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LETTER TO THE EDITOR

Wigner distribution functions and the representation of canonical transformations in quantum mechanics

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Abstract. In this Letter we show how for classical canonical transformations we can pass, with the help of Wigner distribution functions, from their representation U in the configurational Hilbert space to a kernel K in phase space. The latter is a much more transparent way of looking at representations of canonical transformations, as the classical limit is reached when $\hbar \rightarrow 0$ and the successive quantum corrections are related with the power of \hbar^{2n} , $n = 1, 2, \dots$

In recent publications one of the authors (MM) and his collaborators have discussed extensively the representation in quantum mechanics of non-linear and non-bijective canonical transformations (Mello and Moshinsky 1975, Kramer *et al* 1978, Moshinsky and Seligman 1978, 1979a, b). The representations, to be denoted by U , are given in definite Hilbert spaces like, for example, the one associated with coordinate q ; thus the matrix elements $\langle q' | U | q \rangle$ related with specific canonical transformations were derived explicitly. It is not easy though to see from these matrix elements the quantum modifications to the canonical transformations, as the latter are formulated in phase space rather than in Hilbert space. Thus it is interesting to discuss the representation of canonical transformations in the phase space version of quantum mechanics that was developed originally by Wigner (1932), with the help of the distribution functions that now bear his name. We shall do this in the present Letter, illustrating the analysis with the representations of some simple examples of canonical transformations.

We begin by recalling the definition of Wigner's distribution function $f(q, p)$ for a given wavefunction $\psi(q)$, i.e.

$$f(q, p) = (\pi \hbar)^{-1} \int_{-\infty}^{\infty} \langle \psi | q + y \rangle \langle q - y | \psi \rangle \exp\left(\frac{2ipy}{\hbar}\right) dy, \quad (1)$$

where we use Dirac's notation $\langle q | \psi \rangle = \psi(q)$, $\langle \psi | q \rangle = \psi^*(q)$, and restrict ourselves to a single degree of freedom. As is well known (Wigner 1932), the integration of $f(q, p)$ with respect to p or q gives the probability density for the state $|\psi\rangle$ in configuration or momentum space respectively.

We consider now a canonical transformation

$$Q = Q(q, p), \quad P = P(q, p); \quad \{Q, P\} \equiv \frac{\partial Q}{\partial q} \frac{\partial P}{\partial p} - \frac{\partial Q}{\partial p} \frac{\partial P}{\partial q} = 1 \quad (2)$$

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under which a *classical* distribution function $f(q, p)$ would of course transform into $F(q, p)$ given by

$$F(q, p) = f[Q(q, p), P(q, p)]. \tag{3}$$

In quantum mechanics though, the state $|\psi\rangle$ transforms into (Mello and Moshinsky 1975, Kramer *et al* 1978, Moshinsky and Seligman 1978, 1979a, b)

$$|\psi\rangle \rightarrow |\Psi\rangle = U|\psi\rangle, \tag{4}$$

and thus

$$\begin{aligned} F(q, p) &= (\pi\hbar)^{-1} \int_{-\infty}^{\infty} \langle \Psi|q+y\rangle \langle q-y|\Psi\rangle \exp\left(\frac{2ipy}{\hbar}\right) dy \\ &= (\pi\hbar)^{-1} \int \int \int_{-\infty}^{\infty} dz_+ dy dz_- \langle \psi|z_+\rangle \langle z_+|U^\dagger|q+y\rangle \\ &\quad \times \langle q-y|U|z_-\rangle \langle z_-|\psi\rangle \exp\left(\frac{2ipy}{\hbar}\right). \end{aligned} \tag{5}$$

Writing $z_\pm = q' \pm y'$ when it is associated with ψ , and $z_\pm = q' \pm \bar{y}'$ when it is associated with U , and integrating over q', y', \bar{y}', y , with the extra factor

$$\delta(y' - \bar{y}') = (\pi\hbar)^{-1} \int_{-\infty}^{\infty} \exp\left(\frac{2ip'(y' - \bar{y}')}{\hbar}\right) dp',$$

we immediately arrive at the relation

$$F(q, p) = \int \int_{-\infty}^{\infty} dq' dp' f(q', p') \langle q'p'|K|qp\rangle, \tag{6}$$

in which the kernel K is given by

$$\begin{aligned} \langle q'p'|K|qp\rangle &= 2(\pi\hbar)^{-1} \int \int_{-\infty}^{\infty} dy dy' \langle q'+y'|U^\dagger|q+y\rangle \\ &\quad \times \langle q-y|U|q'-y'\rangle \exp\left(\frac{i(2py - 2p'y')}{\hbar}\right), \end{aligned} \tag{7}$$

where from (3) we expect that

$$\lim_{\hbar \rightarrow 0} \langle q'p'|K|qp\rangle = \delta[q' - Q(q, p)] \delta[p' - P(q, p)]. \tag{8}$$

To obtain K we must know U which, *in principle* (Dirac 1947), is determined by the equations (Mello and Moshinsky 1975, Kramer *et al* 1978, Moshinsky and Seligman 1978, 1979a, b)

$$Q(q, p) = UqU^\dagger, \quad P(q, p) = UpU^\dagger, \tag{9}$$

where q, p are now quantum mechanical operators. As $U^\dagger U = I$, we can pass U^\dagger to the left-hand side, and taking matrix elements between a bra $\langle q'|$ and a ket $|q''\rangle$ obtain the

equations (Mello and Moshinsky 1975, Kramer *et al* 1978, Moshinsky and Seligman 1978, 1979a, b)

$$Q\left(q', \frac{\hbar}{i} \frac{\partial}{\partial q'}\right) \langle q' | U | q'' \rangle = q'' \langle q' | U | q'' \rangle, \quad (10a)$$

$$P\left(q', \frac{\hbar}{i} \frac{\partial}{\partial q'}\right) \langle q' | U | q'' \rangle = -\frac{\hbar}{i} \frac{\partial}{\partial q''} \langle q' | U | q'' \rangle. \quad (10b)$$

Of course these equations only make sense when Q, P are well defined operators; otherwise, more sophisticated procedures need to be used (Moshinsky and Seligman 1978, 1979a, b).

