Phase space formalisms of quantum mechanics with singular kernel

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Abstract

The equivalence of the Rivier-Margenau-Hill and Born-Jordan-Shankara phase space formalisms to the conventional operator approach of quantum mechanics is demonstrated. It is shown that in spite of the presence of singular kernels the mappings relating phase space functions and operators back and forth are possible.

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1 Introduction

A wide class of quantum quasi-probability distributions \( F \) of position \( q \) and momentum \( p \) was studied by Cohen \[1\], the Wigner function \[2\] and the Margeneau-Hill functions \[3\] being particular cases. The choice among the \( F \) functions representing the quantum state of a system is similar to the choice of a convenient set of coordinates. However, in order to use safely one of these phase space functions it is necessary to show that the usual operator formulation of quantum mechanics is equivalent to the corresponding phase space formalism. In the later, in addition to the state, it is necessary to specify the functional form of the dynamical variables. In Cohen’s approach each of the distributions \( F \) is obtained with a particular kernel function \( f \) from the quantum density operator \( \hat{\rho} \), \( \hat{\rho} \rightarrow F \). (Operators are represented with an accent “\(^{\circ}\)” and the notation corresponds, as in \[1\], to a particle moving in one spatial dimension.) Cohen gave as well the quantization rule \( g \rightarrow \hat{G} \) that associates with a classical function \( g(q,p) \) a quantum operator \( \hat{G}(\hat{q},\hat{p}) \) in such a way that the expectation value of the operator can be written equivalently as a trace or as a phase space integral (All integrals in this work go from \(-\infty\) to \(\infty\).)

\[
\langle \hat{G}(\hat{q},\hat{p}) \rangle = \text{tr}(\hat{G}) = \int \int F(q,p) g(q,p) dq dp.
\]

(1)

The most frequently used quantization or ordering rules and many others fit into this general scheme (in particular the rules by Weyl \[4,5\], Rivier \[6\], Born-Jordan \[7\], and the set of rules known as normal, antinormal, standard and antistandard \[8-10\]), together with their associated phase space quasi-
probability distributions, see Table 1.

In order to build a quantum formalism in phase space equivalent to the conventional operator approach, rather than considering \( \hat{\rho} \) and \( g \) as primary, a different point of view is required where the primary objects are the state and observable in operator form, \( \hat{\rho} \) and \( \hat{G} \). Their phase space representations, \( F \) and \( g \), are obtained from them using \( \hat{\rho} \rightarrow F \) and the inverse transformation of the quantization rule, i.e., \( \hat{G} \rightarrow g \). Also in this case it is imposed that the expectation value of \( \hat{G}(\hat{q}, \hat{p}) \) is given by (1), but now the function \( g(q, p) \) is not necessarily equal to the classical magnitude; it is simply one the images or representations of \( \hat{G} \) in phase space.

It is also possible to consider \( F \) as a primary object. Then, the transformation \( F \rightarrow \hat{\rho} \) is required to obtain the corresponding density operator. Even though it is not common practice to consider \( F \) as primary in quantum mechanics, there are physical systems of practical importance (semiconductor heterostructures) which are modelled in this fashion \([11,12]\). It is also of interest to note that classical statistical mechanics is a theory formulated in terms of an \( F \) distribution (the classical distribution function) and properties \( g \) (classical magnitudes), so that the transformations \( F \rightarrow \hat{\rho} \) and \( g \rightarrow \hat{G} \) provide a set of equivalent operator formulations of classical statistical mechanics. Their potential applications are yet to be fully explored. One of them, using \( f = 1 \) and associated with the Weyl-Wigner formalism, was examined in \([13]\).

The (formal) full set of transformations that completes Cohen’s two original mappings, has been described by several authors \([14-17]\). Whereas the
transformations $g \rightarrow \hat{G}$ and $\hat{q} \rightarrow F$ involve the kernel function $f$ in a multiple integral, the inverse transformations involve $f^{-1}$. Agarwal and Wolf \cite{15} restricted their detailed study to mappings where the kernel function had no zeroes to avoid the singularities of $f^{-1}$. In fact it has been generally believed that the inverse mappings cannot be performed in these cases \cite{17}. As a consequence the investigation or applications of some of the $f$ functions and their associated quasi-probability distributions and ordering rules have been scarce. Our main objective here is to demonstrate that these singular kernels do not necessarily preclude the existence of the inverse mappings and that indeed equivalent phase space formalisms based on them can be constructed. In other words, we shall show that there is an “inverse operator basis”, see (15) below, in the form of operator valued distributions, associated with these kernels. The need to consider in general the mappings between operators and phase space from a generalized function point of view was already emphasized by Agarwal and Wolf \cite{15}.

