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Phase space functions and correspondence rules

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Abstract. It is shown that positive quantum joint distributions in phase space lead to quantum mechanical operators depending on the state to be considered. It is also shown that a simple requirement of canonical invariance leads to the Weyl correspondence rule as the only allowed one.

1. Introduction

Quantum mechanics can be described in several mathematical forms of which the method of distribution functions in phase space most easily illustrates the connections between quantum mechanics and classical mechanics.

Contrary to the methods of wavefunctions in either coordinate or momentum space the phase space method here presented does not use quantum mechanical operators but ordinary classical functions. The correspondence rule between classical mechanics and quantum mechanics is, so to say, built-in in the phase space function, i.e. starting from a fixed correspondence rule one is led to a definite choice of phase space functions, or *vice versa.*

The Wigner distribution function is the starting point of § 2 of this paper. Some of its well known properties will be reviewed and it will be shown how a generalisation leads to other phase space functions.

Firstly, in § 3, we consider the phase space functions of Cohen (1980) for a particular state and show that they correspond to the definition of operators depending on the actual state. This is not common practice.

In § 4 we reconsider the general phase space functions of § 2 and demonstrate how a simple requirement of canonical invariance of the operators leads to the Wigner function as the only allowed phase space function. This result is in agreement with and a generalisation of a result obtained by Krüger and Poffyn (1976). Also Fairlie (1964) claims that the Wigner function is the phase space function to be used. But his proof does not seem completely convincing, since he postulates that an identity between two integrals taken all over the two-dimensional space also should be valid pointwise.

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2. The Wigner function and generalisations of it

For a state $|s\rangle$, represented in coordinate representation by the wavefunction $\psi(q)$ and in momentum representation by $\phi(p)$, Wigner (1932) introduced the phase space function $F_W(q,p)$ that nowadays bears his name. It plays the role of a quasi-probability distribution in phase space since

$$\int F_W(q,p)\,dp = |\psi(q)|^2 \qquad \int F_W(q,p)\,dq = |\phi(p)|^2 \tag{1}$$

where the integrations everywhere in this paper are to be taken from $-\infty$ to $+\infty$. The prefix 'quasi' indicates that $F_W(q,p)$ may take negative values locally.

Furthermore, as was shown by Groenewold (1946), the expectation value of the quantum mechanical operator $\hat{A}$ can be found by means of the classical counterpart $A(q,p)$ and the phase space function

$$\langle s|\hat{A}|s\rangle = \int\int A(q,p)F_W(q,p)\,dq\,dp \tag{2}$$

when the correspondence rule between the quantum mechanical operator and the classical function is the Weyl correspondence rule (Weyl 1931).

It is now a simple matter to generalise (2) to other correspondence rules by the introduction of other phase space functions. Hence we will here consider the following set of phase space functions which all satisfy (1):

$$F(q,p) = (4\pi^2)^{-1}\int\int\int \exp[i(-\theta q - \tau p + \theta u)]f(\theta,\tau)\psi^*(u-\tfrac{1}{2}\tau)\psi(u+\tfrac{1}{2}\tau)\,d\theta\,d\tau\,du \tag{3}$$

where $f(\theta,\tau)$ is any function satisfying

$$f(0,\tau) = f(\theta,0) = 1. \tag{4}$$

$F_W(q,p)$ is obtained by setting $f(\theta,\tau)=1$.

Using (2) it is possible to find the correspondence rule between the operator $\hat{A}$ and the function A for an arbitrary f. The function f is shown in table 1 for different well known correspondence rules (Essén 1978, Krüger and Poffyn 1976, Mehta 1964, Rivier 1951, Wolf 1975).

When $f(\theta,\tau)$ is independent of $\psi(q)$ it can be shown (Wigner 1971) that in general $F(q,p)$ is not non-negative. Therefore Cohen (1980) allowed $f(\theta,\tau)$ to depend on the

Table 1. The function $f(\theta,\tau)$ for some well known correspondence rules.

Correspondence rule	$f(\theta,\tau)$
Weyl	1
Normal	$\exp[(\theta^2+\tau^2)/4]$
Antinormal	$\exp[-(\theta^2+\tau^2)/4]$
Standard	$\exp(i\theta\tau/2)$
Antistandard	$\exp(-i\theta\tau/2)$
Born–Jordan	$\sin(\frac{1}{2}\theta\tau)/(\frac{1}{2}\theta\tau)$
Rivier	$\cos(\frac{1}{2}\theta\tau)$

state to be considered and thereby introduced non-negative phase space functions, but as we shall see in the following section this leads to quantum mechanical operators also dependent on the state.

