Nonnegative mixed states in Weyl–Wigner–Moyal theory

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Phys. Lett. A **128** (1988), 20–24

Abstract

We classify the gaussian Wigner functions corresponding to mixed states and show that, unlike the case of pure states, not all nonnegative mixed states are gaussian.

A theorem of Hudson [1], generalized to the n-dimensional case by Soto and Claverie [2], establishes that the only nonnegative distribution functions corresponding to pure states in the Weyl–Wigner–Moyal (WWM) formulation of Quantum Mechanics are the Wigner transforms of gaussian wavefunctions.

Recently, Littlejohn [3] posed this problem: which gaussian functions in phase space represent pure quantum states? These are, of course, all of the aforementioned transforms; they are themselves gaussians in phase space. But Littlejohn solved the question essentially by an elegant calculation within the autonomous, algebraic formulation of WWM theory based on the twisted product.

In this letter we enlarge on Littlejohn's work by establishing which gaussians in phase space correspond to states, pure *or mixed*. Furthermore, we show that the analogue of the Hudson–Soto–Claverie–Littlejohn result fails for mixed states: there are non-gaussian nonnegative functions in phase space representing quantum states.

We start by recalling the notion of twisted product of two functions in phase space:

$$(f \times g)(u) := \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} f(v)\, g(w)\, \exp[i(u^t J v + v^t J w + w^t J u)]\, dv\, dw$$

where $u^t = (q_1, \dots, q_n, p_1, \dots, p_n) \in \mathbb{R}^{2n}$ (^{t} denotes transpose), $v, w \in \mathbb{R}^{2n}$, $J = \begin{pmatrix} 0 & 1_n \\ -1_n & 0 \end{pmatrix}$, and $dv = (2\pi)^{-n}\, d^{2n}v$, with $d^{2n}v$ being Lebesgue measure. We have chosen units so that $\hbar = 2$. This is a continuous bilinear operation on $\mathcal{A} := L^2(\mathbb{R}^{2n})$. Let $\mathcal{I} := \{\, f \times g : f, g \in \mathcal{A} \,\}$. $\mathcal{A}$ and $\mathcal{I}$ correspond respectively to the ideals of Hilbert–Schmidt and trace-class operators on $L^2(\mathbb{R}^n)$, via the Weyl correspondence rule. We do not use that correspondence directly here; but we can norm $\mathcal{I}$ so as to be isomorphic to the space of trace-class operators with trace norm. Let $\mathcal{B}$ be the dual normed space of $\mathcal{I}$. We consider $\mathcal{B}$ as the space of quantum-mechanical observables; it is an algebra under the twisted product (isomorphic to the algebra of bounded operators on $L^2(\mathbb{R}^n)$.)

A *state* is an element of $\mathcal{I}$ which is positive in the algebraic sense, i.e.,

$$\langle \rho, f^* \times f \rangle := \int_{\mathbb{R}^{2n}} \rho(u)\, (f^* \times f)(u)\, du \geqslant 0 \quad \text{for all} \quad f \in \mathcal{B}.$$

Then $\rho = \omega^* \times \omega$ for some $\omega \in \mathcal{A}$. Also, one may show that ρ is the Wigner transform of a "density matrix" d:

$$\rho(q, p) = (2\pi)^{-n} \int_{\mathbb{R}^n} d(q + q', q - q') e^{ipq'} \, d^n q'.$$

Pure states are the Wigner transforms of density matrices of the form $\psi^*(q')\psi(q)$ and are identified by the condition $\rho \times \rho = \rho$. Mixed states are (generalized) convex combinations of pure states; our states are thus Wigner functions seen from a different viewpoint.

We remark the important equality:

$$\langle f, g \rangle := \int_{\mathbb{R}^{2n}} f(u)\, g(u)\, du = \int_{\mathbb{R}^{2n}} (f \times g)(u)\, du,$$

true whenever both sides of the equation make sense. We normalize the states by the condition that $2^{-n} \int \rho^2(u)\, du = 1$.

After these preliminaries, we recall Littlejohn's theorem.

Theorem 1 (Littlejohn)**.** *The normalized gaussian*

$$\rho(u) := 2^n (\det F)^{1/4} \exp(-\tfrac{1}{2} u^t F u) \tag{1}$$

is a pure state if and only if the matrix F (necessarily positive definite) is moreover symplectic.

