IL NUOVO CIMENTO VOL. 107 B, N. 7 Luglio 1992

Phase Space Representation of Quantum Mechanics in Terms of Coherent States.

M. CINI (1) and M. SERVA (2)

(1) *Laboratoire de Physique Theorique, Université de Paris XI*
Bâtiment 211, 91405 Orsay, France
Dipartimento di Fisica, Università La Sapienza - Roma, Italia
(2) *Dipartimento di Matematica dell'Università and INFN*
67010 Coppito, L'Aquila, Italia

(ricevuto il 22 Novembre 1991; approvato il 7 Gennaio 1992)

Summary. — The functional representation of the Hilbert space in terms of coherent states is reconsidered with the purpose of studying the connection between quantum states and the corresponding distributions of classical statistical mechanics. The statistical predictions of both theories are compared and the relevance of these results for the conventional interpretation of quantum mechanics is discussed.

PACS 03.65 – Quantum theory; quantum mechanics.
PACS 05.30 – Quantum statistical mechanics.

1. – Introduction.

The first formulation of quantum mechanics in phase space goes back, as is well known, to Wigner [1]. The interest for a formulation of this kind stems from the fact that only in phase space is it possible to establish a connection between quantum mechanics and classical statistical mechanics. Of course the Wigner function $W(p,q)$ is not a probability distribution in phase space, because there cannot be, due to the uncertainty principle, a joint probability distribution in both position and momentum. This limitation shows up in the fact that $W(p,q)$ is not positive definite. The Wigner approach has been extensively used to obtain quantum corrections to classical thermodynamic functions, but it treats the variables p and q on a different footing, loosing therefore an important symmetry of phase space. It has however been a useful tool in the discussion of the quantum measurement problem [2].

More than thirty years later Klauder [3, 4] proposed a different approach to the problem by introducing functional representations of a Hilbert space in terms of overcomplete families of states. For the simple case of one-dimensional particle motion he has shown that, by restricting the Hilbert space to the subspace of coherent states [5], one can reduce the quantum action functional to a classical action functional which, when extremized in this subspace, yields classical equations for the c-number variables $p(t)$ and $q(t)$ which label the coherent states.

An important step has been successively made by Hepp [6] who has rigorously shown that in the limit $\hbar \to 0$ the deviation of expectation values of quantum operators in coherent states from the corresponding classical variables is given by the solution of the quantum harmonic oscillator obtained by linearizing the Heisenberg equations of motion around the classical orbit.

The purpose of the present paper is twofold. We first of all (sect. 2) push forward Klauder's analysis and show that the representative of a Schrödinger wave function in the phase space defined by an overcomplete set of coherent states defines a positive definite probability density. We find the evolution equation of this probability density and show that it reduces to the classical Liouville equation for the harmonic oscillator potential, and, in the limit $\hbar \to 0$, for any potential. We then examine (sect. 3) the connection between the statistical distributions of quantum variables P and Q in a given state and the statistical distributions of the corresponding classical variables p and q and show that quantum expectation values of operators $f(P,Q)$ may be expressed as average values of the same classical functions $f(p,q)$ in phase space plus quantum corrections arising from the reordering of operators in $f(P,Q)$. The classical limit is easily written down in this representation, thereby exhibiting explicitly the connection between a given quantum density matrix and its corresponding classical probability distribution in phase space. Finally (sect. 4) we briefly discuss the relevance of these results on the conventional interpretation of quantum mechanics. Their application to the quantum measurement problem will be dealt with in a separate publication.

2. – Probability density in phase space.

