POSITIVE PHASE SPACE DISTRIBUTIONS AND UNCERTAINTY RELATIONS

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Abstract

In contradistinction to a widespread belief, Wigner's theorem allows the construction of true joint probabilities in phase space for distributions describing the object system as well as for distributions depending on the measurement apparatus. The fundamental role of Heisenberg's uncertainty relations in *Schrödinger* form (including correlations) is pointed out for these two possible interpretations of joint probability distributions. E.g., in order that a multivariate normal probability distribution in phase space may correspond to a Wigner distribution of a pure or a mixed state, it is necessary and *sufficient* that Heisenberg's uncertainty relation in Schrödinger form should be satisfied.

1 Introduction

Joint measurements of conjugate variables q and p are realized in many optical devices. This implies that one can think in this domain of a representation of quantum mechanics by means of joint probability distributions (j.p.d.) in the phase space of conjugate variables q and p [1]. This is perhaps the most convenient way to a realistic underpinning of quantum mechanics. A major advantage is that the incompatible variables q and p are c-numbers. The Wigner distribution function, which is widely used in optics, is the simplest language for coherent and squeezed states [2]. For these states the Wigner function is nonnegative. However, it is well known that the Wigner distribution cannot be considered as a true (nonnegative) probability distribution in general [3]. The aim of this paper is twofold: in the first part (sections 2 and 3) we present an analysis of the central question to consider phase space representations of quantum mechanics as *true* (nonnegative) probability distributions [4, 5] ; in the second part (sections 4 and 5) we emphasize the fundamental role of *Heisenberg's* uncertainty relations in *Schrödinger* form for Gaussian Wigner distributions and compare this with j.p.d. depending on the measurement arrangement (positive operator valued measures).

2 Wigner's theorem

On account of the commutation relations between the operators $\hat{q}$ and $\hat{p}$, there is *no* unique operator corresponding to the monomial $q^n p^m$. As a consequence there is *no* unique construction

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of the j.p.d.. In general, a j.p.d. is completely determined by a given correspondence rule. Notwithstanding this arbitrariness, the existence of true probabilities in phase space is severely restricted by Wigner's theorem [3], which considers the following five requirements:

(1) The j.p.d. is the mean value of an hermitian operator $\hat{K}(q,p)$ depending on the c-numbers q and p: $f(q,p) = \text{tr}[\hat{K}(q,p)\hat{\rho}]$.

(2) The j.p.d. is a linear functional of the density matrix (sesquilinear in the wavefunction): this means that $\hat{K}(q,p)$ is independent of $\hat{\rho}$.

(3) The j.p.d. is a true probability function: $f(q,p) \geq 0$.

(4) When integrating over momentum space, the marginal distributions coincide with the proper quantummechanical probabilities in q: $\int f(q,p)\mathrm{d}p = <q \mid \hat{\rho} \mid q>$.

(5) When integrating over position, the marginal distributions coincide with the proper quantummechanical probabilities in p: $\int f(q,p)\mathrm{d}q = <p \mid \hat{\rho} \mid p>$.

Theorem 1 *The five requirements (1)-(5) are incompatible.*

The requirement (2) is not explicitly present in the original version of Wigner's theorem; the necessity of this requirement was emphasized by Mügür-Schlächter [6], who observed that in the absence of the arbitrary restriction (2) Wigner's theorem cannot be realized. In the stronger version of Kruszynski and de Muynck [7] the requirement on *one* marginal distribution suffices.

3 Realisation of positive phase space distributions

For our purpose, it is sufficient to consider two different interpretations of j.p.d. as functionals of the density matrix.