3. A state independence

By requiring that the correspondence between classical functions and quantum mechanical operators be linear and that the zero operator correspond to the number zero, one obtains

$$\hat{A}=\iint A(q,p)\hat{R}(q,p)\,\mathrm{d}q\,\mathrm{d}p \tag{5}$$

where the set of operators $\hat{R}(q,p)$ describes the actual correspondence rule. It is then immediately found that

$$\langle s|\hat{A}|s\rangle=\iiint \psi^*(q_1)A(q,p)\hat{R}(q,p)\psi(q_1)\,\mathrm{d}q_1\,\mathrm{d}q\,\mathrm{d}p \tag{6}$$

is equal to

$$\langle s|\hat{A}|s\rangle=\iint A(q,p)F(q,p)\,\mathrm{d}q\,\mathrm{d}p. \tag{7}$$

The phase space function can be found from (3), and since the identity between (6) and (7) is to hold for any function $A(q,p)$, we obtain

$$\begin{aligned}\int \psi^*(q_1)\hat{R}(q,p)\psi(q_1)\,\mathrm{d}q_1 &\\ =(4\pi^2)^{-1}\iiint &\exp\{\mathrm{i}[\theta(\tfrac{1}{2}q_1+\tfrac{1}{2}q_2-q)+(q_1-q_2)p]\}f(\theta,q_2-q_1)\\ &\times\psi^*(q_1)\psi(q_2)\,\mathrm{d}q_1\,\mathrm{d}q_2\,\mathrm{d}\theta.\end{aligned} \tag{8}$$

This is to be true for all wavefunctions $\psi(q_1)$, thereby giving

$$\begin{aligned}\hat{R}(q,p)\psi(q_1)=(4\pi^2)^{-1}\iint &\exp\{\mathrm{i}[\theta(\tfrac{1}{2}q_1+\tfrac{1}{2}q_2-q)+(q_1-q_2)p]\}\\ &\times f(\theta,q_2-q_1)\psi(q_2)\,\mathrm{d}q_2\,\mathrm{d}\theta.\end{aligned} \tag{9}$$

Comparing (5) and (9), we see that it is possible in a very simple way to find an expression for any operator in the coordinate representation. We will here consider a particular set of operators, namely the operators $\widehat{q^mp^n}$ where m and n are positive integers.

Multiplying (9) with qp followed by an integration over q and p yields after some manipulations

$$\begin{aligned}\widehat{qp}\psi(q_1)&=\left[\iint qp\,R(q,p)\,\mathrm{d}q\,\mathrm{d}p\right]\psi(q_1)\\ &=\frac{1}{\mathrm{i}}\frac{\partial}{\partial q_1}(q_1\psi(q_1))-\frac{\mathrm{i}}{2}\psi(q_1)+\psi(q_1)\left(\frac{1}{\mathrm{i}}f_{01}q_1-f_{11}\right)\end{aligned} \tag{10}$$

where we have assumed that f can be Taylor expanded,

$$f(\theta, \tau) = \sum_{k,l=0}^{\infty} f_{kl}\theta^k \tau^l. \tag{11}$$

In general the operator $\widehat{q^m p^n}$ can be written as

$$\widehat{q^m p^n}\psi(q_1) = -\mathrm{i}^{n-m} m!\, n!\, f_{mn}\psi(q_1) + \dots \tag{12}$$

where the dots denote terms containing expansion coefficients f_{kl}, $k \leqslant m$, $l \leqslant n$, $(k, l) \neq (m, n)$.

Because of (4) and (11) we are finally led to the conclusion that if we demand the operators $\widehat{q^m p^n}$ to be independent of the state to be considered—which seems quite natural—the function $f(\theta, \tau)$ must be independent of the state too. This is not the case for the positive quantum joint distributions defined by Cohen (1980).