Let P and Q denote the quantum-mechanical momentum and posititon operators of a particle in one-dimensional motion which satisfy the standard commutation relations $[Q, P] = i\hbar$. An overcomplete family of states is generated by the Weyl operator labelled by the c-number variables p, q

$$U(p, q) = \exp[(i/\hbar)(pQ - qP)] \tag{1}$$

acting on a fiducial state $|0\rangle$ such that

$$\langle 0|P|0\rangle = \langle 0|Q|0\rangle = 0\,. \tag{2}$$

The Weyl operator has the property

$$U(p, q)PU^\dagger(p, q) = P - p\,, \tag{3}$$

$$U(p, q)QU^\dagger(p, q) = Q - q\,. \tag{4}$$

Coherent states

$$|q, p\rangle = U(p, q)\,|0\rangle \tag{5}$$

provide a resolution of unity

$$1 = (2\pi\hbar)^{-1}\int \mathrm{d}p\,\mathrm{d}q\,|p, q\rangle\langle p, q| \tag{6}$$

but are not orthogonal

(7) $$\langle p, q | p', q' \rangle = \exp[(-i/\hbar)(pq' - qp')]\langle 0 | p - p', q - q' \rangle .$$

The phase space continuous representation of any state vector $|\Omega\rangle$ is defined by

(8) $$\phi(p, q) = (2\pi\hbar)^{1/2} < p, q | \Omega\rangle .$$

It should be noted that $\phi(p,q)$ is the representative of the state $|\Omega\rangle$ but it is not a wave function in the ordinary sense because it cannot be assigned arbitrarily at a given time as it happens with the representative of $|\Omega\rangle$ in a complete orthogonal basis [7]. In fact $\phi(p,q)$ must satisfy the integral equation

(9) $$\phi(p, q) = (2\pi\hbar)^{-1}\int \mathrm{d}p'\,\mathrm{d}q' \langle p, q | p', q' \rangle \phi(p', q')$$

which is by no means trivial. On the other hand it can be derived easily, once the representative of the fiducial state $|0\rangle$ in an arbitrary complete orthogonal basis $|z\rangle$ is known because

(10) $$\phi(p, q) = \sum_z \langle 0 | U^\dagger(p, q) | z\rangle \langle z | \Omega\rangle$$

and the components $\langle z | \Omega\rangle$ can be assigned arbitrarily at a given time.

Now we come to dynamics. Consider a quantum Hamiltonian of the form

(11) $$\mathscr{H}(P, Q) = (1/2)P^2 + V(Q) .$$

By using the relations

(12) $$\langle p, q | Q | p', q' \rangle = ((q/2) + i\hbar\partial/\partial p)\langle p, q | p', q' \rangle ,$$

(13) $$\langle p, q | P | p', q' \rangle = ((p/2) - i\hbar\partial/\partial q)\langle p, q | p', q' \rangle ,$$

the Hamiltonian (11) leads to the Schrödinger equation for $\phi_t(p, q)$

(14) $$i\hbar\partial\phi_t(p, q)/\partial t = \mathscr{H}\{((p/2) - i\hbar\partial/\partial q), ((q/2) + i\hbar\partial/\partial p)\}\,\phi_t(p, q) .$$

We will show now that the modulus squared $\rho_t(p, q)$ of the amplitude

(15) $$\rho_t(p, q) = |\phi_t(p, q)|^2$$

provides a useful positive-definite distribution function in phase space which is closely connected with the Wigner distribution function $W_t(p, q)$.

To this purpose, the explicit dependence of $\phi_t(p, q)$ on p and q should be exhibited. One possible way of doing it is through the Schrödinger representation (a particular case of eq. (10)):

(16) $$\phi_t(p, q) = \exp[-ipq/2\hbar]\int \mathrm{d}x \langle 0 | x - q\rangle \exp[(-i/\hbar)p(x - q)]\langle x | \Omega(t)\rangle .$$

Then one easily finds

$$(17)\quad \rho_t(p, q) = \iint \mathrm{d}x\,\mathrm{d}x'\langle 0|x\rangle\langle x+q|\Omega(t)\rangle\langle\Omega(t)|x'+q\rangle\langle x'|0\rangle\exp[(-i/\hbar)p(x-x')] =$$

$$= \iint \mathrm{d}z\,\mathrm{d}y\langle 0|z+y/2\rangle\langle z-y/2|0\rangle\langle x+q+y/2|\Omega(t)\rangle\langle\Omega(t)|z+q-y/2\rangle\exp[(-i/\hbar)py].$$

