Wigner distributions in Quantum Mechanics

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Abstract. The Weyl-Wigner description of quantum mechanical operators and states in classical phase-space language is well known for Cartesian systems. We describe a new approach based on ideas of Dirac which leads to the same results but with interesting additional insights. A way to set up Wigner distributions in an interesting non-Cartesian case, when the configuration space is a compact connected Lie group, is outlined. Both these methods are adapted to quantum systems with finite-dimensional Hilbert spaces, and the results are contrasted.

1. Introduction.

It is well known that Quantum Mechanics grew out of the Hamiltonian form of Classical Mechanics, and this was formalized in a procedure called "canonical quantization" [1]. This is a heuristic and suggestive procedure which works for systems whose fundamental variables are continuous and Cartesian. Then the classical configuration space is Euclidean $\mathbb{R}^n$ for n degrees of freedom, while the phase space is $\mathbb{R}^{2n}$. The basic variables q_r, p_r, $r = 1, 2, ..., n$ all lie in the range $-\infty < q_r, p_r < \infty$.

To make the transition to Quantum Mechanics, we replace these classical real variables by Hermitian operators $\widehat{q}_r, \widehat{p}_r$ obeying the canonical commutation relations:

$$[\widehat{q}_r, \widehat{p}_s] = i\delta_{rs}, \quad [\widehat{q}_r, \widehat{q}_s] = [\widehat{p}_r, \widehat{p}_s] = 0 \tag{1}$$

where we have set $\hbar = 1$. These operators act on Schrödinger wave functions $\psi(\mathbf{q})$ belonging to the Hilbert space $\mathcal{H} = \mathcal{L}^2(\mathbb{R}^n)$. General classical dynamical variables, which are real phase space functions $f(\mathbf{q}, \mathbf{p})$, are promoted to Hermitian operators $\widehat{A}$ on $\mathcal{H}$.

Turning now to quantum states, we have pure states described by wave functions $\psi(\mathbf{q})$ and mixed states described by density matrices $\widehat{\rho}$. Pure states can be combined with one another according to the Superposition Principle, while with mixed states only convex combinations can be formed:

$$\begin{aligned}
\psi_1, \psi_2, ... &\rightarrow \psi = c_1 \psi_1 + c_2 \psi_2 + ...; \ c_1, c_2, ... \in \mathbb{C} \\
\widehat{\rho}_1, \widehat{\rho}_2, ... &\rightarrow \widehat{\rho} = p_1 \widehat{\rho}_1 + p_2 \widehat{\rho}_2 + ...; \ p_1, p_2... \in \mathbb{R}^+, \ p_1 + p_2 + ... = 1
\end{aligned} \tag{2}$$

where $\mathbb{R}^+$ stands for the set of non-negative real numbers.

Since the $\widehat{q}$'s and $\widehat{p}$'s do not commute, given a classical dynamical variable $f(\mathbf{q}, \mathbf{p})$ there is "a priori" no unambiguously defined corresponding quantum dynamical variable, as there are factor ordering problems:

$$classical \quad f(\mathbf{q}, \mathbf{p}) \rightarrow \quad quantum \quad f(\widehat{\mathbf{q}}, \widehat{\mathbf{p}}) \quad ambiguous \tag{3}$$

We may think of several rules or prescriptions to resolve this ambiguity, but none is intrinsic to the transition from Classical to Quantum Mechanics. The earliest rule was proposed by Weyl in 1927 [2]. Taking $n = 1$ for simplicity, i.e. one $\widehat{q}$ and one $\widehat{p}$, this rule is to place $\widehat{q}$ and $\widehat{p}$ in all possible relative positions in any expression and then take the average. For monomials, exponentials and general functions, the rule is:

$$\begin{aligned}
i) \ q^m p^n &= \frac{\partial^m}{\partial \lambda^m} \frac{\partial^n}{\partial \mu^n} \frac{(\lambda q + \mu p)^{m+n}}{(m+n)!} \big|_{\lambda=\mu=0} \rightarrow \\
&\rightarrow \frac{\partial^m}{\partial \lambda^m} \frac{\partial^n}{\partial \mu^n} \frac{(\lambda \widehat{q} + \mu \widehat{p})^{m+n}}{(m+n)!} \big|_{\lambda=\mu=0} \\
ii) \ &\exp\left[i(\lambda q + \mu p)\right] \rightarrow \exp\left[i(\lambda \widehat{q} + \mu \widehat{p})\right] \\
iii) \ f(q,p) &= \iint\limits_{-\infty}^{\infty} d\lambda d\mu \ a(\lambda, \mu) \exp\left[i(\lambda q + \mu p)\right] \rightarrow \\
&\rightarrow \widehat{A}_f = \iint\limits_{-\infty}^{\infty} d\lambda d\mu \ a(\lambda, \mu) \exp\left[i(\lambda \widehat{q} + \mu \widehat{p})\right]
\end{aligned} \tag{4}$$