4. A simple canonical invariance

We now go back to the general case (3) without demanding anything but (4) to be fulfilled for the function $f(\theta, \tau)$. Introducing the eigenstates of the $\hat{q}$ operator

$$\hat{q}|q_1\rangle = q_1|q_1\rangle, \tag{13}$$

(3) can be rewritten as

$$\begin{aligned} F(q, p) &= (4\pi^2)^{-1} \iiiint \mathrm{e}^{\mathrm{i}up}\, \delta(q' - q - \tfrac{1}{2}u) \langle s|v - q + q'\rangle \\ &\quad \times \langle v - q + q' - u|s\rangle\, \mathrm{e}^{\mathrm{i}\theta(v-q)} f(\theta, 2q - 2q')\, \mathrm{d}\theta\, \mathrm{d}q'\, \mathrm{d}u\, \mathrm{d}v \\ &= (8\pi^3)^{-1} \iiiiint \mathrm{e}^{\mathrm{i}up} \exp[\mathrm{i}x(q' - q - u/2)] \langle s|v - q + q'\rangle \\ &\quad \times \langle v - q + q' - u|s\rangle\, \mathrm{e}^{\mathrm{i}\theta(v-q)} f(\theta, 2q - 2q')\, \mathrm{d}\theta\, \mathrm{d}q'\, \mathrm{d}u\, \mathrm{d}v\, \mathrm{d}x. \end{aligned} \tag{14}$$

The identity operator

$$1 = \int |q''\rangle\langle q''|\, \mathrm{d}q'' \tag{15}$$

can be applied in obtaining

$$\begin{aligned} F(q, p) &= (8\pi^3)^{-1} \iiiiiint \mathrm{e}^{-\mathrm{i}ux/2}\, \mathrm{e}^{\mathrm{i}xq'}\, \mathrm{e}^{\mathrm{i}(up - xq)} \langle s|v - q + q'\rangle \\ &\quad \times \langle v - q + q' - u|q''\rangle\langle q''|s\rangle\, \mathrm{e}^{\mathrm{i}\theta(v-q)} \\ &\quad \times f(\theta, 2q - 2q')\, \mathrm{d}\theta\, \mathrm{d}q'\, \mathrm{d}u\, \mathrm{d}v\, \mathrm{d}x\, \mathrm{d}q''. \end{aligned} \tag{16}$$

Since

$$\begin{aligned} &\langle q' - q'''|q''\rangle = \langle q'|q'' + q'''\rangle \\ &\mathrm{e}^{\mathrm{i}x\hat{q}}|q'\rangle = \mathrm{e}^{\mathrm{i}xq'}|q'\rangle \qquad \mathrm{e}^{\mathrm{i}x\hat{p}}|q'\rangle = |q' - x\rangle \end{aligned} \tag{17}$$

(16) can be transformed into

$$F(q,p)=(8\pi^3)^{-1}\iiiint\!\!\int \mathrm{e}^{-\mathrm{i}ux/2}\,\mathrm{e}^{\mathrm{i}(up-xq)}\langle s|v-q+q'\rangle\langle q'|\,\mathrm{e}^{\mathrm{i}x\hat{q}}\,\mathrm{e}^{-\mathrm{i}(u-v+q)\hat{p}}|s\rangle\,\mathrm{e}^{\mathrm{i}\theta(v-q)}$$
$$\times f(\theta,2q-2q')\,\mathrm{d}\theta\,\mathrm{d}q'\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}x. \qquad (18)$$

The operator identity (Eriksen 1968, Wilcox 1967)

$$\mathrm{e}^{\mathrm{i}x\hat{q}}\,\mathrm{e}^{\mathrm{i}y\hat{p}}=\mathrm{e}^{\mathrm{i}(x\hat{q}+y\hat{p})}\,\mathrm{e}^{-\mathrm{i}xy/2} \qquad (19)$$

and some manipulations finally transform (18) into

$$F(q,p)=(8\pi^3)^{-1}\iiiint\!\!\int \exp[\mathrm{i}(-up-vp-xq-xv/2)]\langle s|q'+v\rangle$$
$$\times\langle q'|\,\mathrm{e}^{\mathrm{i}(x\hat{q}+u\hat{p})}|s\rangle\,\mathrm{e}^{\mathrm{i}\theta v}f(\theta,2q-2q')\,\mathrm{d}\theta\,\mathrm{d}q'\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}x. \qquad (20)$$

A procedure similar to the one applied in § 3 can be used to obtain the operator corresponding to an arbitrary classical function $A(q,p)$. But first we Fourier transform $A(q,p)$

$$A(q,p)=(2\pi)^{-1}\iint a(s,t)\,\mathrm{e}^{\mathrm{i}(sq+tp)}\,\mathrm{d}s\,\mathrm{d}t. \qquad (21)$$

Inserting (20) and (21) into (15) gives then immediately that the operator $\hat{A}$ corresponding to $A(q,p)$ is given by

$$\hat{A}=(8\pi^3)^{-1}\iiiint\!\!\iiint \exp[\mathrm{i}(-xq-xt/2+xu/2+sq)]|q'+t-u\rangle\langle q'|\,\mathrm{e}^{\mathrm{i}(x\hat{q}+u\hat{p})}$$
$$\times\mathrm{e}^{\mathrm{i}\theta(t-u)}f(\theta,2q-2q')a(s,t)\,\mathrm{d}\theta\,\mathrm{d}q'\,\mathrm{d}u\,\mathrm{d}x\,\mathrm{d}q\,\mathrm{d}s\,\mathrm{d}t. \qquad (22)$$