The freedom of choosing the fiducial state $|0\rangle$ may now be used to assume (conditions (2) are clearly satisfied):

$$(18)\qquad \langle 0|x\rangle = (\pi\hbar/\omega)^{-1/4}\exp[-x^2\omega/2\hbar].$$

By taking into account that

$$(19)\quad \langle z+q+y/2|\Omega(t)\rangle\langle\Omega(t)|z+q+y/2\rangle = \exp[z\,\partial/\partial q][\langle q+y/2|\Omega(t)\rangle\langle\Omega(t)|q-y/2\rangle]$$

and integrating over z, one gets

$$(20)\quad \rho_t(p, q) = \exp[(\hbar/4\omega)\,\partial^2/\partial q^2]\exp[(\hbar\omega/4)\,\partial^2/\partial p^2]\,W_t(q, p) = \iint \mathrm{d}x\,\mathrm{d}y\exp[-(x^2\omega/\hbar)-(y^2/\hbar\omega)\,W_t(q+x, p+y),$$

where $W_t(q, p)$ is the Wigner function

$$(21)\qquad W_t(q, p) = \int \mathrm{d}y\,\langle q+y/2|\Omega(t)\rangle\langle\Omega(t)|q-y/2\rangle\exp[(-i/\hbar)py].$$

The relationship (20) between ρ and W allows us to derive the evolution equation for the first quantity, knowing the evolution equation for the second one. Since

$$(22)\qquad \partial W_t(q, p)/\partial t = L_W W_t(q, p)$$

with

$$(23)\qquad L_W = -p\,\partial/\partial q + (i\hbar)^{-1}\{V[q+(i\hbar/2)\,\partial/\partial p] - V[q-(i\hbar/2)\,\partial/\partial p]\},$$

we obtain

$$(24)\qquad \partial\rho_t(q, p)/\partial t = L_\rho\rho_t(q, p) = \exp[K]L_W\exp[-K]\rho_t(q, p),$$

with

$$(25)\qquad K = K_q + K_p = (\hbar/4\omega)\,\partial^2/\partial q^2 + (\hbar\omega/4)\,\partial^2/\partial p^2.$$

Therefore, from (23), (25) one has

$$(26)\quad L_\rho = -p\,\partial/\partial q - (\hbar\omega/2)(\partial/\partial q)(\partial/\partial p) + (i\hbar)^{-1}\exp[K_q]\{V[q+(i\hbar/2)\,\partial/\partial p] - V[q-(i\hbar/2)\,\partial/\partial p]\}\exp[-K_q].$$

This is the evolution equation in the general case. We show now that when $V(x)$ is the harmonic-oscillator potential with frequency ω eq. (24) reduces to the Liouville equation. In fact in this case we have

$$\begin{cases}(i\hbar)^{-1}\{V[q+(i\hbar/2)\partial/\partial p]-V[q-(i\hbar/2)\partial/\partial p]\}=\omega^2 q\,\partial/\partial p\,,\\ \exp[K_q]\,q\exp[-K_q]=q+(\hbar/2\omega)\,\partial/\partial q\,.\end{cases} \tag{27}$$

With these expressions (24) becomes

$$\partial\rho_t(q,p;t)/\partial t = L\rho_t(q,p;t) \tag{28}$$

with

$$L=-p\,\partial/\partial q+\omega^2 q\,\partial/\partial p\,. \tag{29}$$

Furthermore, we show that eq. (24) for an arbitrary potential can be written as the Liouville equation plus corrections of order $\hbar$. In fact, since

$$(i\hbar)^{-1}\{V[q+(i\hbar/2)\partial/\partial p]-V[q-(i\hbar/2)\partial/\partial p]\}=(\partial V/\partial q)\,\partial/\partial p+O(\hbar^2) \tag{30}$$

and

$$\exp[-K_q]=1+O(\hbar)\,, \tag{31}$$

our statement follows immediately from eqs. (24), (26).

3. – The statistical distribution of quantum variables in phase space.