The quasi-probability distributions in phase space are obtained from $\hat{q}$ as

$$F(q, p) = \frac{1}{4\pi^2} \iint \langle u + \frac{\tau h}{2}|\hat{q}|u - \frac{\tau h}{2}\rangle e^{-i[\theta(q-u)+\tau p]} f(\theta, \tau) d\theta d\tau du. \quad (2)$$

Cohen noted that by imposing the condition

$$f(0, \tau) = f(\theta, 0) = 1, \quad (3)$$

the resulting $F$ function provides the correct “marginal distributions” for $q$ and $p$. A group of $f$ functions and their corresponding quasi-probability distributions are listed in Table 1 \cite{18}. The property (3) is desirable but this condition is not fulfilled by several useful quasi-probability distributions
[such as the $P$-distribution by Sudarshan \[8\] and Glauber \[19\] or the $Q$ (or Husimi \[20\]) distribution.]

The operator $\hat{G}(\hat{q}, \hat{p})$ is given from the phase space function by

$$\hat{G}(\hat{q}, \hat{p}) = \frac{1}{4\pi^2} \int \int \int g(q, p) f(\theta, \tau) e^{-i[\theta(q-\hat{q})+\tau(p-\hat{p})]} \, dq \, dp \, d\theta \, d\tau.$$  \hspace{1cm} (4)

It is an exercise of Fourier transforms to obtain $g$ in terms of $\hat{G}$ from (4),

$$g(q, p) = \frac{\hbar}{2\pi} \int \int \left\langle u + \frac{\tau \hbar}{2} \right| \hat{G} \left| u - \frac{\tau \hbar}{2} \right\rangle e^{-i[\theta(q-u)+\tau(p-u)]} \frac{1}{f(-\theta, -\tau)} \, d\theta \, d\tau \, du.$$ \hspace{1cm} (5)

Similarly

$$\hat{\rho} = \frac{\hbar}{2\pi} \int \int \int F(q, p) f(-\theta, -\tau)^{-1} e^{-i[\theta(q-\hat{q})+\tau(p-\hat{p})]} \, dq \, dp \, d\theta \, d\tau.$$ \hspace{1cm} (6)

The explicit expressions for all the transformations in equations (4), (5), (6) and (7) can be summarized as

$$F = \Lambda[f] \hat{\rho} \hspace{1cm} \hat{\rho} = \{\Lambda[f]\}^{-1} F$$ \hspace{1cm} (7)

$$g = \hbar \Lambda[\tilde{f}^{-1}] \hat{G} \hspace{1cm} \hat{G} = \hbar^{-1}\{\Lambda[\tilde{f}^{-1}]\}^{-1} g$$ \hspace{1cm} (8)

where $\tilde{f} \equiv f(-\theta, -\tau)$.

Here we consider the transformation from $\hat{\rho}$ to $F$ as the reference mapping represented by the “operator” (on the space of density operators) $\Lambda[f]$ which depends functionally on $f$, see (2). The inverse operator $\{\Lambda[f]\}^{-1}$ acts on $F$ to provide the density operator $\hat{\rho}$. Note that $\hat{G} \rightarrow g$ involves, except for a constant, the same operation as $\hat{\rho} \rightarrow F$ but a different kernel, namely $\tilde{f}^{-1}$ \[21\].

These are of course formal results and for every $f$ it is necessary to study if these integrals exist and to determine domains where the transformations
can be performed. Seemingly functions having zeroes, such as \( f(\theta, \tau) = \cos(\theta \tau \hbar/2) \) or \( 2 \sin(\theta \tau \hbar/2)/\theta \tau \hbar \), may be problematic because of the presence of the inverse of \( f \) in the integrands of the transformations \( \hat{G} \to g \) and \( F \to \hat{\varrho} \).

