A NOTE ON THE UNIQUENESS OF THE DISTRIBUTION FUNCTION IN PHASE SPACE

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ABSTRACT

The general situation of quantum distribution functions in phase space and their relation to the correspondence rules is briefly reviewed. It is shown that, contrary to a recent suggestion, the Margenau and Hill distribution is not the distribution indicated by Quantum Mechanics.

RESUMEN

Se hace una breve revisión de la situación general de las funciones de distribución en el espacio fase y su relación con las reglas de correspondencia. Se muestra que, contrariamente a una sugerencia reciente, la distribución de Margenau y Hill no es <u>la</u> distribución indicada por la mecánica cuántica.

1. INTRODUCTION

Nowadays the probabilistic nature of quantum mechanical predic

tions is generally accepted. This motivated the study of the feasibility of reformulating Quantum Mechanics (QM) as a consistent statistical (stochastic) theory which could be described in terms of a distribution function P(p,q) in phase space⁽¹⁻³⁾. Such a probability distribution would make it possible to calculate the expectation value of any operator O{A(p,q)} of the dynamical variables position and momentum represented by the operators \hat{q} and \hat{p} respectively* as

$$\langle O\{A(p,q)\}\rangle = \iint P(p,q)A(p,q)dpdq$$
, (1)

where () denotes the quantum mechanical average or expectation value, and A(p,q) is the classical counterpart of $O{A(p,q)}$. The function P(p,q) would be unique and non negative definite and would yield the quantum marginal distributions when integrated over either of the variables**

$$P(p,q)dp = |\psi(q)|^2$$
, (2.a)

$$P(p,q)dq = |\phi(p)|^2$$
, (2.b)

with $\psi(q)$ and $\varphi(p)$ representing the state of the system proyected into the coordinate or momentum space respectively, being related by a Fourier transform as

$$\psi(q) = \frac{1}{(2\pi\hbar)^{1/2}} \int \phi(p) e^{i/h \ p \cdot q} dp , \qquad (3)$$

where \hbar is Planck's constant divided by 2π . There have been built many functions bilinear in ψ which do satisfy the conditions imposed by Eqs. (2)⁽⁴⁻⁶⁾, the first and most widely known being the Wigner distribution. Nevertheless they are not compatible to each other and QM does not provide enough criteria to single out one among all of them. Furthermore

^{*} All integrals go from $-\infty$ to $+\infty$ and time dependence is not included explicitely.

^{**} This requirement also guarantees the satisfaction of the Heisenberg relations.

they may take negative or even imaginary values. In spite of these limi tations these "quasi-probability" distributions have been recognized as useful tools and are currently used in dealing with certain (quasi-classical) problems in statistical mechanics⁽⁷⁾ where they allow unified investigations of equilibrium and non equilibrium properties for classical and quantal systems. They have also been used in studying the coherence properties of light⁽⁸⁾, but in all cases the choice of the distribution function used is quite arbitrary.

It has recently been indicated $^{(9)}$ that QM suggests a particular joint distribution, namely, the Margenau and Hill distribution $^{(5)}$ given by

$$P(p,q) = \frac{1}{2\pi} \operatorname{Re}\{\psi(q) \int e^{-i\tau p} \psi^*(q-\hbar\tau) d\tau\} \quad . \tag{4}$$

If true, this would imply that the Rivier or symmetrization rule given by

$$O\{p^{n}q^{m}\} = \frac{1}{2} \left[\hat{p}^{n}\hat{q}^{m} + \hat{q}^{m}\hat{p}^{n} \right]$$
(5)

is "the" association rule indicated by QM. In this note it is shown the inaccuracy of this result.

2. DISTRIBUTION FUNCTIONS

The problem of constructing a joint distribution in phase space is closely related to the problem of associating operators to quan tum variables. This becomes clear by writting the expectation value of $O\{e^{i\theta q + i\tau p}\}$ in terms of P(p,q) by using Eq. (1):

$$O\{e^{i\theta q + i\tau p}\} = \iint P(p,q)e^{i\theta q + i\tau p} \, dq dp \quad . \tag{6}$$

This equation can be inverted by a double Fourier transform to obtain P(p,q):

$$P(p,q) = \frac{1}{(2\pi)^2} \iint \langle 0\{e^{i\theta q + i\tau p}\} \rangle e^{-i\theta q - i\tau p} d\theta d\tau$$
(7)

$$= \frac{1}{(2\pi)^2} \sum_{n,m=0}^{\infty} \frac{(i\theta)^n (i\tau)^m}{n! m!} \iint \langle 0\{p^m q^n\} \rangle e^{-i\theta q - i\tau p} d\theta d\tau \quad .$$

