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Wigner quantisation of arrival time and oscillator phase

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Abstract. By means of the Wigner distribution function an expression is derived for the quasiprobability that a free particle in one dimension arrives at the origin during a given time interval and also for the quasiprobability that the phase of a one-dimensional harmonic oscillator lies in a given segment of the circle. It is shown that the best bounds on these quasiprobabilities p are $-0.1559 \leqslant p \leqslant 1.0077$, independent of the size of the interval. It is shown that on disjoint unions of infinitely many intervals the quasiprobabilities may add up to any positive or negative real value. It is briefly indicated how negative probabilities can be avoided altogether in an alternative approach to the quantisation of arrival time and oscillator phase.

1. Introduction

In a classic paper [1] Wigner showed how to construct for each state of a non-relativistic quantum system a function on the phase space of the corresponding classical system, which could be interpreted—with caution—as a probability density. Formally, Wigner's method allows the calculation of expectation values for any classical observable given as a function on phase space. It is one of the basic properties of Wigner functions that the integral of this function over a strip in phase space of the form $\{(p, q)|q \in I\}$ (I a subset of configuration space) coincides with the quantum theoretical probability for the system to be in the set I, calculated with the standard position observable. Similarly, the marginals of Wigner's probability distribution with respect to q coincide with the standard momentum observable. Thus the Wigner function formally provides a joint probability for position and momentum, which is bilinear in the wavefunction (as any quantum theoretical expectation value should be). Hence it is clear from the uncertainty relations that there has to be a drawback in this scheme. The trouble is that the Wigner function is not necessarily positive, so the 'probability' for (p, q) to be in some subset of phase space may turn out to be negative. In fact, one may show by simple examples that the Wigner function need not even be integrable, so that an infinite negative probability and an infinite positive probability cancel formally to give the value one for the total probability. This is the reason for calling the Wigner function a 'quasiprobability density'.

In spite of this occurrence of negative probabilities the Wigner function has proved to be a useful tool in many applications (see [2] for some recent examples and further references). From the beginning [1] an important application has been the study of the semiclassical ($\hbar \to 0$) asymptotics of quantum mechanics [3]. Since a truncated asymptotic expansion of a positive quantity need not be positive, the non-positivity of the Wigner function presents no difficulties in this context. Another area of successful

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applications has been the study of pseudodifferential operators [4], where positivity plays a subordinate role. However, it is a different matter whether the Wigner function provides sensible idealised descriptions of real measuring devices. In this case it is reasonable either to demand an explanation why the quantum states prepared in a laboratory happen to be among those giving positive results, or else to use another theoretical approach giving positive probabilities for all states (see § 5).

In this paper we consider quasiprobabilities calculated from the Wigner function by integrating over a sector in phase space (for one degree of freedom). These quantities have two different simple classical interpretations. On the one hand, $t=-mq/p$ is the time at which a free particle of mass m with initial momentum and position (p, q) will reach (or has reached) the origin $q=0$. Clearly, the lines $t=$ constant are straight lines through the origin and hence the subset of phase space corresponding to $t_1 \leqslant t \leqslant t_2$ and a definite sign of momentum will be a sector with the tip at the origin. On the other hand, a sector corresponds to an interval $\alpha_1 \leqslant \alpha \leqslant \alpha_2$ of the polar angle α in phase space, i.e. the phase of an oscillator with Hamiltonian $H=\frac{1}{2}(p^2+q^2)$. The integrals over sectors have properties between those of integrals over strips on the one hand (where the Wigner function gives sensible results, but yields nothing new beyond the predictions made by the standard observables) and integrals over arbitrary measurable sets on the other hand (where the Wigner function often gives absurd results).

After introducing the necessary notation and listing some basic properties and formulae for the Wigner function in § 2, it will be applied to arrival times and oscillator phases in § 3. In § 4 we will show that the integral over a sector is equal to the expectation value of an operator, which is not positive (so that the catastrophe of negative probabilities does happen in this case) but bounded (so that the catastrophe is in one sense mild) and we will explicitly diagonalise all such operators. We will also show that integrals over unions of sectors may still range from $-\infty$ to $+\infty$, so in general the quasiprobability distributions obtained by this method for arrival time and oscillator phase may be quite useless. In § 5 we briefly indicate how these difficulties may be avoided from the outset by a different approach to the quantisation of classical observables. This approach depends on further details of the system. In particular, the positive operators corresponding to a sector in phase space are now different in the cases of arrival time and oscillator phase.