The Weyl rule does possess the nice property:

$$f(\mathbf{q}, \mathbf{p}) \ real \iff \widehat{A}_f \ hermitian \tag{5}$$

but of course for products:

$$f \rightarrow \widehat{A}_f, \ g \rightarrow \widehat{A}_g \ \nRightarrow \ fg \rightarrow \widehat{A}_f \widehat{A}_g \tag{6}$$

This means that the Weyl correspondence between classical phase-space functions and quantum mechanical operators is not a homomorphism of associative algebras:

$$\widehat{A}_{fg} \neq \widehat{A}_f \widehat{A}_g \tag{7}$$

Indeed, the classical equivalent of operator multiplication in Quantum Mechanics is the non-local Moyal product (see below) of phase-space functions, quite different from the pointwise product; it is associative but of course non-commutative.

At this point let us compare the classical and quantum descriptions of dynamical variables, states and expectation values:

Classical	**Quantum**
Dynamical variable $f(\mathbf{q}, \mathbf{p})$	$\leftarrow Weyl\ rule \rightarrow \widehat{A}_f$
States $\rho(\mathbf{q}, \mathbf{p})$	$\lvert\psi\rangle, \widehat{\rho}$
Expectation values:	
$\langle f\rangle = \iint dq\,dp\, f(\mathbf{q}, \mathbf{p})\, \rho(\mathbf{q}, \mathbf{p})$	$\left\langle \widehat{A}_f\right\rangle = \left\langle \psi\left\lvert \widehat{A}_f\right\rvert \psi\right\rangle, \ Tr\left(\widehat{\rho}\widehat{A}_f\right)$

We have denoted a general classical state by a phase space probability distribution $\rho(\mathbf{q}, \mathbf{p})$. It is now natural to ask: if via the Weyl rule we are able to describe quantum dynamical variables in classical phase space language, what about quantum states? For Cartesian systems, in 1932 Wigner found a way to represent quantum states too by classical real phase space functions [3]. For pure $\lvert\psi\rangle$ or general $\widehat{\rho}$ the corresponding Wigner distributions (for $n = 1$) are:

$$W_\psi(q, p) = \tfrac{1}{2\pi} \int_{-\infty}^{\infty} dq'\, \psi\left(q - \tfrac{1}{2}q'\right) \psi\left(q + \tfrac{1}{2}q'\right)^* e^{iq'p}$$

$$W_{\widehat{\rho}}(q, p) = \tfrac{1}{2\pi} \int_{-\infty}^{\infty} dq'\, \left\langle q - \tfrac{1}{2}q' \left\lvert \widehat{\rho}\right\rvert q + \tfrac{1}{2}q'\right\rangle e^{iq'p} \tag{8}$$

In the pure state case this means that we construct a rank-one projector $\widehat{\rho}$ out of the state vector $\lvert\psi\rangle$ and then use the second definition above.

The mapping (8) is dual to the Weyl map (4) in the sense:

$$f(q, p) \rightarrow \widehat{A}_f\ by\ Weyl,\ \widehat{\rho} \rightarrow W_{\widehat{\rho}}(q, p)\ by\ Wigner\ \Rightarrow$$
$$Tr\left(\widehat{\rho}\widehat{A}_f\right) = \iint dq\,dp\, W(q, p)\, f(q, p) \tag{9}$$

But whereas in the Weyl rule we can take essentially any classical $f(q, p)$ and find its operator counterpart $\widehat{A}_f$, for states the Wigner distributions $W(q, p)$ are highly restricted, on account of the properties of $\widehat{\rho}$ and of the definition (8). A general (real) phase space function is highly unlikely to be $W_{\widehat{\rho}}(q, p)$ for some quantum state $\widehat{\rho}$.

This Weyl-Wigner duality was clarified and developed further by Grönewold and Moyal [4]. In particular Moyal [5] expressed operator multiplication as a nonlocal, associative but non commutative multiplication rule among classical phase space functions, and applied it to quantum dynamics.