It is also possible to relate operators and phase space using a framework complementary to Cohen’s [14-17]: Assume that there is an operator basis \( \hat{B}(\hat{q}, \hat{p}; q, p) \) such that the operator \( \hat{G}(\hat{q}, \hat{p}) \) can be given as

\[
\hat{G} = \iint g_B(q, p) \hat{B}(q, p) \, dq \, dp, \tag{9}
\]

where the “coefficients”, \( g_B(q, p) \), are, as before, the transform, image or representation of the operator in that basis. For a basis \( \hat{B} \) to be practical it must have an inverse \( \hat{B}^{-} \) such that [22]

\[
\text{tr}[\hat{B}^{-}(q, p) \hat{B}(q', p')] = \delta(q - q') \delta(p - p'). \tag{10}
\]

If the density operator is expanded in the inverse basis,

\[
\hat{\varrho} = \iint F_B(q, p) \hat{B}^{-}(q, p) \, dq \, dp, \tag{11}
\]

with expansion coefficients \( F_B(q, p) \), using (10) it follows that

\[
\text{tr}(\hat{G} \hat{\varrho}) = \iint g_B F_B \, dq \, dp \tag{12}
\]

and the coefficients (phase space representations of the state and the observable) are obtained from the operators by taking the traces

\[
F_B(q, p) = \text{tr}(\hat{\varrho} \hat{B}) \tag{13}
\]

\[
g_B(q, p) = \text{tr}(\hat{G} \hat{B}^{-}) \tag{14}
\]
In terms of $f$ these bases are formally given by
\begin{align}
\hat{B}^{-}(q, p) &= \frac{\hbar}{2\pi} \int \int e^{-i[\theta (q - \hat{q}) + \tau (p - \hat{p})]} \frac{1}{f(-\theta, -\tau)} d\theta d\tau \quad (15) \\
\hat{B}(q, p) &= \frac{1}{4\pi^2} \int \int e^{-i[\theta (q - \hat{q}) + \tau (p - \hat{p})]} f(\theta, \tau) d\theta d\tau. \quad (16)
\end{align}

From this perspective each of the phase space formalisms is based on a certain “coordinate system” or “basis” that can be more or less convenient depending on the case. But, as before, the presence of $f^{-1}$ in the expression for the inverse basis seems to impose a limitation when $f$ has zeroes \[17\]. In this way one could be prematurely tempted to discard, for example, phase space formalisms based on the relatively common Rivier quantization rule (or symmetrization rule) and the associated Margeneau-Hill function or on the Born-Jordan quantization rule and the associated Shankara distribution function \[23\]. However the next section shows that the zeroes of $f$ are not actually a problem.

2 Effect of zeroes of $f(\theta, \tau)$

We shall give an explicit expression of the transform of $\hat{q}^n \hat{p}^m$ for arbitrary nonnegative integer values of $n$ and $m$. According to equation (15) the $f$-image of $\hat{q}^n \hat{p}^m$ is obtained by the integral
\begin{align}
g(q, p) &= g(q, p; \hat{q}^n \hat{p}^m; f) \equiv \frac{\hbar}{2\pi} \int \int \int \langle u - \frac{\tau \hbar}{2} | \hat{q}^n \hat{p}^m | u + \frac{\tau \hbar}{2} \rangle \\
&\quad \times e^{i[\theta (q - u) + \tau p]} \frac{1}{f(\theta, \tau)} d\theta d\tau du. \quad (17)
\end{align}

Introducing a closure relation in momentum this takes the form
\begin{align}
g(q, p) &= \frac{1}{4\pi^2} \int \int \int (u - \frac{\tau \hbar}{2})^n p^m e^{i\theta (q - u)} e^{-i\tau (p' - p)} \frac{1}{f(\theta, \tau)} d\theta d\tau du dp'. \quad (18)
\end{align}
Making use of the integral expression of the Dirac delta and of its \( m \)-th order derivative \( \delta^{(m)} \) the integral in \( p' \) is solved,

\[
g(q, p) = \frac{1}{2\pi(-i)^m} \int \int \left(u - \frac{\tau h}{2}\right)^{n} e^{i\theta(q-u)} e^{ip\tau} \frac{1}{f(\theta, \tau)} \delta^{(m)}(\tau) \, d\theta \, d\tau \, du. \tag{19}
\]

The \( \tau \)-integral is carried out next. It is necessary to consider the \( m \)-th derivative of the function

\[
\chi(\tau) = \left(u - \frac{\tau h}{2}\right)^{n} e^{ip\tau} \frac{1}{f(\theta, \tau)}. \tag{20}
\]