The condition on F may be rephrased as follows: $F = S^t S$ for some symplectic matrix S. In fact, if $F = \exp(JB)$ with $B^t = B$, one can take $S = S^t = \exp(\tfrac{1}{2} JB)$.

Thus we assert the next result.

Theorem 2. *A normalized gaussian of the form* (1) *represents a quantum state if and only if there is a symplectic matrix S so that*

$$F = S^t \operatorname{diag}[\lambda_1, \dots, \lambda_n, \lambda_1, \dots, \lambda_n]\, S$$

where $0 < \lambda_i \leqslant 1$ for $i = 1, \dots, n$. Except for trivial translations this gives all states which may be represented by gaussians in phase space.

We break the proof into several steps.

1. Any positive definite real quadratic form is equivalent by symplectic conjugation to one given by the matrix $\operatorname{diag}[\lambda_1, \dots, \lambda_n, \lambda_1, \dots, \lambda_n]$ with $\lambda_i > 0$ for $i = 1, \dots, n$.

   This is a relatively old result in Classical Mechanics [4, 5]. For instance, when $n = 1$, if $F = \begin{pmatrix} a & b \\ b & c \end{pmatrix}$ has $a > 0$, $ac - b^2 > 0$, and if $d = \sqrt{ac - b^2}$, then

   $$F = S^t \begin{pmatrix} d & 0 \\ 0 & d \end{pmatrix} S \quad \text{with} \quad S = \begin{pmatrix} \sqrt{a/d} & b/\sqrt{ad} \\ 0 & \sqrt{d/a} \end{pmatrix}.$$

2. If Ξ is a "unitary" element of $\mathcal{B}$, i.e., $\Xi^* \times \Xi = \Xi \times \Xi^* = 1$, then the inner automorphism $\rho \mapsto \Xi^* \times \rho \times \Xi$ transforms states into states, preserving their pure or mixed character.

3. Linear canonical changes of coordinates in phase space are realized by automorphisms of this form; namely, for any symplectic matrix S there is a unitary $\Xi_S \in \mathcal{B}$ such that

$$(\Xi_S^* \times f \times \Xi_S)(u) = f(Su)$$

for any $f \in \mathcal{B}$ and in particular for a state.

Take $\Xi_S(u) := 2^n \det(1+S)^{-1/2} \exp[\frac{i}{2} u^t J (1+S)^{-1}(1-S)u]$. We shall omit the calculation of Ξ_S, referring instead to [6, 7]. We remark that the functions Ξ_S realize the metaplectic representation of Shale, Segal and Weil [8–10] in the framework of twisted product theory. (The formula should be modified when $\det(1+S) = 0$, but this is immaterial for our purposes.)

Thus we need only consider matrices of the form $\operatorname{diag}[\lambda_1, \dots, \lambda_n, \lambda_1, \dots, \lambda_n]$. In what follows we use the orthonormal basis of functions on phase space given in [11] as follows. For $n = 1$, $k \geqslant l$ (nonnegative integers) and $u = (q, p)$:

$$f_{kl}(u) := 2(-1)^l \sqrt{\frac{l!}{k!}} (q - ip)^{k-l} L_l^{k-l}(q^2 + p^2)\, e^{-(q^2+p^2)/2},$$

where the L_l^{k-l} are Laguerre polynomials; $f_{kl} := f_{lk}^*$ for $k < l$. For $n > 1$, write $u_i := (q_i, p_i)$ and $k = (k_1, \dots, k_n)$, $l = (l_1, \dots, l_n)$; then $f_{kl}(u) := f_{k_1 l_1}(u_1) \cdots f_{k_n l_n}(u_n)$.

The f_{kl} satisfy the important property: $f_{kl} \times f_{rs} = \delta_{lr} f_{ks}$ (Kronecker delta). The "diagonal" elements f_{kk} correspond to pure states of the n-dimensional harmonic oscillator.

4. A function of the form (1) with $F = \operatorname{diag}[\lambda_1, \dots, \lambda_n, \lambda_1, \dots, \lambda_n]$ and some $\lambda_i > 1$ is *not* a state.