A classical canonical transformation will transform the function $A(q,p)$ into a new function depending on the new coordinate and momentum, $A_1(Q,P)$ which is identical with the original one in the sense that $A_1(Q(q,p),P(q,p))=A(q,p)$. Also the operator is transformed when the canonical transformation is applied. But, since the two classical functions are identical, it seems natural to demand the two corresponding operators to be identical too. We will here show that this restriction used on a very simple canonical transformation is sufficient to leave us with the Weyl correspondence rule as the only allowed one.

Out of the set of linear unimodular canonical transformations

$$\begin{aligned} q&\to Q=\alpha q+\beta p\\ p&\to P=\delta q+\gamma p\end{aligned}\qquad \alpha\gamma-\beta\delta=1 \qquad (23)$$

which corresponds to the operator transformations

$$\hat{q}\to\hat{Q}=\alpha\hat{q}+\beta\hat{p}\qquad \hat{p}\to\hat{P}=\delta\hat{q}+\gamma\hat{p} \qquad (24)$$

we choose the very simple one

$$\alpha=\delta=0\qquad \beta=-\gamma=1. \qquad (25)$$

The classical function is transformed into

$$A_1(Q,P)=(2\pi)^{-1}\iint a_1(s,t)\,e^{i(sQ+tP)}\,ds\,dt$$
$$=(2\pi)^{-1}\iint a_1(t,-s)\,e^{i(sq+tp)}\,ds\,dt \tag{26}$$

which is to be identical with (21) giving

$$a_1(s,t)=a(-t,s). \tag{27}$$

The operator $\hat{A}$ is similarly transformed into

$$\hat{A}_1=(8\pi^3)^{-1}\iiiint\iiint \exp[i(-uq+us/2-xu/2+tq)]|q'-s+x\rangle$$
$$\times\langle q'|\,e^{i(x\hat{q}+u\hat{p})}\,e^{i\theta(-s+x)}f(\theta,2q-2q')a(s,t)\,d\theta\,dq'\,du\,dx\,dq\,ds\,dt. \tag{28}$$

Since the two classical functions are identical we now also demand that the two operators are identical. But this identity is to hold for all possible functions $a(s,t)$. Accordingly

$$\iiiint\int \exp[i(-xq-xt/2+xu/2+sq)]|q'+t-u\rangle\langle q'|\,e^{i(x\hat{q}+u\hat{p})}$$
$$\times e^{i\theta(t-u)}f(\theta,2q-2q')\,d\theta\,dq'\,du\,dx\,dq$$
$$=\iiiint\int \exp[i(-uq+us/2-xu/2+tq)]|q'-s+x\rangle\langle q'|\,e^{i(x\hat{q}+u\hat{p})}$$
$$\times e^{i\theta(-s+x)}f(\theta,2q-2q')\,d\theta\,dq'\,du\,dx\,dq \tag{29}$$

for all (s,t).

This is the fundamental identity which we now will show leads to the Weyl correspondence rule as the only allowed one. We multiply from the left with the arbitrarily chosen eigenstate $\langle q_0|$, use the orthonormality of the eigenstates, and use (21) in deriving

$$\iiiint \exp[i(-xq-xt/2+sq+xq_0-xt+2xu)]\langle q_0-t+u|\,e^{iu\hat{p}}\,e^{i\theta(t-u)}$$
$$\times f(\theta,2q-2q_0+2t-2u)\,d\theta\,du\,dx\,dq$$
$$=\iiiint \exp[i(-uq+us/2+tq-x^2+xq_0+xs)]\langle q_0+s-x|\,e^{iu\hat{p}}\,e^{i\theta(-s+x)}$$
$$\times f(\theta,2q-2q_0-2s+2x)\,d\theta\,du\,dx\,dq. \tag{30}$$