The Moyal product $f * g$ of two phase-space functions $f(q, p)$ and $g(q, p)$ is:

$$(f * g)(q, p) = f(q, p) \exp\left\{\frac{\hbar}{2i}\left(\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial q} - \frac{\overleftarrow{\partial}}{\partial q}\frac{\overrightarrow{\partial}}{\partial p}\right)\right\} g(q, p) \tag{10}$$

The first term in the expansion of the exponential gives the ordinary pointwise product of $f(q, p)$ with $g(q, p)$; the second term involves the Poisson bracket of $f(q, p)$ and $g(q, p)$; and the non-local nature is evident.

2. Some properties of Wigner distributions.

To get a "feel" for these phase space functions, we recall some of their important properties:

a)

$$\widehat{\rho}^{\dagger} = \widehat{\rho}, \ Tr\widehat{\rho} = 1 \Rightarrow \ W(q,p) \ real, \ \iint dqdp W(q,p) = 1 \tag{11}$$

b) Recovery of quantum mechanical position and momentum probability distributions as marginals:

$$\int_{-\infty}^{\infty} dp W(q,p) = \langle q\,|\widehat{\rho}|\,q\rangle, \ \int_{-\infty}^{\infty} dq W(q,p) = \langle p\,|\widehat{\rho}|\,p\rangle \tag{12}$$

However in general $W(q,p)$ is not pointwise non negative and so cannot be regarded as a probability distribution. This is generic, indeed (for $n=1$) Hudson's theorem [6] says:

$$W_{\psi}(q,p) \geq 0 \ \forall q,p \ \Rightarrow$$
$$\Rightarrow \psi(q) \ is \ complex \ Gaussian, \ W(q,p) \ is \ real \ Gaussian \tag{13}$$

Further we have a theorem of Folland and Sitaram [7]:

$$W(q,p) \ has \ compact \ support \ \Rightarrow \ W(q,p) = 0 \tag{14}$$

c) At each point in phase space $W(q,p)$ is bounded:

$$|W(q,p)| \leq \frac{1}{\pi} \tag{15}$$

We can see in eqs.(14,15) the great contrast to Schrödinger wave functions $\psi(q)$, which could very well be of compact support, and are certainly not pointwise universally bounded. It is clear that the "Wigner quality" of a phase space function is really delicate.

d) Traciality is a key property: for any two states $\widehat{\rho}$ and $\widehat{\rho}'$:

$$Tr\left(\widehat{\rho}\widehat{\rho}'\right) = \iint dqdp W_{\widehat{\rho}}(q,p) W_{\widehat{\rho}'}(q,p) \tag{16}$$

This ensures that $\widehat{\rho}$ can be reconstructed from, and is completely and faithfully represented by, $W_{\widehat{\rho}}(q,p)$.

e) Turning now to general n, the behavior of $W(\mathbf{q},\mathbf{p})$ under the group of linear canonical transformations is important. These transformations are described by real $2n \times 2n$ matrices S such that the hermitian operators $\widehat{q}'_r, \widehat{p}'_r$ defined by:

$$\left| \begin{array}{c} \widehat{q}'_r \\ \widehat{p}'_r \end{array} \right| = S \left| \begin{array}{c} \widehat{q}_r \\ \widehat{p}_r \end{array} \right| \tag{17}$$

obey the same commutation relations (1) as $\widehat{q}_r, \widehat{p}_r$. Therefore such changes in the basic operators are unitarily implementable. There are unitary operators $\widehat{U}(S)$, $S \in Sp(2n, \mathbb{R})$, determined up to phases and acting on $\mathcal{H}$, such that:

$$\widehat{q}'_r = \widehat{U}(S)^{-1} \widehat{q}_r \widehat{U}(S), \ \ \widehat{p}'_r = \widehat{U}(S)^{-1} \widehat{p}_r \widehat{U}(S) \tag{18}$$

Upon composition, however, and after adjustment of phases, the $\widehat{U}(S)$'s give a unitary representation of the two-fold metaplectic covering group $Mp(2n)$ of the symplectic group

$Sp\,(2n,\mathbb{R})$, not of the latter itself. When a state $\widehat{\rho}$ is transformed in this way, $W_{\widehat{\rho}}\,(\mathbf{q},\mathbf{p})$ transforms very simply:

$$\widehat{\rho}' = \widehat{U}\,(S)\,\widehat{\rho}\,\widehat{U}\,(S)^{-1} \Leftrightarrow W_{\widehat{\rho}'}\left(\left|\begin{array}{c}\widehat{\mathbf{q}}\\\widehat{\mathbf{p}}\end{array}\right|\right) = W_{\widehat{\rho}}\left(S^{-1}\left|\begin{array}{c}\widehat{\mathbf{q}}\\\widehat{\mathbf{p}}\end{array}\right|\right) \tag{19}$$

f) We said above that the "Wigner quality" of a phase space function is quite delicate and subtle. Based on traciality, eq.(16), we can give a necessary and sufficient condition for a given $W\,(\mathbf{q},\mathbf{p})$ to be a Wigner distribution:

$$\begin{array}{c}W\,(\mathbf{q},\mathbf{p})\;\;is\;a\;Wigner\;distribution\;\Leftrightarrow\\[4pt]\iint d^n q\,d^n p\,W\,(\mathbf{q},\mathbf{p})\,W_{\psi}\,(\mathbf{q},\mathbf{p}) \geq 0\;\;\;\forall \psi \in \mathcal{H}\end{array} \tag{20}$$