It evidently suffices to consider the case $n = 1$. The first excited state of the harmonic oscillator is $f_{11}(H) = 2(2H - 1)e^{-H}$ where $H = \frac{1}{2}u^2 = \frac{1}{2}(q^2 + p^2)$. Recalling that $f_{11} \times f_{11} = f_{11}$, we get

$$\begin{aligned} \langle \rho, f_{11}^* \times f_{11} \rangle &= (\text{some positive constant}) \int_0^\infty (2H - 1)\, e^{-(\lambda+1)H}\, dH \\ &= (\text{some positive constant})\, \frac{1 - \lambda}{(1+\lambda)^2} < 0. \end{aligned}$$

5. For $n = 1$, $\beta > 0$, the function $f_\beta(q, p) := 2\sqrt{\tanh(\beta/2)} \exp\bigl(-\frac{1}{2}(q^2 + p^2)\tanh(\beta/2)\bigr)$ is a (mixed) state.

In fact, it is the Gibbs state of the 1-dimensional oscillator at inverse temperature β, since $f_\beta = \sqrt{2\sinh\beta} \sum_{k=0}^\infty e^{-(k+\frac{1}{2})\beta} f_{kk}$.

6. The function $f(u) := 2^n \sqrt{\lambda_1 \cdots \lambda_n} \exp(-\frac{1}{2}\lambda_1(q_1^2 + p_1^2) + \cdots + \lambda_n(q_n^2 + p_n^2))$ is a (mixed) state whenever $0 < \lambda_1 < 1, \dots, 0 < \lambda_n < 1$.

Indeed, with $\beta_i = 2\operatorname{arctanh}\lambda_i$, f is a tensor product of n functions of the previous type: $f(u) = \prod_{i=1}^n f_{\beta_i}(q_i, p_i)$. Thus $f = \sum_k a_k f_{kk}$ (summed over all n-tuples of nonnegative integers); the f_{kk} are (pure) states: and the coefficients $a_k = \prod_{i=1}^n \sqrt{2\sinh\beta_i} \exp(-(k_i + \frac{1}{2})\beta_i)$ are positive and sum to 1.

Theorem 2 follows. □

Remark. The dimension of the manifold of pure gaussian states is $n^2 + n$; the dimension of the manifold of gaussian states is $n^2 + 2n$.

To prove that the collection of nonnegative states found does not include every nonnegative state, an example will suffice. We obtain it from a couple of very interesting results.

Theorem 3 (Bernard *et al* [12])**.** *The convolution of a quantum state with another quantum state is nonnegative.*

For the proof, we remit to [12]. The proof given there is for pure states, but the result extends trivially to the general case.

Theorem 4. *The convolution of a (suitably normalized) nonnegative function with a quantum state is a quantum state.*

Proof. Our argument is a modified version of that in [13], recast in our algebraic framework based on twisted products. The point is that translations may be considered as automorphisms. If δ_v is the Dirac measure on phase space concentrated at v (note that $\delta_v \in \mathcal{B}$) then we can show

$$(\delta_v \times f \times \delta_v)(u) = f(2v - u).$$

Let f be nonnegative and g a state. Then for $h \in \mathcal{B}$ we have

$$\begin{aligned}\langle f * g, h^* \times h\rangle &= \iint f(u)\, g(-u - v)\, (h^* \times h)(-v)\, du\, dv \\ &= \iint f(u)\, (\delta_{-u/2} \times g \times \delta_{-u/2})(v)\, (\delta_0 \times h^* \times h \times \delta_0)(v)\, du\, dv \\ &= \int f(u)\, du \int g(v)\, (k_u^* \times k_u)(v)\, dv \geqslant 0 \quad (\text{with } k_u := h \times \delta_0 \times \delta_{-u/2}). \qquad \square\end{aligned}$$

In contrast to step 2 of Theorem 2, here pure states do not remain pure. The last two results point to a rather mysterious duality between nonnegative functions and quantum states.

Taken together, Theorems 2, 3 and 4 amount to a powerful machine for producing nonnegative mixed states in WWM theory. We now have, for instance, with $n = 1$:

$$(f_\beta * f_{11})(u) = 2e^{-3\beta/2}\sqrt{2\sinh\beta}(1 + u^2 \sinh^2 \tfrac{1}{2}\beta)\exp(-\tfrac{1}{2}u^2 e^{-\beta/2}\sinh\tfrac{1}{2}\beta),$$

which must represent a quantum state and it is not gaussian.

A number of recent articles in this Journal [12–16] have discussed quantum-mechanical nonnegative distributions in phase space. We hope this paper helps to throw some light on these questions.

We gratefully acknowledge support from the Vicerrectoría de Investigación of the Universidad de Costa Rica.

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