In order to evaluate the statistical properties of the quantum operators Q, P and of their functions it is useful to introduce creation and destruction operators acting on the fiducial state $|0\rangle$ (we take for simplicity of notation $\omega=1$):

$$A^\dagger=(2\hbar)^{-1/2}(Q-iP)\,,\qquad A=(2\hbar)^{-1/2}(Q+iP)\,. \tag{32}$$

Then $A|0\rangle=0$.
The Weyl operator (1) can now be written as

$$U(p,q)=\exp[aA^\dagger-a^*A]=\exp[-aa^*/2]\exp[aA^\dagger]\exp[-a^*A]\,, \tag{33}$$

where

$$a=(2\hbar)^{-1/2}(q+ip)\,. \tag{34}$$

In this representation one has for the coherent state $|p,q\rangle$ the form

$$|p,q\rangle=U(p,q)\,|0\rangle=\exp[-(p^2+q^2)/4\hbar]\sum_0^\infty[(2\hbar)^{-1/2}(q+ip)]^n(n!)^{-1/2}|n\rangle \tag{35}$$

with the states $|n\rangle$ defined as usual by

$$|n\rangle=(A^\dagger)^n(n!)^{-1/2}\,|0\rangle\,. \tag{36}$$

The coherent state (35) is now an eigenstate of A with eigenvalue a.

We will now discuss the statistical properties of functions of P and Q for the representation defined by (35). The expectation value of any polynomial in P, Q can now be expressed as a sum of *anti*-ordered products of A and $A^\dagger$ with all the operators A on the left and all the operators $A^\dagger$ to the right. Then, since one has

$$(37)\quad \langle\Omega|A^n A^{\dagger m}|\Omega\rangle = \\ = (2\pi\hbar)^{-1}\int \mathrm{d}p\,\mathrm{d}q\,\langle\Omega|A^n|p, q\rangle\langle p, q|A^{\dagger m}|\Omega\rangle = \int \mathrm{d}p\,\mathrm{d}q\,\rho_t(p, q)\,a^n a^{*m},$$

we can write, for any function

$$(38)\qquad f(P, Q) = \sum_{nm} c(n, m) A^n A^{\dagger m}$$

regular at the origin we have

$$(39)\quad \langle\Omega|f(P, Q)|\Omega\rangle = \sum_{nm} c(n, m)\int \mathrm{d}p\,\mathrm{d}q\,\rho_t(p, q)\,a^n a^{*m} = \\ = \int \mathrm{d}p\,\mathrm{d}q\,\rho_t(p, q) f(p, q) + \mathcal{O}(h) \text{ from antiordering}.$$

The distribution function $\rho_t(p, q)$ is not the classical probability distribution in phase space corresponding to the quantum density matrix $|\Omega\rangle\langle\Omega|$ because it still depends on $\hbar$. Its limit for $\hbar\to 0$, however, is indeed the required phase space probability distribution. Therefore, eq. (39) not only yields a simple and direct calculation of the expected value of any operator $f(P,Q)$, but also gives an easy tool for separating the quantum corrections from the classical average value.

In the simple case of a discrete superposition of coherent states with arbitrary coefficients independent of $\hbar$

$$(40)\qquad |\Omega\rangle = \sum_k c_k\,|r_k, s_k\rangle,$$

we easily obtain

$$(41)\qquad \lim_{\hbar\to 0}\rho_t(p, q) = \sum_k |c_k|^2\,\delta(p - r_k(t))\,\delta(q - s_k(t)),$$

because the cross terms $\langle r_j, s_j|r_k, s_k\rangle$ $(k\neq j)$ vanish exponentially in the limit $\hbar\to 0$ and the arbitrary coefficients c_k are independent of $\hbar$. The expression on the right-hand side of eq. (41) is indeed the classical probability distribution in phase space corresponding to a statistical mixture of a superposition of classical oscillators of coordinates and momenta $r_k s_k$.