2. The Wigner function

For simplicity we shall consider only systems with one degree of freedom. Let D be a density matrix describing a possibly mixed quantum state, i.e. an operator $D \geqslant 0$ with $\operatorname{Tr} D=1$. Such an operator is given by an integral kernel $D(\cdot,\cdot): \mathbb{R}^2 \to \mathbb{C}$ in momentum space. If $D=\Sigma_i \lambda_i |\psi_i\rangle\langle\psi_i|$ with $\lambda_i \geqslant 0$ and $\Sigma_i \lambda_i \|\psi_i\|^2=1$ is a decomposition of D into pure states, then this kernel equals $D(p_1, p_2)=\Sigma_i \lambda_i \overline{\psi_i(p_1)}\psi_i(p_2)$. In terms of this kernel the Wigner function $\rho(D;\cdot,\cdot)$ is defined as

$$\rho(D; p, q)=\int \mathrm{d}p' \,\mathrm{e}^{-\mathrm{i}p'q} D(p+\tfrac{1}{2}p', p-\tfrac{1}{2}p'). \tag{1}$$

Here we have chosen the normalisation $(2\pi)^{-1}\int \mathrm{d}p\, \mathrm{d}q\, \rho(D; p, q)=\operatorname{Tr} D$. An alternative definition of ρ is [5]

$$\rho(D; p, q)=2 \operatorname{Tr}(D W(p, q) \Pi W(p, q)^*) \tag{2}$$

where $(\Pi\psi)(p)=\psi(-p)$ is the parity operator and $W(p, q)$ the Weyl operator

$$(W(p, q)\psi)(p')=\exp(\tfrac{1}{2}\mathrm{i}pq-\mathrm{i}p'q)\psi(p'-p). \tag{3}$$

The operators $W(p, q)$ are unitary and are determined up to unitary equivalence and multiplicities [6] by the Weyl relation

$$W(p_1, q_1)W(p_2, q_2)=\exp[\tfrac{1}{2}\mathrm{i}(p_1q_2-q_1p_2)]W(p_1+p_2, q_1+q_2). \tag{4}$$

The bracket in the exponent, considered as a bilinear form in the two vectors (p_i, q_i), is called the symplectic form and is to be considered as a fundamental geometric feature of phase space.

The expression (2) shows that ρ is everywhere bounded by 2, which agrees with the intuition that the phase space probability density of a quantum state cannot have high peaks. Since $W(p, q)\Pi W(p, q)^*=W(2p, 2q)\Pi$, the quantum version of the Riemann–Lebesgue lemma [7, proposition 3.4(6)] implies that ρ is always continuous and goes to zero at infinity. Moreover, since D is a Hilbert–Schmidt operator, $\rho(D;\cdot,\cdot)$ is a square integrable function on phase space [7, proposition 3.4.(4)]. We say that a density matrix D is tempered if all partial derivatives of $D(p_1, p_2)$ fall off faster than any power at infinity. In this case the Wigner function, being a partial Fourier transform of D with respect to the difference variable, has the same property. In particular, $\rho(D;\cdot,\cdot)$ is integrable for tempered density matrices. However, the Wigner function may fail to be integrable, as the example $D=|\psi\rangle\langle\psi|$ with $\psi(p)=1$ for $|p|<1$ and $\psi(p)=0$ otherwise shows. For further topological properties of Wigner functions and the associated Wigner–Weyl correspondence between tempered distributions on phase space and quadratic forms in Hilbert space the reader is referred to [8, 9].

When $D=|\psi\rangle\langle\psi|$ is a pure state, ρ is positive if and only if ψ is a complex Gaussian [10, 11]. It is an open problem to give a characterisation of mixed states D with positive Wigner functions. A remarkable property of Wigner functions, which is best understood in terms of the calculus developed in [7], is that the convolution of two Wigner functions is positive and integrable. Thus, in a sense, the non-negativity of Wigner functions is a phenomenon peculiar to small regions in phase space (compared to the limits set by the Heisenberg inequality), which is washed out if the function is averaged with a Gaussian of sufficiently large spread.

An important property of the Wigner correspondence is its covariance with respect to the group G of affine symplectic transformations: it is clear from (2) that a phase-space translation $D\mapsto W(p, q)DW(p, q)^*$ of a state D becomes a shift $\rho(p', q')\mapsto\rho(p'-p, q'-q)$ of Wigner functions. A similar property holds for linear maps $\sigma:\mathbb{R}^2\to\mathbb{R}^2$ preserving the symplectic form. For such maps the operators $\tilde{W}(p, q)=W(\sigma(p, q))$ again satisfy the Weyl relations. Hence von Neumann's uniqueness theorem [6] implies the existence of a unitary operator U_σ (unique up to a phase) satisfying $U_\sigma W(p, q)U_\sigma^*=W(\sigma(p, q))$. Obviously, the operators U_σ form a representation up to a factor of the group of symplectic linear transformations. Together with the Weyl operators representing the translations we thus have a representation of the affine symplectic group G, which is sometimes called the metaplectic representation. Classically as well as quantum mechanically the generators of one-parameter subgroups of G are precisely the Hamiltonians which are at most quadratic in position and momentum. Since the parity operator Π commutes with U_{G}, equation (2) implies the covariance property

$$\rho(U_\sigma DU_\sigma^*; p, q)=\rho(D;\sigma^{-1}(p, q)). \tag{5}$$

Special one-parameter subgroups of G needed later are the free time evolution $U_t = \exp(\mathrm{i}tP^2/2m)$ corresponding to the maps $(p, q) \mapsto (p, q+pt/m)$, the time evolution of the oscillator $U_\alpha = \exp[\mathrm{i}\alpha\frac{1}{2}(P^2+Q^2)]$ corresponding to $(p, q) \mapsto (p\cos\alpha + q\sin\alpha, -p\sin\alpha + q\cos\alpha)$, and the dilatation group $U_\lambda = \exp[\mathrm{i}\lambda\frac{1}{2}(PQ+QP)]$ corresponding to $(p, q) \mapsto (\mathrm{e}^\lambda p, \mathrm{e}^{-\lambda} q)$.