Since s, t, and q_0 can be chosen arbitrarily, we choose

$$t=q_0=-s \tag{31}$$

yielding

$$\iiiint \exp[i(-xq - xq_0/2 - qq_0 + 2xu)]\langle u|\, e^{iu\hat{p}}\, e^{i\theta(q_0-u)} f(\theta, 2q-2u)\, d\theta\, du\, dx\, dq$$

$$= \iiiint \exp[i(-uq - uq_0/2 + qq_0 - x^2)]\langle -x|\, e^{iu\hat{p}}\, e^{i\theta(q_0+x)}$$

$$\times f(\theta, 2q+2x)\, d\theta\, du\, dx\, dq. \tag{32}$$

We multiply from the right with the eigenstate of the $\hat{p}$ operator $|p_0\rangle$ and since

$$\langle u|p_0\rangle \propto \exp(iup_0) \tag{33}$$

we obtain after some manipulations

$$\iint \exp[2ix(q_0-p_0)] f(\theta, q_0-2x)\, e^{i\theta x}\, dx\, d\theta$$

$$= \iint \exp\{i[x(2q_0-p_0)-x^2]\} f(\theta, 2p_0-3q_0+2x)\, e^{i\theta x}\, dx\, d\theta. \tag{34}$$

The arbitrary p_0 is chosen:

$$p_0 = 0 \tag{35}$$

which leads to

$$\iint e^{2ixq_0} f(\theta, q_0-2x)\, e^{i\theta x}\, dx\, d\theta = \iint e^{2ixq_0} f(\theta+x, -3q_0+2x)\, e^{i\theta x}\, dx\, d\theta. \tag{36}$$

The identity theorem for Fourier transforms yields then firstly

$$\int e^{2ixq_0} f(\theta, q_0-2x)\, dx = \int e^{2ixq_0} f(\theta+x, -3q_0+2x)\, dx \tag{37}$$

and secondly

$$f(\theta, q_0-2x) = f(\theta+x, -3q_0+2x). \tag{38}$$

Since this is true for all (θ, x, q_0) we finally end up with

$$f(\theta, \tau) = f(\theta, 0) = 1 \tag{39}$$

for all (θ, τ).

This finishes the proof and shows, as we have already mentioned, that the Weyl correspondence possesses a canonical invariance property that is not possessed by any other correspondence rule. Finally, returning to (22), with $f(\theta, \tau)$ determined by (39), the Weyl correspondence is found in the well known form

$$\hat{A} = (2\pi)^{-1} \iint e^{i(s\hat{q}+t\hat{p})}\, a(s, t)\, ds\, dt. \tag{40}$$

This form is easily seen to be invariant under any of the transformations (23)–(24).

5. Conclusion

It has been shown, as was also found by Krüger and Poffyn (1976), that the Weyl correspondence rule has some special properties that allow one to call this the 'best' correspondence rule. Accordingly one should use Wigner's phase space function whenever phase space functions are required.

It should here be pointed out that a completely different approach can be reached by considering the inversion operators $\hat{\Pi}(q, p)$ in phase space (Royer 1977, Grossmann 1976, Dahl 1982a, b). It turns out that the Wigner distribution function can be written as

$$F_W(q, p) = \pi^{-1}\langle s|\hat{\Pi}(q, p)|s\rangle. \tag{41}$$

Accordingly $F_W(q, p)$ describes how a state is distributed around a particular phase space point. This interpretation, which is not possible for other phase space functions, gives us a picture where it is meaningful that the phase space function is both positive and negative.

Hence, independent of using phase space functions or correspondence rules as the starting point, we are left with the Weyl–Wigner formalism as the 'best' one.

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References

Cohen L 1980 *J. Math. Phys.* **21** 794
Dahl J P 1982a *Phys. Scr.* **25** 499
—— 1982b *Physica* A **114** 439
Eriksen E 1968 *J. Math. Phys.* **9** 790
Essén H 1978 *Am. J. Phys.* **46** 983
Fairlie D B 1964 *Proc. Camb. Phil. Soc.* **60** 581
Groenewold H J 1946 *Physica* **12** 405
Grossmann A 1976 *Commun. Math. Phys.* **48** 191
Krüger J G and Poffyn A 1976 *Physica* A **85** 84
Mehta C L 1964 *J. Math. Phys.* **5** 677
Rivier D C 1951 *Phys. Rev.* **83** 862
Royer A 1977 *Phys. Rev.* A **15** 449
Weyl H 1931 *The Theory of Groups and Quantum Mechanics* (New York: Dover)
Wigner E 1932 *Phys. Rev.* **40** 749
—— 1971 in *Perspectives in Quantum Theory* ed W Yourgrau and A van der Merwe (Cambridge, MA: MIT)
Wilcox R M 1967 *J. Math. Phys.* **8** 962
Wolf K B 1975 in *Group theory and its Applications* ed E M Loebl (New York: Academic)