function or its integral, when considered over all pure states, must also be best possible upper or lower bounds when considered over all mixed states, although a bound that is *attainable* over pure states may not in general be attainable over mixed states. Bearing this in mind, we restrict attention in what follows to pure states.

Best possible bounds on the Wigner function itself are known [2]:

$$-\frac{1}{\pi} \leq W_\psi(q, p) \leq \frac{1}{\pi} \tag{7}$$

for all normalized ψ, for all $(q, p) \in \Gamma$. It is easily seen that $W_\psi = \pm 1/\pi$ at the point (q, p) if and only if

$$\psi(q - x)e^{ipx} = \pm\psi(q + x)e^{-ipx} \quad \text{for all } x. \tag{8}$$

The problem of interest here is to find best possible bounds on the "quasiprobability functional" corresponding to the subregion S, defined as

$$Q_S[W_\psi] = \int_S W_\psi(q, p)\, dq\, dp$$
$$= \int_\Gamma \chi_S(q, p) W_\psi(q, p)\, dq\, dp, \tag{9}$$

where χ_S is the function with the value 1 on S, and the value 0 on the complement of S.

It follows at once from (7) and (9) that

$$-\frac{A_S}{\pi} \leq Q_S[W_\psi] \leq \frac{A_S}{\pi}, \tag{10}$$

where $A_S = \int_S dq\, dp$ is the area of S.

In order to obtain stronger bounds than (10), recall that each real-valued function $T(q, p)$ on Γ can be associated with a Hermitian operator $\hat{T}$ such that

$$(\psi, \hat{T}\psi) = \int_\Gamma T(q, p) W_\psi(q, p)\, dq\, dp, \tag{11}$$

where (ψ_1, ψ_2) is the usual scalar product of wave functions. Here $\hat{T}$ can always be written as a Fredholm integral operator,

$$(\hat{T}\psi)(x) = \int_{-\infty}^{\infty} K_T(x, y)\psi(y)\, dy, \tag{12}$$

with Hermitian kernel given in terms of the real-valued function $T(q, p)$ as

$$K_T(x, y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} T[(x + y)/2, p]e^{ip(x-y)}\, dp. \tag{13}$$

Consider now the case when $T(q, p) = \chi_S(q, p)$. Comparison of (9) and (11) shows that

$$Q_S[W_\psi] = (\psi, \hat{K}_S\psi), \tag{14}$$

$$(\hat{K}_S\psi)(x) = \int_{-\infty}^{\infty} K_S(x, y)\psi(y)\, dy, \tag{15}$$

$$K_S(x, y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \chi_S[(x + y)/2, p]e^{ip(x-y)}\, dp. \tag{16}$$

It follows at once from (14) that the extremal values of $Q_S[W_\psi]$ are determined by the eigenvalue problem $\hat{K}_S\psi = \lambda\psi$ with $\hat{K}_S$ as in (15). In particular,

$$\inf Q_S = \lambda_{\min}, \qquad \sup Q_S = \lambda_{\max}, \tag{17}$$

where $\lambda_{\min}$ and $\lambda_{\max}$ are the least and greatest eigenvalues of $\hat{K}_S$, respectively (or more generally, the infimum and supremum of the spectrum of $\hat{K}_S$). Thus the problem of interest now becomes the determination of $\lambda_{\min}$ and $\lambda_{\max}$.

In order to proceed, suppose that the subregion $S \subset \Gamma$ has the general form shown in Fig. 1.

Here F_1 and F_2 are real-valued functions defined for $b \leq q \leq c$, and satisfying $F_1(b) = F_2(b)$, $F_1(c) = F_2(c)$, and $F_2(q) \geq F_1(q)$ for $b < q < c$. Each function need only be piecewise continuous, and $b = -\infty$ and/or $c = \infty$ is allowed. For such a subregion, the characteristic function has the form

$$\chi_S(q, p) = \begin{cases} 1 & b < q < c, \quad F_1(q) < p < F_2(q), \\ 0 & \text{otherwise}, \end{cases} \tag{18}$$
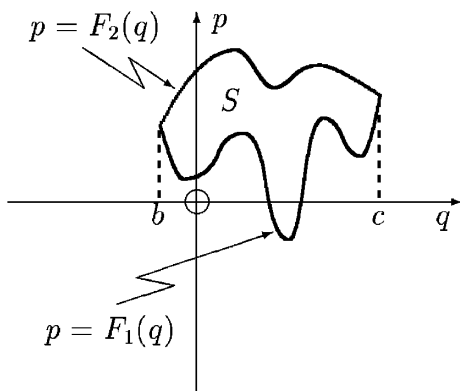
FIG. 1.   A typical region S in the phase plane.