3. Quantisation of arrival time and oscillator phase

Now let $f: \mathbb{R} \to \mathbb{R}$ represent some function of the classical arrival time $t = -q/p$, i.e. the time determined from the equation $q + pt = 0$. (From now on we choose units so that the mass m of the particle is $m = 1$.) We are interested in the expectation values of all these functions, i.e. in

$$
\begin{aligned}
(2\pi)^{-1} \int & \mathrm{d}p\,\mathrm{d}q f(-q/p)\rho(D; p, q) \\
&= (2\pi)^{-1} \int \mathrm{d}p\,\mathrm{d}q\,\mathrm{d}p' f(-q/p)\exp(-\mathrm{i}qp')D(p+\tfrac{1}{2}p', p-\tfrac{1}{2}p') \\
&= (2\pi)^{-1} \int \mathrm{d}p\,\mathrm{d}p'\,\mathrm{d}t|p| f(t)\exp(\mathrm{i}tpp')D(p+\tfrac{1}{2}p', p-\tfrac{1}{2}p') \\
&= (2\pi)^{-1} \int \mathrm{d}t f(t) \int \mathrm{d}p_1\,\mathrm{d}p_2\,\tfrac{1}{2}|p_1+p_2| \exp[\tfrac{1}{2}\mathrm{i}t(p_1^2-p_2^2)]D(p_1, p_2).
\end{aligned}
$$

Thus

$$
\rho_T(D; t) = (2\pi)^{-1} \int \mathrm{d}p_1\,\mathrm{d}p_2\,\tfrac{1}{2}|p_1+p_2| \exp[\tfrac{1}{2}\mathrm{i}t(p_1^2-p_2^2)]D(p_1, p_2) \tag{6}
$$

represents the quasiprobability density for arrival at the origin at time t. The exponential factor in this integral expresses the covariance of this density with respect to the free time evolution: we have $\rho_T(D; t) = \rho_T(U_t^* D U_t; 0)$ where U_t denote the unitary time evolution operators. The density $\rho_T(D; 0)$ is determined by the kernel $p_1, p_2 \mapsto \frac{1}{2}|p_1+p_2|$. This kernel is not positive definite, so it is clear that ρ_T may become negative for suitable D.

It is interesting to consider the special case of density matrices which are supported by the quadrant $p_1 \geq 0$, $p_2 \geq 0$. Thus all particles in the ensemble described by D 'travel to the right'. In this case the absolute value in (6) may be omitted. If $D = |\psi\rangle\langle\psi|$ is a pure state with $\psi(p) = 0$ for $p \leq 0$, and

$$
\hat{\psi}_t(x) = (2\pi)^{-1/2} \int \mathrm{d}p \exp(\mathrm{i}px - \tfrac{1}{2}\mathrm{i}tp^2)\psi(p)
$$

denotes the wavefunction in position space at time t, then

$$
\rho_T(D; t) = (1/2\mathrm{i})(\overline{\hat{\psi}_t(0)}\hat{\psi}_t'(0) - \overline{\hat{\psi}_t'(0)}\hat{\psi}_t(0)) \tag{7}
$$

coincides with the usual probability current at position $x = 0$, where the prime denotes the derivative. Integrating this over time and observing that for $t \to -\infty$ $\hat{\psi}_t$ is concentrated on the negative half-axis [12] we obtain

$$
\int_{-\infty}^{t} \mathrm{d}t'\,\rho_T(D, t') = \int_0^\infty \mathrm{d}x |\hat{\psi}_t(x)|^2. \tag{8}
$$

This formula has the classical interpretation that among particles travelling to the right those arriving at $x=0$ before t are the same as those located in the positive half-axis at time t. The Wigner quantisation of arrival time is in accordance with this intuition. What is paradoxical, however, is that ρ_T may be negative even if ψ contains only positive momenta. Hence there may be a net flow of probability from the positive to the negative axis in position space. In the next section we shall compute a uniform bound on the size of the integrated flow over any time interval, and we shall show that the absolute variation of $t\mapsto\int_0^\infty dx|\hat{\psi}_t(x)|^2$ may be infinite.

We now turn to the derivation of an expression for the quasiprobability density $\rho_\Phi(D;\alpha)$ for the oscillator phase α. The covariance of the density ρ_T with respect to the free-particle time evolution was manifest in (6), because the evolution operators act by multiplication in momentum space. Similarly, we have the following formula for the density ρ_Φ in terms of the eigenbasis $|n\rangle$, $n\in\mathbb{N}$, of the Hamiltonian $\frac{1}{2}(P^2+Q^2)$.