When the state $|\Omega\rangle$ is given by a continuous superposition of coherent states we can write

$$(42)\qquad |\Omega(t)\rangle = (2\pi\hbar)^{-1}\int \mathrm{d}r\,\mathrm{d}s\,|r, s\rangle\langle r, s|\Omega(t)\rangle = \int \mathrm{d}r\,\mathrm{d}s\,c_t(r, s)|r, s\rangle,$$

which is the equivalent of (40). The correspondent of (41) is

$$(43)\qquad \lim_{\hbar\to 0}\rho_t(p, q) = \lim_{\hbar\to 0}\int \mathrm{d}r\,\mathrm{d}s\,|c_t(r, s)|^2\,\delta(p - r)\,\delta(q - s),$$

which is however a simple identity, because the coefficients $c(r,s)$ in general depend on $\hbar$. We have therefore to work out the limit for $\hbar\to 0$ for each case.

As an example we take for $|\Omega\rangle$ the eigenstate $|n\rangle$ of $\mathscr{H}$ with eigenvalue $W = \hbar(n + (1/2))$. In this case we have

$$\rho_t(p, q) = (2\pi\hbar)|\langle p, q|n\rangle|^2 = (2\pi\hbar)\exp\{-[(p^2 + q^2)/2\hbar]\}[(p^2 + q^2)/2\hbar]^n/n! . \tag{44}$$

To perform the limit $\hbar \to 0$ we have to be careful. In fact, if we keep n fixed the energy of the state would tend to zero with $\hbar$. Only if we keep the energy W constant we obtain the correct limit. Therefore, we write

$$\rho_t(p, q) = (2\pi\hbar)\exp[-[(p^2 + q^2)/2\hbar]][(p^2 + q^2]/2\hbar]^{W/\hbar - 1/2}/(W/\hbar - 1/2)! . \tag{45}$$

Since $\rho_t(p, q)$ depends only on $(p^2 + q^2)$, we go to polar coordinates

$$q + ip = (2E)^{1/2}\exp[i\alpha]; \qquad q - ip = (2E)^{1/2}\exp[i\alpha]; \qquad dp\, dq = dE\, d\alpha .$$

Then the classical limit of the expectation value of any function $f(P,Q)$ may be written as

$$\lim_{\hbar\to 0}\int dp\, dq\, \rho_t(p, q) f(p, q) = \tag{46}$$

$$= \lim_{\hbar\to 0}\int dE \exp[-E/\hbar](E/\hbar)^{W/\hbar}/(W/\hbar)! \int d\alpha f(E, \alpha) = (2\pi)^{-1}\int d\alpha f(W, \alpha) .$$

This means that we can write

$$\lim_{\hbar\to 0}\rho_t(p, q)\, dp\, dq = (2\pi)^{-1}\delta[(p^2 + q^2)/2 - W]\, dp\, dq . \tag{47}$$

This is indeed the classical phase space probabiblity distribution with constant energy W (microcanonical ensemble).

When $|\Omega\rangle$ is a superposition of energy eigenstates

$$|\Omega\rangle = \sum_n c_n \exp[-int]|n\rangle = \sum_n b_n |n\rangle , \tag{48}$$

we can work out the classical limit by taking into account that the sum over n lies in a limited range ΔN around a value N which will be taken very large. Going again to polar coordinates we have

$$\rho_t(p, q) = \sum_n\sum_{n'} b_n b_{n'}^* \exp[-E/\hbar](\sqrt{E/\hbar})^{n+n'}\exp[i\alpha(n - n')]/\sqrt{n!}\sqrt{n'!} = \tag{49}$$

$$= \sum_n |c_n|^2 \exp[-E/\hbar](E/\hbar)^n/n! + \sum_n \sum_{\Delta n \neq 0} \mathscr{B}_{n,\Delta n}(E, \alpha) .$$

The first term gives the sum of the phase space probability distributions of the microcanonical ensembles corresponding to the different energies W_n. For simplicity we discuss explicitly the second term in the case in which the superposition has only two eigenstates with energies W_1 and W_2. Then we set $(W_1 + W_2)/2 = W$ and $W_1 - W_2 = \Delta$. Then $(n! \approx n^n)$

$$\sum_n \sum_{\Delta n \neq 0} \mathscr{B}_{n,\Delta n}(E, \alpha) = \exp[-E/\hbar](E/W)^{W/\hbar}|c_1 c_2|\cos[(\alpha - t)\Delta/\hbar + \gamma] , \tag{50}$$

where γ is the phase difference between c_1 and c_2. This gives an oscillating time-dependent contribution corresponding to a microcanonical probability distribution corresponding to the mean energy W.