(1) The j.p.d. $f(q,p)$ is interpreted as the probability that the variables q and p have certain values, the variable considered as a property possessed by the object system. In this case, two possibilities are left open for the construction of true j.p.d.:

(1.1) $f(q,p)$ *is a linear functional of $\hat{\rho}$.*

In this case the requirements (1)-(5) are only compatible with a restricted class of functions. E.g. for the Weyl correspondence rule, the restricted class of functions are Gaussons (see section 4). The Wigner distribution cannot be considered as a true probability distribution in general, because e.g. it takes necessarily negative values for pure states that are not Gaussons. However, one can easily construct positive non-Gaussian Wigner j.p.d. corresponding to *mixed* states. For a representation of quantum mechanics by means of true Wigner j.p.d. one can add the new requirement that only nonnegative j.p.d. are physical states . This means e.g. that a one photon state is represented by a mixed state [10]. This idea is made plausible by the experimental fact that it is impossible to prepare a pure state with 100 % efficiency.

(1.2) $f(q,p)$ *is a nonlinear functional of $\hat{\rho}$.*

J.p.d. which are a nonlinear functional of the density matrix are not restricted by Wigner's theorem. The j.p.d. which is the product of the proper quantum mechanical marginal distributions is a trivial example: $f(q,p) = <q \mid \hat{\rho} \mid q><p \mid \hat{\rho} \mid p>$. Non-trivial examples with correlations exist also in the literature [11].In this case the j.p.d. is a *multilinear* functional of the density matrix. We have considered a complete analysis of true distributions which are *quadratic* functional

of the density matrix [5]. This results in a new concept of j.p.d. which is based on a consistent phase space interpretation of the energy eigenstates of the wave function.

(2) The j.p.d. $f(q, p)$ is not function of the object system alone, but may also depend on the measurement arrangement of two incompatible observables Q and P. The measurements mutually influence each other in such a way that the singly measured quantum probability functions cannot be reproduced from the measurement results. In this case it is no longer desirable that the marginal probability distributions equal the single measured ones, hence Wigner's theorem does not restrict this class of j.p.d. and $f(q, p)$ may be a linear function of the density matrix. The optimal stochastic phase-space representations introduced by Prugovečki [12] are an example of this class. In general the distributions of class (2) can be considered in the framework of positive operator valued measures [13].

4   Heisenberg's uncertainty relation in Schrödinger form and coherent and squeezed Wigner distributions

We consider case (1.1) for the Weyl correspondence rule. In this case the construction of true j.p.d. for pure states is restricted by the remarkable and important theorem which was proven by Hudson [8] for one-dimensional systems and generalized by Soto and Claverie [9] for systems with an arbitrary number of degrees of freedom.

Theorem 2 *The necessary and sufficient condition for the Wigner distribution function of a pure state to be nonnegative is that the corresponding wave function $< q|\psi >$ is the exponential of a quadratic form.*

As a consequence the wave function represents a coherent or a squeezed state and the j.p.d. is a bivariate or a multivariate normal (Gaussian) distribution in phase space. Conversely, in two--dimensional phase space of the conjugate random variables q and p the most general normalised bivariate normal probability distribution with mean values $\bar{q}$ and $\bar{p}$ can be put in the standard form

$$f(q, p) = \frac{1}{2\pi\sqrt{\Delta}} \exp\left\{ -\frac{1}{2\Delta} \left[\sigma_p (q - \bar{q})^2 - 2\sigma_{q,p}(q - \bar{q})(p - \bar{p}) + \sigma_q (p - \bar{p})^2 \right] \right\}, \tag{1}$$

where σ_q and σ_p and $\sigma_{q,p}$ represent respectively the variances and the covariance $\sigma_q = E[(q - \bar{q})^2]$, etc.; E denotes the expectation value and Δ is the determinant of the covariance matrix: $\Delta = \sigma_q \sigma_p - \sigma_{q,p}^2 \geq 0$. Schrödinger derived a more general and stronger form of Heisenberg's uncertainty relation including the correlation $\sigma_{q,p}$:

$$\sigma_q \sigma_p - \sigma_{q,p}^2 \geq \hbar^2/4, \tag{2}$$

which we call "Heisenberg's uncertainty relation in *Schrödinger* form". It is easy to derive and to diagonalise the corresponding density matrix. $f(q, p)$ may now represent a pure *or* a mixed state. The eigenfunctions $< q|\psi >$ are oscillator eigenfunctions functions multiplied by a common q-dependent phase factor which is characteristic for the correlation. We can show explicitly that there is a close connection between a Gaussian distribution in phase space, quadratic Hamiltonians and temperature dependent oscillator states. This implies a connection between physical and

statistical parameters. The eigenvalues of the corresponding density matrix are $(1 - z)z^n$ with $z = (\Delta - \hbar/2)/(\Delta + \hbar/2)$, which leads to a *sufficient* condition for a bivariate normal probability distribution to be a quantum state:

Theorem 3 *In order that a bivariate normal probability distribution in phase space with variances σ_q, σ_p and covariance $\sigma_{q,p}$ may correspond to a Wigner distribution of a pure or a mixed state, it is necessary and sufficient that Heisenberg's uncertainty relation in Schrödinger form $\sigma_q \sigma_p - \sigma_{q,p}^2 \geq \hbar^2/4$ should be satisfied [4, 14].*

It is very remarkable that the Schrödinger form of Heisenberg's uncertainty relation, which is a necessary condition to be fulfilled for every Wigner distribution function, is also a *sufficient* condition in the case of a bivariate normal probability distribution. Indeed, to be a Wigner distribution function, $f(q, p)$ must satisfy an infinite set of KLM [15] or equivalent conditions in general, but for the two-dimensional Gaussian distribution the infinite set reduces to *one* simple *necessary and sufficient* physical condition. In this respect, the uncertainty relation in Schrödinger form is *more fundamental* than Heisenberg's relation in the usual, less stronger form $\sigma_q \sigma_p \geq \hbar^2/4$. Moreover, the Schrödinger form is *invariant* for linear canonical transformations (in general $Sp(2n, R)$ invariant transformations), while the usual form is not. Finally, for quadratic Hamiltonians, which are closely related to the Gaussian Wigner distribution, the Schrödinger form remains *invariant* during the motion if the variances and the covariance are dependent on time. Indeed, in this case the quantum Liouville equation is equivalent to the classical Liouville equation and therefore $\bar{q}$, $\bar{p}, \sigma_q, \sigma_p$ and $\sigma_{q,p}$ have the same time dependence as in the classical case. These are further reasons why the uncertainty relation in Schrödinger form is *more relevant* than Heisenberg's relation in the usual form.

For systems with an arbitrary number of degrees of freedom the strong form of Heisenberg's uncertainty relation is derived from the inequality $\text{tr}(a^\dagger \hat{\rho} a) \geq 0$ where the vector a is given by $a = A(\hat{q} - \bar{q}) + B(\hat{p} - \bar{p})$, A and B being arbitrary matrices, and which takes the form:

$$\begin{vmatrix} A^\dagger \\ B^\dagger \end{vmatrix} \begin{vmatrix} \sigma_{q,q} & \sigma_{q,p} - i\hbar/2 \\ \sigma_{p,q} - i\hbar/2 & \sigma_{p,p} \end{vmatrix} \begin{vmatrix} A \\ B \end{vmatrix} \geq 0. \tag{3}$$

Therefore Heisenberg's uncertainty relation in Schrödinger form takes now the matrix form:

$$\sigma - i\hbar\beta/2 \geq 0. \tag{4}$$

where σ is the covariance matrix $\begin{vmatrix} \sigma_{q,q} & \sigma_{q,p} \\ \sigma_{p,q} & \sigma_{p,p} \end{vmatrix}$ and β the fundamental symplectic matrix $\begin{vmatrix} 0 & 1 \\ -1 & 0 \end{vmatrix}$.