Lemma 1. Let D be the density matrix with Wigner function $\rho(D;\cdot,\cdot)$. Then

$$(2\pi)^{-1}\int r\,dr\,d\alpha\, f(\alpha)\rho(D;r\cos\alpha, r\sin\alpha)=(2\pi)^{-1}\int d\alpha\, f(\alpha)\rho_\Phi(D;\alpha)$$

with

$$\rho_\Phi(D;\alpha)=\sum_{n,m}\Omega_{nm}\langle m|D|n\rangle\exp[i(m-n)\alpha] \tag{9}$$

and

$$\Omega_{nm}=(n!m!)^{1/2}\,i^{n-m}\sum_{k\leq n,m}(-1)^k 2^{(n+m)/2-k}\frac{\Gamma(\frac{1}{2}(n+m)-k+1)}{(n-k)!(m-k)!k!}. \tag{10}$$

Sketch of proof. The easiest way to obtain the coefficients Ω_{nm} is to use the non-normalised coherent vectors $C(u)=\sum_n u^n(n!)^{-1/2}|n\rangle$ $(u\in\mathbb{C})$ as a generating function. These vectors satisfy the relations $\langle C(u),C(v)\rangle=\exp(\bar{u}v)$ and $W(p,q)C(u)=\exp[-\bar{z}(u+\frac{1}{2}z)]C(u+z)$ with $z=(1/\sqrt{2})(q+ip)$. Hence with formula (2) we obtain for coherent dyads $D=|C(u)\rangle\langle C(v)|$ the Wigner function

$$\rho(|C(u)\rangle\langle C(v)|;p,q)=2\exp(-2|z|^2+2\bar{v}z+2\bar{z}u+\bar{v}u).$$

Inserting this into the first equation of the lemma and carrying out the radial integration we get with $r\,e^{-i\alpha}=\sqrt{2}z$ and $\zeta=i\bar{v}\,e^{-i\alpha}-i\,e^{i\alpha}u$:

$$\sum_{nm}\Omega_{nm}u^m\bar{v}^n(n!m!)^{-1/2}\exp[i(m-n)\alpha]=e^{-\bar{v}u}\int 2r\,dr\exp(-r^2+\sqrt{2}\zeta r)$$
$$=\left(\sum_k\frac{(-\bar{v}u)^k}{k!}\right)\left(\sum_n\frac{(\sqrt{2}\zeta)^n}{n!}\int 2r\,dr\,r^n\exp(-r^2)\right).$$

The integral is equal to $\Gamma(\frac{1}{2}n+1)$. Expanding the binomial ζ^n and comparing coefficients of $\bar{v}^n$ and u^m we find (10) and the lemma is proved.

From the α dependence of (9) it is immediately clear that $\rho_\Phi(D;\alpha)=\rho_\Phi(U_\alpha^* DU_\alpha,0)$, where U_α now denotes the time evolution operators for the oscillator Hamiltonian. Setting $n=m$ in (10) we obtain $\Omega_{nn}=1$, so that $(2\pi)^{-1}\int d\alpha\,\rho_\Phi(D;\alpha)=\sum_n\langle n|D|n\rangle=\mathrm{Tr}\,D$ as required of a probability density. The positivity properties of ρ_Φ now hinge on the positive definiteness of the matrix Ω and will be considered below.

4. Negative probabilities

By a pointed sector in phase space we mean a convex set bounded by two non-parallel straight lines extending to infinity. An example is $S=\{(p,q)|t_1\leqslant -(q/p)\leqslant t_2;\ p\geqslant 0\}$, i.e. the set of classical states describing particles which travel to the right and reach the origin between the times t_1 and t_2. By a double sector we mean the union of two 'opposite' sectors with the same tip and the same bounding straight lines, like $S'=\{(p,q)|t_1\leqslant -(q/p)\leqslant t_2\}$. If we can calculate the integral of all Wigner functions over a given sector S, then we can calculate such integrals for all sectors obtained from S by affine symplectic transformations by using the basic covariance property (5). It is easy to see any two pointed (respectively double) sectors are connected by an affine symplectic transformation. The following proposition makes use of the fact that for every sector S there is an essentially unique one-parameter group of affine symplectic transformations leaving S invariant. If the tip of S is the origin, the generator of this group is given by a matrix with zero trace, whose eigenvectors point along the sides of S.

Proposition 2. Let $S\subset\mathbb{R}^2$ be a pointed or double sector in phase space. Then there is a unique bounded Hermitian operator A_S such that for any tempered density matrix

$$(2\pi)^{-1}\int_{(p,q)\in S} \mathrm{d}p\,\mathrm{d}q\,\rho(D;p,q)=\mathrm{Tr}(DA_S).$$

Moreover, the spectrum of A_S is purely absolutely continuous. For pointed sectors the spectrum is equal to the union of the intervals $[-s_-,0]$ with multiplicity 2 and $[0,s_+]$ with multiplicity 1. For double sectors the spectrum is an interval of the form $[-s,1+s]$ with multiplicity 2.

The constants are $s_-\approx 0.155\,940$, $s_+\approx 1.007\,678$ and $s\approx 1.236\,824$.

Proof. By the above remarks it suffices to consider one particular sector of each kind. As the prototype of a pointed sector we shall take $S=\{(p,q)|p\geqslant 0,q\geqslant 0\}$. The one-parameter group leaving this sector invariant is the group of transformations $(p,q)\mapsto(\mathrm{e}^{\lambda}p,\mathrm{e}^{-\lambda}q)$. The idea of the proof is to diagonalise the operators A_S together with the unitarities representing this group.

