Phase Space Formulation of Quantum Mechanics

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Lecture 1 Introduction:
— from the coordinate representation to the phase space representation; the Weyl-Wigner transform

Lecture 2 The Wigner function:
— nonpositivity; quantum tomography

Lecture 3 Classical and quantum dynamics:
— the Groenewold operator; semiquantum mechanics
Introduction:

QM has many representations

- coordinate rep, momentum rep, Bargmann rep, Zak’s $kq$ - rep, ...

- each has its own advantages — most are equivalent
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  - each has its own advantages — most are equivalent
- The phase space rep is different in character
  - not equivalent to the above
  - prominent in recent years for applications to quantum optics,
    quantum information theory, quantum tomography, …
  - also for questions re foundations of QM and classical mechanics (CM)
    - QM as a deformation of CM, the nature of the QM-CM interface, …
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- The development of the theory is associated with a very long list of names: Weyl, Wigner, von Neumann, Groenewold, Moyal, Takabayasi, Stratonovich, Baker, Berezin, Pool, Berry, Bayen \textit{et al.}, Shirokov, \ldots

Our treatment will necessarily be \textit{very} selective \ldots
Start with some familiar reps of QM, related by unitary transformations.

Consider how we form the coordinate rep for a quantum system with one linear degree of freedom — dynamical variables $\hat{q}, \hat{p}$. 
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— scalar product $\langle \varphi | \psi \rangle$. 
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Consider how we form the coordinate rep for a quantum system with one linear degree of freedom — dynamical variables \( \hat{q}, \hat{p} \).

• Start with abstract \( \mathcal{H} \): complex Hilbert space of state vectors \( |\varphi\rangle, |\psi\rangle, \ldots \)
  — scalar product \( \langle \varphi|\psi \rangle \).

• Introduce generalized eigenvectors of \( \hat{q} \):
  \( \hat{q}|x\rangle = x|x\rangle \)
  — orthonormal \( \langle x|y \rangle = \delta(x - y) \) and complete \( \int |x\rangle \langle x| dx = \hat{1} \)
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Introduce generalized eigenvectors of $\hat{q}$: $\hat{q}|x\rangle = x|x\rangle$

— orthonormal $\langle x | y \rangle = \delta(x - y)$ and complete $\int |x\rangle\langle x| \, dx = \hat{I}$

Define a unitary mapping $\mathcal{H} \xrightarrow{u} \mathcal{H}' = L_2(C, dx)$, $|\varphi\rangle \xrightarrow{u} \varphi = u|\varphi\rangle$

by setting

$\varphi(x) = \langle x | \varphi \rangle$. 
Inverse

$$|\varphi\rangle = u^{-1} \varphi = \int |x\rangle \langle x|\varphi\rangle \, dx$$

$$= \int \varphi(x)|x\rangle \, dx.$$ 

Unitarity is evident — $u^{-1} = u^\dagger$:

$$\langle \varphi|\psi \rangle = \int \langle \varphi|x \rangle \langle x|\psi \rangle \, dx = \int \varphi(x)^* \psi(x) \, dx.$$
Inverse

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Unitarity is evident — 

\[ u^{-1} = u^\dagger: \]

\[ \langle \varphi|\psi \rangle = \int \langle \varphi|x\rangle \langle x|\psi \rangle \, dx = \int \varphi(x)^*\psi(x) \, dx. \]

In the same way we can form the momentum rep:

\[ \hat{p}|p\rangle = p|p\rangle \]

\[ \tilde{\varphi} = v|\varphi\rangle \in L_2(C, dp), \quad \tilde{\varphi}(p) = \langle p|\varphi \rangle \]

\[ v^\dagger\tilde{\varphi} = |\varphi\rangle = \int |p\rangle \tilde{\varphi}(p) \, dp \]
Then the coordinate and momentum reps are also related by a unitary transformation:

\[ \varphi = u |\varphi\rangle = uv^\dagger \hat{\varphi} \]

\[ \varphi(x) = \int \langle x|p\rangle \hat{\varphi}(p) \, dp \]

— the Fourier Transform:

\[ \langle x|p\rangle = \frac{1}{\sqrt{2\pi}} e^{ixp/\hbar} \]

All very familiar — dates back (at least) to Dirac’s book.
Before we move on, consider what happens to operators, e.g. in the coordinate rep:

\[ \hat{a} \rightarrow \hat{a}' = u \hat{a} u^\dagger \]

\[ (\hat{a}' \varphi)(x) = (u \hat{a} u^\dagger \varphi)(x) = \int \langle x | \hat{a} | y \rangle \varphi(y) \, dy. \]

— integral operator with kernel \( a_K(x, y) = \langle x | \hat{a} | y \rangle \).