This last equation shows explicitly how the choice of a characteristic function $\langle 0\{e^{i\theta q + i\tau p}\}\rangle$ or equivalently of an association rule $0\{p^nq^m\}$ determines uniquely the joint probability distribution. In this respect QM does not provide a general consistent way of associating operators to quantum variables. There are some general criteria such as the hermiticity condition for operators in order to ensure real expectation values, their coincidence with their classical counterparts in the limit $\hbar + 0$, and so on; nevertheless more than one association rule fits these requirements. A review of the many possible rules can be found somewhere else^(10,11). Sutherland⁽⁹⁾ has used an alternative method to construct the joint distribution based on the general relation

$$P(p,q) = P(q) P(p|q) , \qquad (8)$$

where P(p|q) is a conditional probability of p being between p and p + dpwhen q is between q and q + dq; therefore P(p|q) includes the correlations between q and p. From Eq. (1) the expectation value of $O\{e^{i\tau p}\}$ can be written as

$$\langle e^{i\tau \hat{p}} \rangle = \iint P(p,q)e^{i\tau p} dq dp$$
 (9.a)

$$= \int P(q) \left[e^{i\tau p} \right]_{q} dq , \qquad (9.b)$$

where $\left[e^{i\tau p}\right]_q$ represents the classical conditional mean value at position q defined by

$$\left[e^{i\tau p}\right]_{q} \equiv \int P(p|q)e^{i\tau p} dp$$
(10)

On the other hand, according to QM this expectation value is given by

$$\langle e^{i\tau \hat{p}} \rangle = \int \psi^*(q) e^{i\tau \hat{p}} \psi(q) dq$$

If $P(q) = |\psi(q)|^2$ is used, this equation can then be written in a form similar to Eq. (9.b):

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$$\langle e^{i\tau\hat{p}}\rangle = \int P(q) \langle e^{i\tau\hat{p}} \rangle_{q} dq$$
,

and $(e^{i\tau \hat{p}})_{q}$, the quantum counterpart of $[e^{i\tau p}]_{q}$, is found to be

$$\langle e^{i\tau\hat{p}}\rangle_{q} = \frac{1}{\psi(q)} e^{i\tau\hat{p}} \psi(q) = \frac{1}{\psi(q)} \psi(q+\hbar\tau)$$
 (11)

Therefore, by using $[e^{i\tau p}]_q = \langle e^{i\tau \hat{p}} \rangle_q$,

$$\langle e^{i\tau \hat{p}} \rangle_{q} = \int P(p|q) e^{i\tau p} dp$$
 (12)

This last equation, if inverted, gives

 $P(p|q) = \frac{1}{2\pi} \int \langle e^{i\tau \hat{p}} \rangle_q e^{-i\tau p} d\tau$,

and if P(p|q) is known, P(p,q) can be obtained by using Eq. (8). This reasoning leads to the standard distribution and therefore to the standard ordering rule $O\{p^nq^m\} = \hat{q}^m \hat{p}^n$. If we impose the additional requirement that expectation values should be real or equivalently that operators should be hermitian (this can be done by taking the real part of the distribution or by symmetrizing the operators respectively), the previous procedure leads unambiguously to the Margenau and Hill distrib<u>u</u> tion.

The problem with this derivation is that although Eq. (12) can be formally inverted, $\langle e^{i\tau \hat{p}} \rangle_{q}$ does not contain enough elements to generate P(p|q). This is evident from the fact that the P(p,q) thus constructed cannot be isolated in Eq. (9.a) from which it was obtained, that is, it is meaningful only when integrated over q:

$$\frac{1}{2\pi} \int \langle e^{i\tau \hat{p}} \rangle_{q} e^{-i\tau p} d\tau = \int P(p,q) dq$$

If instead this method had been applied to Eq. (6) (which can indeed be inverted), we would have obtained

$$\left[e^{i\theta q + i\tau p} \right]_q \equiv \int P(p|q)e^{i\theta q + i\tau p} dp$$
,

with its quantum counterpart given by

$$\langle 0\{e^{i\theta q + i\tau p}\}\rangle_q = \frac{1}{\psi(q)} 0\{e^{i\theta q + i\tau p}\} \psi(q) \quad .$$

Therefore

$$\int P(p|q)e^{i\theta q + i\tau p} dp = \frac{1}{\psi(q)} O\{e^{i\theta q + i\tau p}\} \psi(q) ,$$

from which P(p,q) can be obtained by making a Fourier transform of this last equation and multiplying P(p|q) by $P(q) = |\psi(q)|^2$, that is:

$$P(p,q) = P(q)P(p|q)$$
$$= \frac{e^{-i\theta q}}{2\pi} \int \psi(q) \ O\{e^{i\theta q + i\tau p}\} \ \psi(q)e^{-i\tau p} \ d\tau$$

This equation corroborates that there can be constructed as many distribution functions as association rules may be proposed.

3. FINAL REMARKS

For completeness, it should be added that it has been demonstrated⁽¹²⁾ the impossibility of constructing a positive definite joint distribution bilinear in ψ . On the other hand it has been identified⁽¹³⁾ an infinite class of positive definite functions (not bilinear in ψ) satisfying Eq. (2), which lead to non linear association rules for the crossed products $O\{p^nq^m\}$, but they are constructed merely on mathematical grounds. The question of uniqueness remains opened.

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