We begin by calculating the expectation I^{ε} of $F_{\varepsilon}(p,q)=\Theta(p)\Theta(q)\,\mathrm{e}^{-\varepsilon pq}$ with respect to the Wigner function of a pure state $D=|\psi\rangle\langle\psi|$, where Θ denotes the unit step function with $\Theta(x)=1$ for $x\geqslant 0$ and $\Theta(x)=0$ otherwise. In the limit $\varepsilon\to 0$ F_{ε} becomes the characteristic function of the sector S and for tempered functions ψ the limit $\lim_{\varepsilon\to 0} I^{\varepsilon}$ exists and is equal to $(2\pi)^{-1}\int_{(p,q)\in S}\mathrm{d}p\,\mathrm{d}q\,\rho(D;p,q)$ by dominated convergence. Then

$$\begin{aligned}
I^{\varepsilon}&=(2\pi)^{-1}\int \mathrm{d}p\,\mathrm{d}q\,\Theta(p)\Theta(q)\,\mathrm{e}^{-\varepsilon pq}\int \mathrm{d}p'\,\mathrm{e}^{-\mathrm{i}p'q}\bar{\psi}(p+\tfrac{1}{2}p')\psi(p-\tfrac{1}{2}p')\\
&=(2\pi)^{-1}\int \mathrm{d}p_1\,\mathrm{d}p_2\,\Theta(p_1+p_2)\bar{\psi}(p_1)\psi(p_2)\\
&\qquad\times\int_0^{\infty}\mathrm{d}q\,\exp[-\mathrm{i}(p_1-p_2)q-\tfrac{1}{2}\varepsilon(p_1+p_2)q]\\
&=(2\pi)^{-1}\int \mathrm{d}p_1\,\mathrm{d}p_2\,\bar{\psi}(p_1)\psi(p_2)\frac{\Theta(p_1+p_2)}{\frac{1}{2}\varepsilon(p_1+p_2)+\mathrm{i}(p_1-p_2)}.
\end{aligned}$$

This integral is the sum of the four integrals $I^\varepsilon(\sigma_1, \sigma_2)$ over quadrants distinguished by $\sigma_i = \operatorname{sgn}(p_i) = \pm 1$. In each of these integral we shall substitute $p_i = \sigma_i\, e^{2\lambda_i}$, obtaining

$$I^\varepsilon(\sigma_1, \sigma_2) = (2\pi)^{-1} \int_{-\infty}^{+\infty} d\lambda_1 \int_{-\infty}^{+\infty} d\lambda_2\, \overline{\sqrt{2}\, e^{\lambda_1}\psi(\sigma_1\, e^{2\lambda_1})}\, \sqrt{2}\, e^{\lambda_2}\psi(\sigma_2\, e^{2\lambda_2}) K^\varepsilon_{\sigma_1,\sigma_2}(\lambda_1 - \lambda_2)$$

with

$$K^\varepsilon_{\sigma_1,\sigma_2}(\lambda) = \frac{2\Theta(\sigma_1\, e^{\lambda} + \sigma_2\, e^{-\lambda})}{\frac{1}{2}\varepsilon(\sigma_1\, e^{\lambda} + \sigma_2\, e^{-\lambda}) + i(\sigma_1\, e^{\lambda} - \sigma_2\, e^{-\lambda})}.$$

Thus

$$K^\varepsilon_{++}(\lambda) = 2(\varepsilon \cosh(\lambda) + 2i \sinh(\lambda))^{-1} \qquad K^\varepsilon_{+-}(\lambda) = 2\Theta(\lambda)(\varepsilon \sinh(\lambda) + 2i \cosh(\lambda))^{-1}$$

$$K^\varepsilon_{-+}(\lambda) = \overline{K^\varepsilon_{+-}(-\lambda)} \qquad K^\varepsilon_{--}(\lambda) = 0.$$

Since $I^\varepsilon(\sigma_1, \sigma_2)$ is the expectation of a convolution kernel, we pass to the Fourier transforms

$$\tilde{\psi}_\sigma(\eta) := (2\pi)^{-1/2} \int d\lambda\; e^{i\lambda\eta}\sqrt{2}\, e^{\lambda}\psi(\sigma\, e^{2\lambda})$$

$$\hat{K}^\varepsilon_{\sigma_1,\sigma_2}(\eta) := (2\pi)^{-1} \int d\lambda\; e^{i\lambda\eta} K^\varepsilon_{\sigma_1,\sigma_2}(\lambda)$$

so that

$$I^\varepsilon = \sum_{\sigma_1,\sigma_2} I^\varepsilon(\sigma_1, \sigma_2) = \int_{-\infty}^{+\infty} d\eta \sum_{\sigma_1,\sigma_2} \overline{\tilde{\psi}_{\sigma_1}(\eta)}\hat{K}^\varepsilon_{\sigma_1,\sigma_2}(\eta)\tilde{\psi}_{\sigma_2}(\eta).$$

Since the functions $K^\varepsilon_{\sigma_1,\sigma_2}$ fall off exponentially as $\lambda \to \pm\infty$, their Fourier transforms are bounded. Moreover, the transform of ψ is normalised such that $\int d\eta(|\tilde{\psi}_+(\eta)|^2 + |\tilde{\psi}_-(\eta)|^2) = \int dp|\psi(p)|^2 = \|\psi\|^2$. We shall show that the functions $\hat{K}^\varepsilon_{\sigma_1,\sigma_2}(\eta)$ stay uniformly bounded and converge pointwise to a limit $\hat{K}_{\sigma_1,\sigma_2}(\eta)$ as $\varepsilon \to 0$. Hence I^ε converges to a limit, which is a bounded quadratic form in ψ, i.e. $I = \langle\psi, A_S\psi\rangle$ for a unique bounded operator A_S.