(this is of course in addition to reality and normalization). However from a practical point of view, this is rather unwieldy. In case $W\,(\mathbf{q},\mathbf{p})$ is a Gaussian, the condition can be made explicit in terms of its covariance matrix by exploiting the behavior (19) under symplectic transformations [8]. A real normalizable Gaussian on a $2n$ dimensional phase space can without loss of generality be taken to be of the form:

$$W_{\mathbb{G}}\,(\mathbf{q},\mathbf{p}) \sim \exp\left\{-\left|\begin{array}{cc}\mathbf{q} & \mathbf{p}\end{array}\right|\mathbb{G}\left|\begin{array}{c}\mathbf{q}\\\mathbf{p}\end{array}\right|\right\} \tag{21}$$

with $\mathbb{G}$ a real symmetric and positive definite $2n \times 2n$ matrix. By a nice theorem due to Williamson [9], such a matrix can be brought to diagonal form by some $S \in Sp\,(2n,\mathbb{R})$ of the kind discussed in property e) above:

$$S^T \mathbb{G} S = diag\,(k_1, k_2, ..., k_n, k_1, k_2, ..., k_n),\;\; k_j > 0 \tag{22}$$

This is generally not a similarity transformation as S may not belong to $SO\,(2n,\mathbb{R})$, therefore it is not isospectral and the k_j's are generally not eigenvalues of $\mathbb{G}$. The condition now reads:

$$W_{\mathbb{G}}\,(\mathbf{q},\mathbf{p})\;\;is\;a\;Wigner\;distribution\;\Leftrightarrow\;0 < k_j \leq 1\;\forall j \tag{23}$$

One can see how strong these conditions are - they are essentially the Heisenberg uncertainty relations for the n modes. For other treatments of Gaussian Wigner functions one may consult Ref. [10].

These then are some important properties of Wigner distributions in the Cartesian case. Both in Quantum Optics and Quantum Chemistry, Wigner distributions have been widely used.

3. Finite dimensions.

For a long time there has been considerable interest in extending these ideas to quantum systems with finite-dimensional state spaces. One can also consider extensions in infinite-dimension to non Cartesian systems.

Some early attempts in the finite-dimensional case are by R.Jagannathan in his unpublished 1976 thesis; Hannay and Berry in 1980; and Feynman as well as Wootters in 1987 [11]. Our work exploring approaches to setting up Wigner distributions in various situations consists of four interconnected parts:

Infinite dimensions, continuous variables	Finite dimension N
(i) New "Dirac" method, two-step procedure	(iii) Any N
(ii) Quantum Mechanics on compact	(iv) Any *odd* N
Lie groups as configuration spaces	

It is important to point out that (iii) and (iv) are adaptations of (i) and (ii) respectively; and interestingly our results in (iii) for odd N are in general different from the results in (iv), the latter displaying greater flexibility.

We now briefly outline our methods and results in the four situations.

4. (i) "Dirac" approach in Cartesian case [12].

For simplicity alone we assume one degree of freedom, $n = 1$. In the Weyl-Wigner approach, we can see that three desirable aims are attained all at once:

- Classical phase space descriptions for quantum variables and states;
- Recovery of quantum-mechanical probabilities as marginals;
- Translation of operator Hermiticity into reality of phase-space functions.

In contrast, the Dirac-inspired method uses two steps to achieve these. It exploits the essential similarity of position $\widehat{q}$ and momentum $\widehat{p}$ in the Cartesian case, in fact they are unitarily related by Fourier transformation.