4. – Conclusions.

Our result can be summarized by saying that for any state $|\Omega\rangle$ and for any operator $f(P,Q)$ of the form (38) we find a positive phase space density $\rho_t(p, q)$ and a variable

(51) $$\mathscr{f}(p, q) = \sum_{nm} c(n, m)\, a^n\, a^{\dagger m}$$

such that

(52) $$\langle\Omega\,|\,f(P, Q)\,|\,\Omega\rangle = \int \mathrm{d}p\, \mathrm{d}q\, \rho_t(p, q)\, \mathscr{f}(p, q)\,.$$

Therefore the expectation value of a quantum operator $f(P,Q)$ in any quantum state $|\Omega\rangle$ satisfying the Schrödinger equation with Hamiltonian (11) can always be expressed as the sum of an explicit classical term plus quantum corrections of order h

(53) $$\langle\Omega\,|\,f(P, Q)\,|\,\Omega\rangle = \int \mathrm{d}p\, \mathrm{d}q\, \mathscr{L}(p, q) f(p, q) + O(\hbar)\,,$$

where

(54) $$\mathscr{L}(p, q) = \lim_{\hbar \to 0} \rho_t(p, q)$$

is the classical phase space probability distribution corresponding to the density matrix $|\Omega\rangle\langle\Omega|$.

This result is clearly relevant to all discussions on the classical limit of quantum mechanics. We only wish to stress here that both the uncertainties $\langle\Omega\,|\,(\Delta Q)^2\,|\,\Omega\rangle$ and $\langle\Omega\,|\,(\Delta P)^2\,|\,\Omega\rangle$ in coordinate and momentum may be expressed in form (53) [8]. This means that for semiclassical states $|\Omega\rangle$ (such that the Heisenberg product $\Delta Q\, \Delta P \gg h$) the uncertainty of the localization of the system in phase space is essentially of classical statistical origin, being only the expression of incomplete knowledge on the actual system state, and cannot be ascribed to the impossibility of defining the position and momentum of a particle before having measured one or the other. Of course there is always a fundamental uncertainty of quantum origin which prevents perfect localization, but this uncertainty is always confined within areas of order h. It is therefore incorrect to assert, as the conventional interpretation of quantum mechanics holds, that only after a measurement a particle acquires a position or a velocity within given ranges. It is in fact meaningful to say that even before any measurement had been performed, the system coordinate and momentum were bounded within a region in phase space $\approx h$, the effect of a measurement having been therefore the one of reducing our ignorance on its localization in phase space from a region $\gg \hbar$ to its minimum possible value $\approx \hbar$.

* * *

One of us (MC) is indebted to Prof. R. Omnès for useful discussions and for having made possible his permanence at Orsay through a grant of the French C.N.R.S.

REFERENCES

[1] E. P. WIGNER: *Phys. Rev.*, 40, 479 (1932).
[2] M. CINI and M. SERVA: *Quantum Mechanics without Reduction*, edited by M. CINI and J. M. LEVY-LEBLOND (Hilger, London), p. 103.
[3] R. J. KLAUDER: *J. Math. Phys.*, 4, 1055 (1963).
[4] R. J. KLAUDER: *J. Math. Phys.*, 4, 1058 (1963).
[5] R. J. KLAUDER: *J. Math. Phys.*, 5, 177 (1964).
[6] K. HEPP: *Commun. Math. Phys.*, 35, 265 (1974).
[7] R. J. KLAUDER: *Coherent States* (World Scientific, Singapore), p. 8.
[8] M. CINI and M. SERVA: *Found. Phys. Lett.*, 3, 129 (1990).