and the kernel (16) becomes

$$K_S(x, y) = \frac{1}{2\pi} \int_{F_1(x+y/2)}^{F_2(x+y/2)} e^{ip(x-y)} \, dp$$

$$= \frac{e^{i(x-y)F_2(x+y/2)} - e^{i(x-y)F_1(x+y/2)}}{2\pi i(x - y)}, \quad (19)$$

for $2b < (x + y) < 2c$, and 0 otherwise. Note that the singularity at $x = y$ is only apparent. Then (15) becomes

$$(\hat{K}_S \psi)(x) = \int_{2b-x}^{2c-x} \frac{e^{i(x-y)F_2(x+y/2)} - e^{i(x-y)F_1(x+y/2)}}{2\pi i(x - y)}$$

$$\times \psi(y) \, dy. \quad (20)$$

More generally, the subregion S may consist of several nonintersecting parts $S_1, S_2, \ldots$ of the same general type, even on overlapping q intervals. It is easily seen that in such a case $\hat{K}_S = \hat{K}_{S_1} + \hat{K}_{S_2} + \cdots$ However, in general $[\hat{K}_{S_1}, \hat{K}_{S_2}] \neq 0$, etc., so that the bounds associated with different subregions cannot be added.

Note also that the extremal values of Q_S and $Q_{S'}$ are the same if S is transformed into S' by a canonical transformation of Γ of the form

$$q' = \alpha q + \beta p + \gamma, \qquad p' = \mu p + \nu q + \rho, \quad (21)$$

where α, β, γ, μ, ν, and ρ are real constants satisfying $\alpha\mu - \beta\nu = 1$. In particular, the case of any circular or elliptical region of area πa^2 can be reduced to the case of a circular disk of radius a, centered at the origin.

In this case, the operator $\hat{K}_S$ (let $\hat{K}_a$ denote it now) is given from (20) by

$$(\hat{K}_a \psi)(x) = \int_{-2a-x}^{2a-x} \frac{\sin[(x - y)\sqrt{a^2 - (x + y)^2/4}]}{\pi(x - y)}$$

$$\times \psi(y) \, dy, \quad (22)$$

for $-\infty < x < \infty$, and it is not hard to check that $\hat{K}_a$ commutes with the simple harmonic oscillator Hamilton-

ian operator $\hat{H}$ defined by

$$\hat{H} \psi(x) = -\frac{d^2\psi(x)}{dx^2} + x^2\psi(x). \quad (23)$$

This is explained by the fact that $\hat{H}$ generates transformations of the wave function corresponding to rotations in the phase plane, which leave the disk invariant. It follows that for *every* value of a the eigenfunctions of $\hat{K}_a$ are the oscillator eigenfunctions

$$\psi_n(x) = H_n(x)e^{-x^2/2}, \qquad n = 0, 1, \ldots, \quad (24)$$

where H_n is the Hermite polynomial [13].

According to (14), the eigenvalue $\lambda_n(a)$ of $\hat{K}_a$ corresponding to the eigenfunction (24) must equal the total quasiprobability on the disk of radius a, as determined by the Wigner function W_n (say) corresponding to that eigenfunction. Since it is known [2,12] that

$$W_n(q, p) = (-1)^n \pi^{-1} L_n(2[p^2 + q^2])e^{-(p^2+q^2)}, \quad (25)$$

where L_n is the Laguerre polynomial [13], it follows that

$$\lambda_n(a) = (-1)^n \int_0^{a^2} L_n(2u) \, e^{-u} \, du. \quad (26)$$

Thus $\lambda_0(a) = 1 - e^{-a^2}$, $\lambda_1(a) = 1 - (1 + 2a^2)e^{-a^2}$, $\lambda_2(a) = 1 - (1 + 2a^4)e^{-a^2}$, $\lambda_3(a) = 1 - (1 + 2a^2 - 2a^4 + \frac{4}{3}a^6)e^{-a^2}$, etc.

In summary,

$$\int_{-2a-x}^{2a-x} \frac{\sin[(x - y)\sqrt{a^2 - (x + y)^2/4}]}{\pi(x - y)} \psi_n(y) \, dy$$

$$= \lambda_n(a)\psi_n(x), \quad (27)$$

with ψ_n as in (24) and λ_n as in (26).