By using Leibniz’s formula for the \( m \)-th derivative of a product twice and putting \( \tau = 0 \) one obtains

\[
\frac{d^m \chi}{d\tau^m} = \sum_{l=0}^{m} \left( \begin{array}{c} m \\ l \end{array} \right) \prod_{j=0}^{l} \left( \begin{array}{c} l \\ j \end{array} \right) (ip)^j \frac{n!}{(n + j - l)!} u^{n-l+j}(-h/2)^{j-l} \frac{d^{m-l}f^{-1}}{d\tau^{m-l}} \bigg|_{\tau = 0}, \tag{21}
\]

which is used to integrate over \( \tau \) with the aid of the derivatives of the delta function. Then the \( u \)-integral is carried out,

\[
g(q, p) = (-1)^n \sum_{l=0}^{m} \sum_{j=0}^{l} \frac{1}{(m+n-l)\left( \begin{array}{c} m \\ l \end{array} \right) \left( \begin{array}{c} l \\ j \end{array} \right)} \frac{n!}{(n + j - l)!} (h/2)^{j-l} \times \int e^{i\theta q} \frac{d^{m-l}f^{-1}}{d\tau^{m-l}} \bigg|_{\tau = 0} \delta^{(n-l+j)}(\theta) \, d\theta. \tag{22}
\]

The derivatives of \( f^{-1} \) with respect to \( \tau \) at \( \tau = 0 \) can be performed by using the formula for the derivative of arbitrary order, say \( m-l \), of the inverse of a function \[24\]. This formula involves \( f^{-1}(\tau = 0) \),

\[
\frac{d^{m-l}f^{-1}}{d\tau^{m-l}} \bigg|_{\tau = 0} = (m-l)!(-1)^{m-l} \frac{1}{f^{m-l+1}(\tau = 0)} D_{m-l} \tag{23}
\]
where
\[ D_{m-l} \equiv \begin{vmatrix} a_1 & a_0 & 0 & 0 & \cdots & 0 \\ a_2 & a_1 & a_0 & 0 & \cdots & 0 \\ a_3 & a_2 & a_1 & a_0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & a_0 \\ a_{m-l} & a_{m-l-1} & a_{m-l-2} & \cdots & a_2 & a_1 \end{vmatrix} \tag{24} \]

and
\[ a_n = a_n(\theta) = \left. \frac{1}{n!} \frac{d^n f}{d\tau^n} \right|_{\tau=0} \tag{25} \]

Finally the integration over \( \theta \) is performed using the derivatives of the delta function, and taking the condition (3) into account. Again, Leibniz’s theorem is used to arrive at the lengthy but explicit expression
\[ g(q,p;\hat{q}^m \hat{p}^n; f) = \sum_{l=0}^{m} \sum_{j=0}^{n-l+j} (-1)^{m-j} \frac{(m-l)!}{l!} i^{j-k-m} (\hbar/2)^{l-j} \binom{m}{l} \binom{l}{j} \times \binom{n-l+j}{k} \frac{n!}{(n+j-l)!} p^j q^{n-l-j} D_{m-l} \frac{d^k}{d\theta^k} \bigg|_{\theta=0} \tag{26} \]

where only mixed partial derivatives of the \( f \) function at the origin (\( \theta = 0, \tau = 0 \)) are to be considered.

We conclude that provided that Cohen’s condition (3) is satisfied and \( f \) is analytical at the origin \( g(q,p;\hat{q}^m \hat{p}^n; f) \) is well defined in spite of the possible zeroes of \( f \). The expression corresponding to the operators in reverse order, \( g(q,p;\hat{p}^m \hat{q}^n; f) \), is the same except for a the change of sign \( (\hbar/2)^{l-j} \rightarrow (-\hbar/2)^{l-j} \).

Examples of images of \( \hat{q}^2 \hat{p}^2 \) for several \( f \) using (24) are
\[ g(q,p;\hat{q}^2 \hat{p}^2; f = 1) = p^2 q^2 + 2i\hbar pq - \frac{\hbar^2}{2} \]
\[ g[q,p;\hat{q}^2 \hat{p}^2; f = \cos(\theta \tau \hbar/2)] = p^2 q^2 + 2i\hbar pq \]
\[
g \left[ q, p; \hat{q}^2 \hat{p}^2 ; f = 2 \sin\left(\theta \tau / 2\right)/(\theta \tau h) \right] = p^2 q^2 + 2 i h p q - \frac{h^2}{3}
\]
\[
g \left[ (q, p; \hat{q}^2 \hat{p}^2 ; f = e^{-i(\theta \tau h / 2)} \right] = p^2 q^2
\]
\[
g \left[ q, p; \hat{q}^2 \hat{p}^2 , f = e^{i(\theta \tau h / 2)} \right] = p^2 q^2 + 4 i h p q - 2 h^2
\]