The first two properties listed above can both be achieved by a practically trivial first step. Next, in a rather interesting second step, the Hermiticity-reality connection is secured. The key fact is that the wave function of an (ideal) momentum eigenstate is always non-zero:

$$\langle q|p \rangle = \frac{1}{\sqrt{2\pi}} \exp(iqp) \neq 0 \tag{24}$$

An operator $\widehat{A}$ is in any case completely determined by its mixed matrix elements $\left\langle q \left| \widehat{A} \right| p \right\rangle$, so it is (trivially!) a classical phase space description of $\widehat{A}$! Taking advantage of eq.(24), however, we define, following Dirac:

$$\widehat{A} \to A_l(q,p) =: \left\langle q \left| \widehat{A} \right| p \right\rangle \langle p|q \rangle = \frac{\left\langle q \left| \widehat{A} \right| p \right\rangle}{2\pi \langle q|p \rangle} \tag{25}$$

since this allows us to express $\widehat{A}$ as an ordered function of operators $\widehat{q}$ and $\widehat{p}$, the former always placed to the left of the latter:

$$\widehat{A} = 2\pi A_l(\widehat{q}, \widehat{p}) \tag{26}$$

Recovering the marginals is equally trivial:

$$\int\limits_{-\infty}^{\infty} dp A_l(q,p) = \left\langle q \left| \widehat{A} \right| q \right\rangle; \quad \int\limits_{-\infty}^{\infty} dq A_l(q,p) = \left\langle p \left| \widehat{A} \right| p \right\rangle \tag{27}$$

However, in general:

$$\widehat{A} \ \text{Hermitian} \ \nRightarrow \ A_l \ \text{real} \tag{28}$$

To tackle this we look at the trace of the product of two operators:

$$Tr\left(\widehat{A}\widehat{B}\right) =$$
$$= (2\pi)^2 \iiiint dq\,dp\,dq'\,dp'\, A_l(q,p) \langle q|p \rangle \langle p|q' \rangle \langle q'|p' \rangle \langle p'|q \rangle B_l(q',p') =$$
$$= \iiiint dq\,dp\,dq'\,dp'\, A_l(q,p) K_l(q-q', p-p') B_l(q',p') \tag{29}$$
$$K_l(q-q', p-p') = \exp\{i(q-q')(p-p')\}$$

The kernel K_l has interesting properties: symmetry under the interchange $(q,p) \leftrightarrow (q',p')$; invariance under phase space translations; unitarity in a suitable sense. The exponent is the area of a phase space rectangle, and so it is a geometric phase. To transform this kernel away,

we need a "square root" kernel in a convolution sense, having similar invariances, such that its use preserves the recovery of marginals as in eq.(27).

This is easily achieved in essentially unique fashion, as the same expression with a change in scale will do:

$$K_l\left(q-q',p-p'\right) = \iint\limits_{-\infty}^{\infty} dq''dp''\xi\left(q-q'',p-p''\right)\xi\left(q'-q'',p'-p''\right)$$

$$\xi\left(q-q'',p-p''\right) = \sqrt{2/\pi}\exp\left\{2i\left(q-q''\right)\left(p-p''\right)\right\} \tag{30}$$

Using this in the trace expression (29) and associating one factor with each of A_l and B_l we get:

$$\widehat{A} \to A_l\left(q,p\right) \to A\left(q,p\right) = \sqrt{2\pi}\iint\limits_{-\infty}^{\infty} dq'dp'\xi\left(q-q',p-p'\right)A_l\left(q',p'\right)$$

$$Tr\left(\widehat{A}\widehat{B}\right) = \tfrac{1}{2\pi}\iint\limits_{-\infty}^{\infty} dqdp A\left(q,p\right)B\left(q,p\right) \tag{31}$$

This is indeed the Weyl-Wigner definition with all three characteristic properties. Thus we have a new route to an old result, bringing out the underlying structure from a fresh point of view.

To repeat: in this approach, the introduction of phase space descriptions and recovery of marginals constitute the essentially trivial first step; then in the second step we secure reality from Hermiticity and get the Weyl-Wigner result essentially uniquely.

5. (ii) **Quantum Mechanics on a compact Lie Group** [13].

In the non Cartesian situation the definition of canonical momenta and construction of a phase space suitable for handling quantum mechanical quantities are both subtle, they are not as immediate and automatic as in the Cartesian case. We might anticipate that this is even more so in the finite-dimensional situation. The canonical commutation relations no longer hold, and the canonical quantization procedure has to be modified. We describe first what happens in an interesting continuous non Cartesian case.