For diagonalising A_S it suffices to diagonalise for each $\eta \in \mathbb{R}$ the Hermitian 2×2 matrix $\hat{K}(\eta)$. A_S is thus unitary equivalent to a direct sum of the two multiplication operators on $\mathfrak{L}^2(\mathbb{R}, d\eta)$ multiplying with the eigenvalues $\Lambda_\pm(\eta)$ of the matrix $\hat{K}(\eta)$. For determining $\Lambda_\pm(\eta)$ we need to calculate the Fourier transforms $\hat{K}^\varepsilon_{\sigma_1,\sigma_2}$. In the Fourier integral for $\hat{K}^\varepsilon_{+-}$ the limit $\varepsilon \to 0$ can be carried out under the integral sign. The limit can be expressed by a Ψ function of Euler and is thus not an elementary function of η. $\hat{K}^\varepsilon_{++}$ can be evaluated by means of the residue theorem using the periodicity $K^\varepsilon_{++}(\lambda + i\pi) = -K^\varepsilon_{++}(\lambda)$. For this one considers a path along the real axis and back along the line $\operatorname{Im}\lambda = \pi$. The result is

$$\hat{K}_{++}(\eta) = (1 + e^{-\pi\eta})^{-1} \qquad \hat{K}_{--}(\eta) = 0$$

$$\hat{K}_{+-}(\eta) = \frac{1}{2\pi i}\int_0^\infty d\lambda\; e^{i\lambda\eta}\frac{1}{\cosh\lambda} = \overline{\hat{K}_{-+}(\eta)}$$

$$\Lambda_\pm(\eta) = \tfrac{1}{2}\hat{K}_{++}(\eta) \pm (\tfrac{1}{4}\hat{K}_{++}(\eta)^2 + |\hat{K}_{+-}(\eta)|^2)^{1/2}.$$

It is clear that $\Lambda_-(\eta)$ is negative and $\Lambda_+(\eta)$ is positive for all η. As $\eta\to+\infty$ $\hat{K}_{++}$ tends to 1 exponentially, whereas $\hat{K}_{+-}(\eta)$ tends to zero only like η^{-1}. Hence $\Lambda_+(\eta)\geq 1$ for sufficiently large η. The values $-s_-=\min_\eta \Lambda_-(\eta)$ and $s_+=\max_\eta \Lambda_+(\eta)$ given in the proposition are calculated numerically.

The case of double sectors is completely analogous. The operator A_{-S} belonging to the sector $-S=\{(p,q)|p\leq 0, q\leq 0\}$ is obtained from A_S by exchanging the signs of momenta. Thus A_S+A_{-S} is the operator of multiplication with the matrix

$$\tilde{K}_{\sigma_1,\sigma_2}(\eta)=\hat{K}_{\sigma_1,\sigma_2}(\eta)+\hat{K}_{-\sigma_1,-\sigma_2}(\eta)$$

with eigenvalues

$$\tilde{\Lambda}_\pm(\eta)=\hat{K}_{++}(\eta)\pm 2\,\mathrm{Re}\,\hat{K}_{+-}(\eta).$$

Again $s=\max_\eta \tilde{\Lambda}_+(\eta)$ is determined numerically. Proposition 2 is proved.

By this proposition the quasiprobability for sectors may be defined as $\mathrm{Tr}(DA_S)$ even if the Wigner function $\rho(D;\cdot,\cdot)$ is not integrable, and the integral $\int_{(p,q)\in S}\mathrm{d}p\,\mathrm{d}q\,\rho(D;p,q)$ makes no sense as it stands. One might try to extend this procedure to the definition of quasiprobabilities for more general sets $S_M=\{(p,q)|-q/p\in M\}$ for Borel sets $M\subset\mathbb{R}$. Clearly, this procedure works for finite unions of sectors. However, the following proposition shows that, as the number of sectors in a disjoint union increases, the total negative quasiprobability may diverge so that there is no hope for defining the quasiprobability for general sets S_M and all density matrices D.

Proposition 3. There is a unit vector $\psi\in\mathfrak{H}$ with the following property: for any $R\in\mathbb{R}$, $0<R<\infty$ there is a family of disjoint sectors S_ν ($\nu=1,\ldots,n$) in phase space such that

$$\sum_{\nu=0}^{n}\langle\psi, A_{S_\nu}\psi\rangle<-R.$$

Proof. Consider the family $\mathfrak{U}$ of operators of the form $\Sigma_{\nu=1}^n A_{S_\nu}$ for finite disjoint collections of sectors S_ν. Suppose to the contrary that for all unit vectors ψ the set of numbers $\{\langle\psi, A\psi\rangle|A\in\mathfrak{U}\}$ is bounded below. Then it is also bounded above, since for each collection $\{S_\nu\}$ there is a complementary collection $\{S'_\nu\}$ with $\Sigma_\nu A_{S_\nu}+A_{S'_\nu}=\mathbb{1}$. Hence by the uniform boundedness theorem [13] there is a constant C such that $\|A\|\leq C$ for all $A\in\mathfrak{U}$. Thus the proposition is proven by contradiction if we exhibit a sequence ψ_k of unit vectors and a sequence $A_k\in\mathfrak{U}$ such that $\langle\psi_k, A_k\psi_k\rangle\to-\infty$.