We shall now consider two simple examples of canonical transformations. The first will be the linear one

$$Q = aq + bp, \quad P = cq + dp; \quad ad - bc = 1, \quad b > 0, \quad (11)$$

where the constants are all real. We have then (Moshinsky and Quesne 1971)

$$\langle q' | U | q'' \rangle = (2\pi b)^{-1/2} \exp[(-i/2b)(aq'^2 - 2q'q'' + dq''^2)], \quad (12)$$

which satisfies equations (10) if we note from (11) that $c = (ad - 1)/b$. Introducing (12) in (7) and using the relation $\langle q' | U^\dagger | q'' \rangle = \langle q'' | U | q' \rangle^*$ we immediately obtain

$$\langle q' p' | K | qp \rangle = \delta[q' - (aq + bp)] \delta[p' - (cq + dp)]. \quad (13)$$

Thus for the linear canonical transformation the kernel coincides with its classical limit (8), in agreement with the fact that for this type of transformation Poisson and Moyal (1949) brackets coincide.

In the second example we take Q as the Hamiltonian of a linear potential (Landau and Lifshitz 1958), and thus we have the canonical transformation

$$Q = (p^2/2m) - F_0q, \quad P = -p/F_0, \quad (14)$$

where m is the mass, F_0 a constant of the dimension of force, and $\{Q, P\} = 1$. Equation (10a) leads then to an Airy function (Landau and Lifshitz 1958), and we also satisfy (10b) and get a normalised (Landau and Lifshitz 1958) unitary representation if we write

$$\langle q' | U | q'' \rangle = A \Phi(-\xi), \quad (15a)$$

$$\xi = [q' + (q''/F_0)](2mF_0/\hbar^2)^{1/3}, \quad (15b)$$

$$A = (2m)^{1/3} \pi^{-1/2} F_0^{-1/6} \hbar^{-2/3}, \quad (15c)$$

$$\Phi(\xi) = (4\pi)^{-1/2} \int_{-\infty}^{\infty} \exp\{i[(u^3/3) + u\xi]\} du. \quad (15d)$$

Substituting (15a) into (7) and making use of (15d) we can show straightforwardly that for the canonical transformation (14) the kernel K becomes

$$\langle q' p' | K | qp \rangle = \left\{ 2 \left(\frac{m}{\hbar^2 F_0^2} \right)^{1/3} \pi^{-1/2} \Phi \left[2 \left(\frac{m}{\hbar^2 F_0^2} \right)^{1/3} \left(\frac{p^2}{2m} - F_0q - q' \right) \right] \right\} \delta \left(p' + \frac{p}{F_0} \right). \quad (16)$$

We note first that when $\hbar \rightarrow 0$ the function Φ becomes (Landau and Lifshitz 1958) either very small or very rapidly oscillating except when $q' \approx (p^2/2m) - F_0q$. Furthermore, with the help of (15d) we easily see that $\pi^{-1/2} \int_{-\infty}^{\infty} \Phi(x) dx = 1$. Thus the expression in

{ } in (16) tends to a δ function in the limit $\hbar \rightarrow 0$, so that the kernel K goes into its classical limit (8), where Q and P are given by (14).

To see what the quantum corrections are, it is best to apply the K of (16) to a smooth distribution function $f(q, p)$, rather than study it directly. We choose

$$f(q, p) = (\pi ab)^{-1} \exp[-(q^2/a^2) - (p^2/b^2)], \quad (17)$$

where from (1) we will have the relation $b = \hbar/a$ if f is obtained from a Gaussian state in configuration space. Again using (15d) we obtain for the new distribution function $F(q, p)$ the expression

$$F(q, p) = f(Q, P) \sum_{k=0}^{\infty} \frac{\hbar^{2k} F_0^{2k} m^{-k}}{(2a)^{3k}} \left(\sum_{\substack{t=0 \\ 3k-t \text{ even}}}^{3k} \frac{(-1)^{(3k-t)/2} (2Q)^t (3k)!}{a^t t! [(3k-t)/2]! k! 3^k} \right), \quad (18)$$

where Q, P are given by (14). As indicated in (3), $f(Q, P)$ is the classical change in the distribution function due to the canonical transformation, and it will be the only one remaining in (18) if $\hbar \rightarrow 0$. Thus the terms associated with the higher powers of \hbar^2 indicate the successive quantum corrections to the distribution function when we perform the canonical transformation.

The examples discussed in this Letter are very specialised, but they clearly indicate the procedure to be followed in general. Among the more interesting cases where this formalism can be applied are those of non-bijective (Kramer *et al* 1978, Moshinsky and Seligman 1978, 1979a, b) canonical transformations. The concepts of ambiguity group and ambiguity spin used in the derivation of the representation U can then give interesting insights into the structure of phase space as a carrier of canonical transformations, as will be discussed in future publications.

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