Assume the configuration space is a compact Lie group G of dimension n, with coordinates α^r, $r = 1, 2, ..., n$, of the nature of angles. Also assume for definiteness that G is simple. The classical canonical momenta are like angular momenta, they are generators of G in the classical sense; each of them, J_r, $r = 1, 2, ..., n$ can have any real value:

$$\begin{aligned} classical\ configuration\ space &=\ compact\ Lie\ group\ G \Rightarrow \\ classical\ phase\ space &=\ T^*G \simeq G \times \mathbb{R}^n \end{aligned} \tag{32}$$

with α^r as coordinates over G, and J_r as coordinates over the factor $\mathbb{R}^n$. We can present the basic classical Poisson bracket relations symbolically in this manner:

$$\begin{aligned} \{f_1\left(\alpha\right), f_2\left(\alpha\right)\} &= 0 \\ \{f\left(\alpha\right), J^r\} &=\ linear\ first\ order\ differential \\ & \quad\ operator\ acting\ on\ f\left(\alpha\right) \\ \{J_r, J_s\} &= c_{rs}^t J_t \end{aligned} \tag{33}$$

Here the c's are the structure constants of G. We see here a new feature: the momenta have non-zero brackets with one another, they are non-Abelian for non-Abelian G. So coordinates and momenta have very different natures and properties.

When we make the transition to Quantum Mechanics, it is natural to assume that Schrödinger wave functions are complex functions on G with an invariant inner product. Denoting elements of G by $g, g', ...$, we have:

$$\text{wave functions } \sim \psi(g), \ g \in G$$
$$\|\psi\|^2 = \int_G dg \, |\psi(g)|^2 \tag{34}$$

with dg a normalized left and right translation invariant volume element on G. The operators $\widehat{J}_r$ are the hermitian generators of, say, left group action on ψ:

$$e^{-i\alpha^r \widehat{J}_r}\psi(g) = \psi\left(g(\alpha)^{-1}g\right) \tag{35}$$

This is like Cartesian momenta $\widehat{p}_r$ generating translations in $\widehat{q}_r$. The difference is their non commutativity:

$$\left[\widehat{J}_r, \widehat{J}_s\right] = ic_{rs}^t \widehat{J}_t \tag{36}$$

Turning to eigenvalues and eigenfunctions of momenta, we need the representation theory of G. Generalizing the notations of quantum angular momentum theory, denote the various inequivalent unitary irreducible representations (UIR) of G by j, of dimension N_j. Within a UIR label rows and columns by $m, n, m', ...$ So we have various unitary representation matrices $D_{mn}^j(g)$. We then say:

$$\text{momentum eigenvalues } \sim \text{ discrete set of labels } jmn$$
$$\text{momentum eigenfunctions } \sim D_{mn}^j(g) \tag{37}$$

Now it is a fact that any wave function $\psi(g)$ can be expanded in terms of the D-functions, an extension of Fourier analysis called harmonic analysis:

$$\psi(g) = \sum_{jmn} \psi_{jmn} N_j^{1/2} D_{mn}^j(g)$$
$$\psi_{jmn} = N_j^{1/2} \int_G dg D_{mn}^j(g)^* \psi(g) \tag{38}$$
$$\|\psi\|^2 = \int_G dg \, |\psi(g)|^2 = \sum_{jmn} |\psi_{jmn}|^2$$

We may then view $\psi(g)$ and ψ_{jmn} as configuration and momentum space wave functions respectively, and $|\psi(g)|^2$, $|\psi_{jmn}|^2$ as the corresponding complementary probability distributions. In this situation we pose the question: for a given wave function $\psi(g)$, can we set up a corresponding Wigner distribution of the general form $\psi\psi^*$, some expression $\widetilde{W}(g; ...)$ where the dots are suitable "momentum variables", which is real in a suitable sense and the marginals give us the known probability distributions:

$$\int dg\widetilde{W}(g; ...) \sim |\psi_{jmn}|^2, \quad \sum_{...} \widetilde{W}(g; ...) \sim |\psi(g)|^2 \ ? \tag{39}$$

This can be done using one key idea: given two group elements g' and g, we need a definition of their "midpoint" $s(g', g)$ with reasonable properties:

$$g', g \in G \rightarrow s(g', g) \in G$$
$$\text{symmetry: } s(g', g) = s(g, g')$$
$$\text{identity: } s(g, g) = g$$
$$\text{covariance: } s(g_1 g' g_2, g_1 g g_2) = g_1 s(g, g') g_2 \tag{40}$$

One can see that basically we need to define the square root of a general group element, covariant under conjugation. If we take $s(g, g')$ to be the midpoint on the geodesic connecting g to g', then (except possibly on a set of measure zero) all these conditions are met.

Remark. This "midpoint " rule allows to solve our specific problem. However, for more general situations its use is more subtle. Mathematically oriented readers may consult Ref.[14]. For the non-compact case, within the time-frequency Wigner function (signal analysis) see Ref.[15] for a critical discussion of this subtle point.