Let $|\psi_k\rangle=(1/\sqrt{2})(|0\rangle+|k\rangle)$, where $|n\rangle$ denotes the nth eigenstate of the oscillator. Then $\rho_\Phi(|\psi_k\rangle\langle\psi_k|;\alpha)=:\rho(\alpha)=\frac{1}{2}(\Omega_{00}+\Omega_{kk}+\mathrm{e}^{\mathrm{i}k\alpha}\Omega_{0k}+\mathrm{e}^{-\mathrm{i}k\alpha}\Omega_{k0})=1+|\Omega_{0k}|\cos[k(\alpha-\frac{1}{2}\pi)]$ with $\Omega_{0k}=\mathrm{i}^k|\Omega_{0k}|$ from lemma 1. We shall see below that $|\Omega_{0k}|\geq 1$ for large k, so ρ is negative on k disjoint intervals $[\alpha_\nu,\beta_\nu]$. On each of these intervals we have $\int_{\alpha_\nu}^{\beta_\nu}\mathrm{d}\alpha\;\rho(\alpha)=-k^{-1}\int_{-\gamma}^{+\gamma}\mathrm{d}\alpha(|\Omega_{0k}|\cos\alpha-1)=-2k^{-1}(|\Omega_{0k}|\sin\gamma-\gamma)\leq-2k^{-1}(|\Omega_{0k}|^2-1)^{1/2}+k^{-1}\pi$ with $\gamma=\cos^{-1}(|\Omega_{0k}|^{-1})\leq\pi/2$. Let S_ν, $\nu=1,\ldots,k$, denote the corresponding sectors in phase space. Then

$$\sum_\nu\langle\psi_k, A_{S_\nu}\psi_k\rangle=\int_{\rho(\alpha)<0}\mathrm{d}\alpha\,\rho(\alpha)\leq-2(|\Omega_{0k}|^2-1)^{1/2}+\pi.$$

It remains to be shown that $|\Omega_{0k}|$ is unbounded. From lemma 1 we have $|\Omega_{0k}| = 2^{k/2}\Gamma(\frac{1}{2}k+1)(k!)^{-1/2}$. Evaluating this with Stirling's formula we obtain $\ln(|\Omega_{0k}|) = \frac{1}{4}\ln(k\pi/2) + O(k^{-1})$.

5. Covariant observables

In this section we briefly describe how the negative probabilities of the Wigner quantisation of arrival time and oscillator phase can be avoided. A positive quantisation rule must assign to each density matrix D a suitable probability measure μ_D on some parameter space, which is equal to $\mathbb{R}$ for arrival times and equal to the circle S^1 for the oscillator phase. We require in addition that mixtures $\lambda D_1 + (1-\lambda)D_2$ $(\lambda \in [0, 1])$ of density matrices are mapped to the corresponding mixtures of probability measures. Hence for any Borel set σ the assignment $D \mapsto \mu_D(\sigma)$ is a positive affine functional on the set of density matrices, which implies the existence of a positive bounded operator $F(\sigma)$ with $\mu_D(\sigma) = \mathrm{Tr}[D \cdot F(\sigma)]$. Since each $\mu_D(\cdot)$ is supposed to be a probability measure, the set function $\sigma \mapsto F(\sigma)$ is a measure with values in the positive operators on Hilbert space, satisfying the normalisation condition $F(\mathbb{R}) = \mathbb{1}$ (respectively $F(S^1) = \mathbb{1}$). In the following we shall use the term 'observable' [14, 15] for such measures. We do not require each operator $F(\sigma)$ to be a projection, since this condition is not necessary for a statistical interpretation and is too restrictive for the constructions below.

We shall demand of an arrival time observable that it transforms correctly under the time translations. By this we mean that preparing the system earlier results in a shift of the arrival time distributions given by the observable, i.e. $\mathrm{Tr}(U_t D U_t^* F(\sigma)) = \mathrm{Tr}(D \cdot F(\sigma + t))$. Since this equation must hold for all states D, we have $U_t F(\sigma) U_t^* = F(\sigma + t)$. This covariance property was also noted for the Wigner quantisation of arrival time after (6). For a quantisation of the oscillator phase we shall impose the analogous condition $U_\alpha F(\sigma) U_\alpha^* = F(\sigma + \alpha)$ where the shift $\sigma \mapsto \sigma + \alpha$ is to be understood mod 2π.

There is a well developed theory of observables satisfying a covariance condition of this kind [16, 17]. It is based on a dilation construction by Naimark [18], which reduces the problem of constructing all covariant observables to finding only the projection valued covariant observables. These in turn have been thoroughly studied by Mackey under the name of 'systems of imprimitivity' [19]. In the two cases at hand one gets a complete classification of covariant observables by combining these two ideas.