It can be checked -via eq. (11) with the corresponding \( f \) for each case- that the operator obtained from these phase space functions is indeed \( \hat{q}^2 \hat{p}^2 \), and that, once \( f \) has been chosen, the relation between operators and phase space images is biunivocal for arbitrary (non-negative) values of \( m \) and \( n \). It is possible in summary to map into phase space functions at least operators of \( \hat{p} \) and \( \hat{q} \) in polynomial form or given by expansions in \( \hat{q}^n \hat{p}^m \) or \( \hat{p}^m \hat{q}^n \). A broad set of bounded operators admits such expansions [10].

Note that (26) is non-linear in \( f \) so that if \( f = a f_1 + b f_2 \), in general \( g_f \neq a g_{f_1} + b g_{f_2} \). In particular, the images obtained with the inverse of Rivier’s rule are not given by the average of the phase space representations using the inverses of the standard and antistandard rules.

The arguments for demonstrating the feasibility of the inverse transformation \( F \rightarrow \hat{\varrho} \) are analogous, based on expanding \( F \) in power series \( \sum_{nm} b_{nm} q^n p^m \) and transforming each \( q^n p^m \) term independently to obtain the density operator as \( \sum_{nm} b_{nm} \hat{\varrho}_{nm} \). Also in this case the singularity is avoided due to the delta functions. The result is

\[
\hat{\varrho}_{nm} = h \frac{m}{l=0} \frac{n}{k=0} \frac{n-k}{j=0} \binom{m}{l} \binom{n}{k} \binom{n-k}{j} l! j^l + k (-1)^l 2^{k-n} \times \frac{d^k D_l}{d q^k} \bigg|_{q=0} \hat{q}^n \hat{p}^m \hat{q}^{n-k-j} \tag{28}
\]

Moreover, using (13) and (14) it is easy to check that (14) is verified. In
other words, Rivier’s rule, as well as other rules based on functions \( f \) with derivatives at the origin have an inverse basis in a generalized sense. Eq. (13) is a symbolic expression that results from trying to fit the transformation (\( \Psi \)), whose calculation is possible as shown above, into the scheme of eq. (14). The fit requires a formal change in the order of integration. This generally illegitimate procedure is allowed when dealing with generalized functions. In this regard it is worth recalling that the integral form of the a delta function \( [(2\pi)^{-1} \int \! dx \, \exp (ixy)] \) is in fact a symbol that is not to be interpreted “literally”. The origin of this symbol is again a formal change of integration when performing two successive Fourier transformations. In the actual computation the order of integration is reversed, see the illustrative discussion in [24], or a rigorous and more general analysis in [26]—especially sec. 7.9—. In the same vein, the actual order of integration when using (13) is to be reversed so that it is never performed over \( \theta \) and \( \tau \) first. This avoids the possible singularities of \( f^{-1} \) at the zeroes of \( f \).

In summary, the number of phase space formalisms equivalent to the conventional operator approach is broader than it had been generally believed. Zeroes of \( f \) do not preclude the possibility of a set of biunivocal transformations between operators and phase space representations.

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| f                                      | F                               | quantization rule |
|----------------------------------------|---------------------------------|-------------------|
| $\cos(\theta \tau \hbar/2)$           | Wigner                          | Margenau-Hill     |
| $2 \sin(\theta \tau \hbar/2)/\theta \tau \hbar$ | Shankara                        | Born-Jordan       |
| $e^{-\nu(\theta \tau \hbar/2)}$       | Kirkwood $f_K^+$                | standard          |
| $e^{\nu(\theta \tau \hbar/2)}$       | Kirkwood $f_K^-$                | antistandard      |
| $e^{\pm \frac{\lambda}{2}(\tau \lambda)^2 + (\theta/\lambda)^2}$ | P-function(Sudarshan-Glauber)   | normal            |
| $e^{-\frac{\lambda}{4}(\tau \lambda)^2 + (\theta/\lambda)^2}$ | Q-function(Husimi)              | antinormal        |

TABLE 1 CAPTION: $\lambda$ is a real parameter different from zero.