We define now, to begin with, for given $\psi(g)$:

$$\widetilde{W}(g; jmnm'n') =$$
$$= N_j \int_G dg' \int_G dg'' \psi(g') D^j_{m'n'}(g')^* \delta\left(g^{-1}s(g', g'')\right) D^j_{mn}(g'') \psi(g'')^* \tag{41}$$

where $\delta(..)$ is the invariant Dirac delta function going with the volume element dg, and find as consequences:

$$\widetilde{W}(g; jmnm'n')^* = \widetilde{W}(g; jm'n'mn)$$
$$\sum_{jmn} \widetilde{W}(g; jmnmn) = |\psi(g)|^2 \tag{42}$$
$$\int_G dg \widetilde{W}(g; jmnm'n') = \psi_{jm'n'} \psi^*_{jmn}$$

We can therefore adopt this as a good definition of the Wigner distribution in this continuous, non Cartesian situation. Even traciality is assured but actually it turns out that what has been defined above is overcomplete and a somewhat simpler expression will suffice. This is a result of the non-Abelian nature of G, something we do not see in the familiar Cartesian case. Namely, instead of $\widetilde{W}$ above, we can work with:

$$W(g; jmm') = \frac{1}{N_j} \sum_n \widetilde{W}(g; jmnm'n) =$$
$$= \int_G dg' \int_G dg'' \psi(g') D^j_{mm'}\left(g''g'^{-1}\right)^* \delta\left(g^{-1}s(g', g'')\right) \psi(g'')^* \tag{43}$$

and then, after straightforward extension to a general operator, we have:

$$Tr\left(\widehat{A}\widehat{B}\right) = \sum_{jmm'} N_j \int_G dg W_{\widehat{A}}(g; jmm') W_{\widehat{B}}(g; jm'm) \tag{44}$$

In summary, a complete Weyl-Wigner isomorphism can be set up. Notice that the domain of definition of these objects is not the classical phase space T^*G with $2n$ continuous coordinates α^r, J_r, but what we may call a "semi-quantized phase space" in which the momenta are already quantized. The important differences compared to the Cartesian situation are quite evident. In particular there is no rôle for the symplectic group $Sp(2n, \mathbb{R})$, and the Dirac approach seems unavailable.

Remark. Our treatment of Quantum Mechanics on compact Lie groups uses T^*G as a generalization of $T^*\mathbb{R}^n$. We prefer this point of view because T^*G is a Drinfeld double "Morita equivalent" [16] to the complexification of G. Other approaches are available in the literature

where the momentum map associated with the canonical action of G on T^*G gives rise to the orbit method advocated by A. Kirillov. In this context one may use the definition of Wigner functions with coordinates on coadjoint orbits, and the Fourier transform as it is done in Refs. [17] and [18].

6. (iii) Quantum Mechanics in N-dimensional state spaces [12].

For any finite dimension N, the Dirac method can be adapted, since "position" and "momentum" can be defined to have similar properties. Each vector $|\psi>$ in a Hilbert space $\mathcal{H}^{(N)}$ of dimension N is a column vector with complex entries $\psi(q)$ thought of as the "position space" wave function of $|\psi>$:

$$\psi(q) = \langle q|\psi\rangle, \; q = 0, 1, ..., N-1$$
$$\langle \psi|\psi \rangle = \sum_{q=0}^{N-1} |\psi(q)|^2 \tag{45}$$

We then set up a conjugate "momentum basis" of vectors $|p\rangle$ by a finite Fourier transformation:

$$|p\rangle = \tfrac{1}{\sqrt{N}}\sum_q e^{2\pi i p q/N}\,|q\rangle, \quad p = 0, 1, ..., N-1$$
$$\langle q|p\rangle = \tfrac{1}{\sqrt{N}}e^{2\pi i p q/N} \tag{46}$$

So, we have two orthonormal bases $\{|q\rangle\}, \{|p\rangle\}$ for $\mathcal{H}^{(N)}$; and $\widetilde{\psi}(p) = \langle p|\psi\rangle$ is the "momentum space" wave function. The "phase space" description of an operator $\widehat{A}$ on $\mathcal{H}^{(N)}$, an $n \times n$ matrix $\left(\left\langle q'|\widehat{A}|q\right\rangle\right)$ in the position description, is initially taken to be:

$$\widehat{A} \to A_l(q, p) = \left\langle q|\widehat{A}|p \right\rangle \langle p|q\rangle = \frac{1}{N}\frac{\left\langle q|\widehat{A}|p \right\rangle}{\langle q|p\rangle} \tag{47}$$