The result of this analysis is the following: all covariant arrival time observables are given by the following analogue of (6):

$$\rho_T(D; t) = (2\pi)^{-1} \int \mathrm{d}p_1\, \mathrm{d}p_2\, k(p_1, p_2) \exp[\tfrac{1}{2}\mathrm{i}t(p_1^2 - p_2^2)] D(p_1, p_2) \tag{11}$$

where the kernel $\frac{1}{2}|p_1 + p_2|$ is replaced by a positive-definite kernel $k(p_1, p_2)$ satisfying the normalisation condition $k(p, p) = |p|$. The simplest example of this kind is the replacement of the arithmetic mean $\frac{1}{2}|p_1 + p_2|$ by the geometric mean $|p_1 p_2|^{1/2}$. We shall see below that this choice is even canonical in a sense to be specified. Similarly, all covariant observables for the oscillator phase are given by (9) where Ω is any positive-definite matrix satisfying the normalisation condition $\Omega_{nn} = 1$. An example in this case is the choice $\Omega_{nm} = 1$ for all $n, m \in \mathbb{N}$.

Thus there are infinitely many covariant observables for arrival time and oscillator phase. An analogous phenomenon is well known from quantisation rules in phase space: there are very many observables jointly measuring position and momentum in the sense that they are covariant with respect to phase space translations [7, proposition 3.3]. (However, none of them shares the extremely high symmetry (5) of the Wigner function.) This non-uniqueness of arrival time observables is physically quite reasonable since there are many different kinds of counters. So the choice of a particular arrival time observable will depend on the detailed description of the counter [19]. On the other hand, one may try to find observables for 'optimal' measurements of arrival time, which are more 'canonical'.

One criterion that can be used for this purpose is based on the observation that some of the covariant observables are very 'smeared out'. For example, choosing $\Omega_{nm}=\delta_{nm}$ in (9) assigns the uniform distribution to every density matrix. Therefore a good criterion should force the observable to be as sharp as possible under the constraint of covariance. One criterion of this kind has been introduced in [16]: for any observable F, any measurable function f on the parameter space of F, and any ψ in Hilbert space, we have the inequality:

$$\int |f(x)|^2\langle\psi, F(\mathrm{d}x)\psi\rangle - \left\| \int f(x)F(\mathrm{d}x)\psi \right\|^2 \geqslant 0. \tag{12}$$

This expression, called the variance form of F with respect to f, measures the intrinsic uncertainties associated with the observable F. It vanishes for projection valued observables F, but its vanishing on a dense domain for certain unbounded functions f does not imply that the observable is projection valued. We say that an observable has minimal variance in a certain class of observables, if for no other observable the variance form is smaller in all states. Those phase space observables for which the variances with respect to the coordinate functions p and q become minimal are precisely the observables formed with coherent states [16, 21]. In the case of arrival time observables the minimal variance condition, together with some symmetry requirements for reflections, which are necessary for distinguishing arrival at the origin from arrival at some other place, single out the arrival time observable with kernel $|p_1p_2|^{1/2}$. The proof is entirely analogous to the proof given in [16] for an analogue in three space dimensions. It turns out that for this observable the variance form is zero on its natural domain.

For the case of phase observables for the oscillator it is natural to demand that the variance with respect to the function $\mathrm{e}^{\mathrm{i}\alpha}$ be minimal, i.e. that

$$\|\psi\|^2 - \left\| \int \mathrm{e}^{\mathrm{i}\alpha}F(\mathrm{d}\alpha)\psi \right\|^2$$

cannot be decreased for all states ψ simultaneously by choosing another F. By using Naimark's construction [18] one can show that this condition implies that $\Omega_{nm} = \exp(\mathrm{i}\gamma_n - \mathrm{i}\gamma_m)$ for real numbers γ_n. Imposing covariance with respect to antiunitary time inversion forces γ_n to be a multiple of π, so $\Omega_{nm}=\pm 1$. Thus we arrive at a discrete set of phase observables, among which the choice $\Omega_{nm}\equiv 1$ appears to be distinguished.

All positive phase space observables can be obtained by averaging the Wigner function with suitable integrable functions [7]. Thus it is natural to ask whether the convolution of the densities ρ_T and ρ_Φ with suitable integrable functions can be one of the positive observables discussed in this section. At least for arrival time observables it is easy to see that this is not the case: the convolution of an observable specified by a kernel k (or the Wigner arrival time distribution) with an integrable function ξ gives another covariant observable with kernel $\tilde{k}(p_1, p_2) = \hat{\xi}(\frac{1}{2}(p_1^2 - p_2^2))k(p_1, p_2)$, where $\hat{\xi}$ denotes the Fourier transform of ξ with $\hat{\xi}(0) = 1$. We claim that the kernel $\hat{\xi}(\frac{1}{2}(p_1^2 - p_2^2))\frac{1}{2}(p_1 + p_2)$ is not positive definite for any ξ. For if it were positive, we should have for every p_1, p_2: $[\hat{\xi}(\frac{1}{2}(p_1^2 - p_2^2))\frac{1}{2}(p_1 + p_2)]^2 \leq p_1 p_2$. In the limit $p_2 \to 0$ with constant p_1 this implies $\hat{\xi}(\frac{1}{2}p_1^2) = 0$ for all p_1, i.e. $\xi = 0$, which is the claimed contradiction.

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