Figure 2 shows the graphs of λ_n *versus* a for $n = 0, 1, 2, 3$, and also the graphs of $\lambda_{\max}$ and $\lambda_{\min}$ (bold lines). Note that $\lambda_{\max}(a) = \lambda_0(a) = 1 - e^{-a^2}$, whereas the graph of $\lambda_{\min}$ has the peculiar scalloped shape shown, because $\lambda_{\min}(a) = \lambda_1(a)$ for $0 \leq a < a_1$, $\lambda_{\min}(a) = \lambda_2(a)$ for $a_1 \leq a < a_2$, etc., where a_1 is the greatest value of a at which $\lambda_1(a) = \lambda_2(a)$, a_2 is the greatest value of a at which $\lambda_2(a) = \lambda_3(a)$, etc. Thus $a_1 = 1$, $a_2 = \sqrt{(3 + \sqrt{3})/2}$, etc.

With the introduction of the appropriate dimensional factors, the result is that the integral of any pure-state or mixed-state Wigner function over any circular or elliptical region with area $\pi a^2\hbar$ in the phase plane lies in the interval $[\lambda_{\min}(a), \lambda_{\max}(a)]$, in contrast to the integral of any classical density, which lies in $[0, 1]$. According to quantum mechanics, any quasiprobability distribution determined by quantum tomography (in particular) is described by a Wigner function [8–10]. For such a
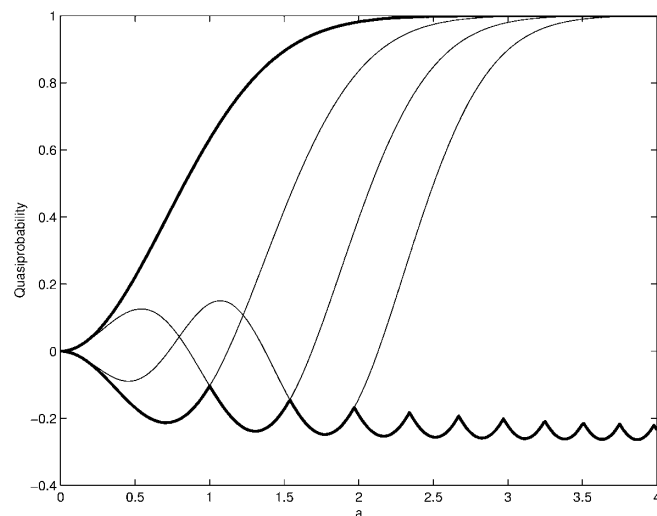
FIG. 2.   Left to right: graphs of λ_n for $n = 0, 1, 2, 3$, and also of $\lambda_{\max}$, $\lambda_{\min}$ (bold lines).

distribution, the quasiprobability on disks of various radii, centered on regions where the distribution is most negative, for example, could be estimated and checked for consistency against the theoretical bounds. Of course, experimental data are inevitably subject to noise for various reasons. While there are known techniques to allow for noise in the reconstruction of densities from more primitive data [8,14], this would obviously limit the power of the proposed check. A more subtle complication is that reconstruction algorithms may invoke quantum mechanical arguments [8–10], and any check would be satisfied trivially in a given case if these arguments *forced* a reconstructed density to satisfy the theoretical bounds. Any given reconstruction algorithm would have to be analyzed carefully in this regard to ensure that a check was meaningful.

If these difficulties could be overcome, might the proposed check be elevated to the level of a test of quantum mechanics itself? The assumptions underlying the theory of the Wigner function are very few: the linear vector space of states, the Born interpretation, and the conjugate relations between coordinates and momenta. However, quantum mechanics has been so well tested at the energy scales of the present experiments that any violations, if indeed there are any, must surely be exceedingly small, and very probably beyond present capabilities of resolution amidst noise.

Eigenvalue problems corresponding to other shapes such as squares and triangles are easily formulated, but do not seem to be exactly solvable. They could be tackled numerically. Exact results for disks can be extended to the case of an annular region (and more generally the case of several concentric annuli), because the operators $\hat{K}_a$ commute for different a, and have common eigenfunctions. This may be particularly useful in checking distributions determined by the "ring method" [6].

These ideas can be extended to systems with more degrees of freedom, and to systems with spin.

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