Note that

\[ \hat{a} \hat{b} \rightarrow u \hat{a} \hat{b} u^\dagger = u \hat{a} u^\dagger u \hat{b} u^\dagger = \hat{a}' \hat{b}' \]

— so these unitary transformations preserve the product structure of the algebra of operators on \( \mathcal{H} \)

— they define algebra isomorphisms.
To define the phase space rep, we have a different starting point:

Consider $\mathcal{T}$: complex Hilbert space of linear operators $\hat{a}$ on $\mathcal{H}$ s.t.

$$\text{Tr}(\hat{a}^\dagger \hat{a}) < \infty$$

— Hilbert-Schmidt operators

— scalar product

$$((\hat{a}, \hat{b})) = \text{Tr}(\hat{a}^\dagger \hat{b})$$
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The importance of $\mathcal{T}$ stems from the fact that it contains the density operator (matrix)

$$\hat{\rho}(t) = \begin{cases} 
|\psi(t)\rangle\langle\psi(t)| & \text{pure state} \\
\sum_r p_r |\psi_r(t)\rangle\langle\psi_r(t)| & \text{mixed state}
\end{cases}$$

$$p_r > 0, \quad \sum_r p_r = 1$$

$$\hat{\rho}(t)^\dagger = \hat{\rho}(t), \quad \hat{\rho}(t) \geq 0, \quad \text{Tr}(\hat{\rho}(t)) = 1$$
In fact
\[(\hat{\rho}(t), \hat{\rho}(t))) \equiv \text{Tr}(\hat{\rho}(t)^2) \leq 1,\]
so \(\hat{\rho}(t)\) is in \(\mathcal{T}\).

Furthermore, we can calculate the expectation value of any observable \(\hat{a} \in \mathcal{T}\) as
\[\langle \hat{a} \rangle (t) = \text{Tr}(\hat{\rho}(t)\hat{a}) = ((\hat{\rho}(t), \hat{a})).\]

Unfortunately, \(\mathcal{T}\) does not contain \(\hat{I}, \hat{q}, \hat{p}, \ldots\)
We overcome this by ‘rigging’ $\mathcal{T}$:

Consider $S \subset \mathcal{T}$ with $\overline{S} = \mathcal{T}$. Then $\mathcal{T}^* \subset S^*$, so

$$S \subset \mathcal{T} \equiv \mathcal{T}^* \subset S^*$$

or, with an abuse of notation,

$$S \subset \mathcal{T} \subset S^*$$

Gel’fand triple

Choosing e.g.

$$S = \text{linear span}\{|m\rangle\langle n|\}$$

in terms of the number states $|m\rangle$ for $m, n = 0, 1, 2, \ldots$, it is easy to see that $S^*$ contains all polynomials in $\hat{I}, \hat{q}, \hat{p}$.

We can extend the definition of $(\cdot,\cdot)$ to $S^*$ in a natural way. Then we can calculate

$$\langle \hat{a}\rangle(t) = ((\hat{\rho}(t), \hat{a}))$$

for most observables of interest.
Question: Do we need $\mathcal{H}$, the space of state vectors, to do QM, or can we get by with $\mathcal{T}$ (or more precisely, with $S^*$)?