Theorem 4 *The necessary and sufficient conditions for a Gaussian phase space function to be a Wigner distribution is that the covariance matrix σ satisfies Heisenberg's uncertainty relation in Schrödinger form: $\sigma - i\hbar\beta/2 \geq 0$ [4].*

Analogous remarks as for the bivariate j.p.d. are valid for the multivariate j.p.d., the eq. 4 is now $Sp(2n, R)$ invariant. The theorem entails a considerable simplification with respect to the theorem of Simon, Sudarshan and Mukanda [17], where $Sp(2n, R)$ invariant powers of $\beta\sigma^{-1}$ satisfy n complicated inequalities. The difference between a pure and a mixed state is given by a theorem of Littlejohn [16]:

Theorem 5 *The necessary and sufficient condition for a Gaussian Wigner distribution to be a pure state is that the matrix $2\sigma/\hbar$ is a symplectic matrix: $\sigma\beta\sigma = (\hbar^2/4)\beta$.*

In two dimensions the matrix relation reduces to $\sigma_q \sigma_p - \sigma_{q,p}^2 = \hbar^2/4$.

5 Heisenberg's uncertainty relation in Schrödinger form for j.p.d. depending on the measurement arrangement

It was argued in section 3 that the construction of j.p.d. of class (2) is not restricted by Wigner's theorem. Requiring Galilei invariance, linearity and positivity for any density matrix describing the object system, we have for the most general form of the j.p.d.:

$$f(q,p) = \hbar^{-n}\text{tr}(\hat{D}^{\dagger}_{q,p}\hat{\rho}_{meas}\hat{D}_{q,p}\hat{\rho}_{obj}) \tag{5}$$

where $\hat{\rho}_{meas}$ and $\hat{\rho}_{obj}$ are the density matrices describing exhaustively the measurement apparatus and the object system and $\hat{D}_{q,p}$ represents the displacement operator. If both $\hat{\rho}_{meas}$ and $\hat{\rho}_{obj}$ are pure states then $f(q,p)$ reduces to the transition probability $f(q,p) = \hbar^{-n}\text{tr}(\psi_{meas}, \hat{D}_{q,p}\psi_{obj})$. The marginal distributions are always given by the convolution of two true probability densities:

$$\int f(q,p)\text{d}p = < q \mid \hat{\rho}_{meas} \mid q > \star < q \mid \hat{\rho}_{obj} \mid q >, \tag{6}$$

$$\int f(q,p)\text{d}q = < p \mid \hat{\rho}_{meas} \mid p > \star < p \mid \hat{\rho}_{obj} \mid p >, \tag{7}$$

which can be seen as accuracy calibrations given by the confidence functions $< q \mid \hat{\rho}_{meas} \mid q >$ and $< p \mid \hat{\rho}_{meas} \mid p >$. The couple $q, < q \mid \hat{\rho}_{meas} \mid q >$ together with $p, < p \mid \hat{\rho}_{meas} \mid p >$ can also be interpreted as a fuzzy sample point in phase space [12]. Remark also that, for these j.p.d. the ordening of operators is equivalent with a measuring procedure. One can also write the j.p.d. as a convolution of two Wigner distributions:

$$f(q,p) = f_{meas}(q,p) \star f_{obj}(q,p), \tag{8}$$

the first one representing the measurement procedure and the second one describing the object system. This "smoothing" or "coarse graining" of the Wigner distribution eliminates fast oscillations in $\hbar$ and gives therefore a better representation in the classical limit [18]. Another consequence of the last formula is that the covariance matrix σ is the sum of the covariance matrix σ_{obj} of the object system and the σ_{meas} of the measurement procedure. Hence we obtain the "operational" uncertainty relation

$$\sigma - \imath\hbar\beta \geq 0. \tag{9}$$

which reduces in one dimension to $\sigma_q\sigma_p - \sigma_{q,p}{}^2 \geq \hbar^2$. This operational uncertainty relation is in accordance with the experimental uncertainty relation $(\Delta q)_{ex}(\Delta p)_{ex} \sim \hbar$ [19]. Comparing this with the uncertainty relations for the j.p.d. of the preceding section, we observe that the inequalities are the same, except for the essential difference that $\hbar$ replaced by $2\hbar$, expressing the presence of extra noise due to the measurement procedure.

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