This leads to recovery of marginals and the trace formula:

$$\sum_p A_l(q, p) = \left\langle q\left|\widehat{A}\right|q\right\rangle; \; \sum_q A_l(q, p) = \left\langle p\left|\widehat{A}\right|p\right\rangle$$
$$Tr\left(\widehat{A}\widehat{B}\right) = \sum_{qpq'p'} A_l(q, p)\, K_l(q - q', p - p')\, B_l(q', p') \tag{48}$$
$$K_l(q - q', p - p') = \exp\left\{2\pi i (q - q')(p - p')/N\right\}$$

Except for the discrete and finite range for the q's and p's, these are similar to the Cartesian case. One can now ask if a "square root" ξ of K_l can be extracted in the form:

$$K_l\left(q - q', p - p'\right) = \sum_{q''p''} \xi\left(q, p; q'', p''\right) \xi\left(q', p'; q'', p''\right) \tag{49}$$

with suitable properties. Then in the trace formula (48) we attach one ξ factor with each of A_l and B_l and define:

$$\widehat{A} \to A_l(q, p) \to A(q, p) = \frac{1}{\sqrt{N}}\sum_{q'p'} \xi\left(q, p; q', p'\right) A_l\left(q', p'\right) \tag{50}$$

so that:

$$Tr\left(\widehat{A}\widehat{B}\right) = N\sum_{qp} A(q, p)\, B(q, p) \tag{51}$$

We would like to choose ξ so that:

$$\widehat{A}\ Hermitian\ \Leftrightarrow\ A(q,p)\ real$$
$$\sum_p A(q,p) = \left\langle q \left| \widehat{A} \right| q \right\rangle ;\ \sum_q A(q,p) = \left\langle p \left| \widehat{A} \right| p \right\rangle \tag{52}$$

A detailed study shows that such a "square root" kernel ξ can indeed be constructed. However, in contrast to the continuum case, there is a fair amount of freedom in choices of signs in the construction of ξ; and for any choices we get an acceptable Weyl-Wigner description. We may point out that in comparison to the results of Hannay and Berry [11], for an N level system our phase space is a set of just N^2 points, while they need $4N^2$ points.

7. (iv) Quantum Mechanics in $\mathcal{H}^{(N)}$ for odd N [19].

This is the last of our four cases. Here the Lie group method can be adopted, but only in odd dimensions. Whenever for such N we can find a finite group G of order N, via its representation theory we can set up an acceptable Wigner distribution formalism. The definitions and properties are:

$$|\psi\rangle = \{\psi(g)\} \rightarrow W(g;jmm') = W(g;jm'm)^* =$$
$$= \sum_{g'} \psi\left(g'^{-1}g\right) D^j_{mm'}\left(g'^2\right) \psi(g'g)^*$$
$$\frac{1}{N}\sum_{jm} N_j W(g;jmm) = |\psi(g)|^2 \tag{53}$$
$$\frac{N_j}{N}\sum_{g} W(g;jmm') = \sum_n \psi_{jm'n}\psi^*_{jmn}$$

Here the ψ_{jmn}'s are given by the expansion:

$$\psi(g) = \sum_{jmn} \sqrt{\frac{N_j}{N}} \psi_{jmn} D^j_{mn}(g) \tag{54}$$

The expressions for operators and traces are as expected.

The limitation to odd dimensions N comes from the fact that the midpoint construction works only in such situations. We may also note that for a given odd N we may have more than one distinct choice of group G, and it may be non Abelian with multidimensional UIR's. Then we have something new not seen in the results of the Dirac method which works uniformly for all dimensions.

8. Concluding Remarks.

We see that the Weyl-Wigner formalism is a robust feature of Quantum Mechanics, always present in one or more forms in every interesting case, and may be considered as an alternative picture of Quantum Mechanics which allows for an easy treatment of the quantum-classical transition on the same carrier space (the "phase space"). However, from our analysis it follows that we cannot easily find an "axiomatic" setting "à la par" of the Dirac Hilbert space approach or the $\mathbb{C}^*$-algebraic approach to Quantum Mechanics.

But there is one unifying theme: the Dirac "square root" concept familiar from the relativistic electron wave equation. Here we deal with the square root of a kernel in the continuous Cartesian

case, of a group element in the Lie group case, of a discrete kernel in any finite number of dimensions, and again of a group element in the odd-dimensional case.

In the finite-dimensional situations we see quite a lot of freedom in choice of definitions, and number theoretic features as well. It seems worthwhile to use these results in problems of quantum information theory and the study of entanglement.

Dedication and Acknowledgements

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