(Berry phase? Charge quantization? ....)
• Suppose that we can get by with $\mathcal{T}$. Then we can proceed to consider unitary transformations of $\mathcal{T}$, just as we did in the case of $\mathcal{H}$:

$$
\mathcal{T} \xrightarrow{U} \mathcal{T}' \quad \hat{a} \xrightarrow{U} \hat{a}' = U(\hat{a})
$$

$$
((\hat{a}', \hat{b}'))_{\mathcal{T}'} = ((U(\hat{a}), U(\hat{b})))_{\mathcal{T}'} = ((\hat{a}, \hat{b}))_{\mathcal{T}}.
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• The previously-defined transformations of operators, induced by transformations of vectors in $\mathcal{H}$, provide examples:

$$U(\hat{a}) = u \hat{a} u^\dagger$$

$$((\hat{a}', \hat{b}'))_{\mathcal{T}'} = \text{Tr}(u \hat{a} u^\dagger, u \hat{b} u^\dagger)_{\mathcal{T}'} = \text{Tr}(\hat{a}, \hat{b}) = ((\hat{a}, \hat{b}))_{\mathcal{T}}.$$ 

However, it is important to see that not every possible $U(\hat{a})$ is of the form $u \hat{a} u^\dagger$. 
• Then we have a complication:

How is $U(\hat{a}\hat{b})$ related to $U(\hat{a})$ and $U(\hat{b})$?

There may not even exist \textit{\`a priori} a well-defined product of $U(\hat{a})$ and $U(\hat{b})$ in $\mathcal{T}'$!
Then we have a complication:

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There may not even exist \( \text{\`a priori} \) a well-defined product of \( U(\hat{a}) \) and \( U(\hat{b}) \) in \( \mathcal{T}' \)!

To recover the situation, we have to define a product in \( \mathcal{T}' \):

\[
U(\hat{a}) \star U(\hat{b}) \overset{\text{def}}{=} U(\hat{a}\hat{b})
\]

Then since \( \hat{a}\hat{b} \neq \hat{b}\hat{a} \) in general, we have

\[
U(\hat{a}) \star U(\hat{b}) = U(\hat{a}\hat{b}) \neq U(\hat{b}\hat{a}) = U(\hat{b}) \star U(\hat{a})
\]

— non-commutative star-product in \( \mathcal{T}' \).
To set up the unitary $U$ defining the phase space rep, consider the (hermitian) kernel operator \cite{Stratonovich} 

\[ \hat{\Delta}(q,p) = 2 \hat{P} e^{2i(q\hat{p} - p\hat{q})/\hbar} = 2e^{-2iqp/\hbar} \hat{P} e^{-2ipq/\hbar} e^{2iqp/\hbar} = 2e^{2iqp/\hbar} \hat{P} e^{2iqp/\hbar} e^{-2ipq/\hbar} \]

where $\hat{P}$ is the parity operator: $\hat{P} |x\rangle = |-x\rangle$. 


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The kernel sits in $S^*$ and defines a continuous generalized basis for $\mathcal{T}$.

Orthonormal:

\[
((\hat{\Delta}(q, p), \hat{\Delta}(q', p')))) = \text{Tr}(\hat{\Delta}(q, p)\dagger\hat{\Delta}(q', p')) = 2\pi\hbar \delta(q - q')\delta(p - p').
\]

Complete:

\[
\frac{1}{2\pi\hbar} \int \hat{\Delta}(q, p)((\hat{\Delta}(q, p), \hat{a})) \, dq \, dp = \hat{a} \quad \forall \hat{a} \in \mathcal{T}.
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$$

cf. $\langle x|y \rangle = \delta(x - y)$, $\int |x\rangle \langle x|\varphi \rangle \, dx = |\varphi\rangle$ $\forall |\varphi\rangle \in \mathcal{H}$. 
We now define the phase space rep by setting

\[ A(q, p) = ((\hat{\Delta}(q, p), \hat{a})) = \text{Tr}(\hat{\Delta}(q, p)\dagger \hat{a}) \]

— symbolically, \[ A = \mathcal{W}(\hat{a}) \quad \mathcal{W} = \text{Weyl-Wigner transform.} \]
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• Then

\[ ((\hat{a}, \hat{b})) \xrightarrow{\mathcal{W}} \frac{1}{2\pi \hbar} \int A(q, p)^* B(q, p) \, dq \, dp , \]

so that \( T' = L_2(C, dq dp) = \mathcal{K} \), say.
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so that \( \mathcal{T}' = L_2(C, dqdp) = \mathcal{K}, \) say.

• The inverse mapping is

\[ \hat{a} = \mathcal{W}^{-1}(A) = \frac{1}{2\pi\hbar} \int \hat{\Delta}(q, p) A(q, p) \, dq \, dp. \]
• cf.

\[ \varphi(x) = \langle x | \varphi \rangle \]

— symbolically, \( \varphi = u | \varphi \rangle \).

• Then

\[ \langle \varphi | \psi \rangle \xrightarrow{u} \int \varphi(x)^* \psi(x) \, dx \]

so that \( \mathcal{H'} = L_2(C, dx) \).

• The inverse transformation is

\[ | \varphi \rangle = u^{-1} \varphi = \int |x\rangle \varphi(x) \, dx . \]
In the case of $\mathcal{W}$, there is a natural product in $T' = \mathcal{K}$, namely the ordinary product of functions $A(q,p)B(q,p)$

— but clearly this is not the image of $\hat{a}\hat{b}$, because it is commutative.

So in the case of the phase space rep, we will need to use

$$A \star B = \mathcal{W}(\hat{a}\hat{b}) \neq AB$$

$$(A \star B)(q,p) = ((\Delta(q,p), \hat{a}\hat{b})).$$
In particular, we have to use the star product to describe

- **Quantum Dynamics:**

\[
\begin{align*}
\frac{i\hbar}{\partial t} \hat{\rho}(t) &= [\hat{H}, \hat{\rho}] \\
\Rightarrow i\hbar \frac{\partial W(q, p, t)}{\partial t} &= H(q, p) \star W(q, p, t) - W(q, p, t) \star H(q, p)
\end{align*}
\]

where \( W = \mathcal{W}(\frac{1}{2\pi\hbar} \hat{\rho}) \) — the Wigner function. (Wigner, 1932)
In particular, we have to use the star product to describe

- Quantum Dynamics:

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i\hbar \frac{\partial \hat{\rho}(t)}{\partial t} = [\hat{H}, \hat{\rho}]
\]

\[
\mathcal{W} \quad \rightarrow \quad i\hbar \frac{\partial \mathcal{W}(q, p, t)}{\partial t} = H(q, p) \star \mathcal{W}(q, p, t) - \mathcal{W}(q, p, t) \star H(q, p)
\]

where \( \mathcal{W} = \mathcal{W}(\frac{1}{2\pi\hbar}\hat{\rho}) \) — the Wigner function. (Wigner, 1932)

- Quantum symmetries:

\[
\hat{a}' = \hat{u}_g \hat{a} \hat{u}_g^\dagger
\]

\[
\mathcal{W} \quad \rightarrow \quad U_g(q, p) \star A(q, p) \star U_g(q, p)^*
\]

\[
\hat{u}_g \hat{u}_g^\dagger = \hat{u}_g^\dagger \hat{u}_g = \hat{1}, \quad \mathcal{W} \quad \rightarrow \quad U_g \star U_g^* = U_g^* \star U_g = 1.
\]

— star-unitary representations of groups on phase space. (Fronsdal, 1978)
To get $A(q, p)$ more explicitly, make use of the coordinate rep:–

$$(\hat{a}\varphi)(x) = \int a_K(x, y)\varphi(y) \, dy, \quad a_K(x, y) = \langle x | \hat{a} | y \rangle.$$ 

$$\Delta_K(x, y) = \langle x | \hat{\Delta}(q, p) | y \rangle = 2e^{2iqp\hbar} \langle x | \hat{P} e^{2iq\hat{p}/\hbar} e^{-2ip\hat{q}/\hbar} | y \rangle$$

$$= 2e^{2iqp\hbar} e^{2ipy/\hbar} \langle -x | e^{2iq\hat{p}/\hbar} | y \rangle$$

$$= e^{2ip(q-y)/\hbar} \delta\left(\frac{x+y}{2} - q\right).$$
To get $A(q, p)$ more explicitly, make use of the coordinate rep:

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Then

$$\text{Tr}(\hat{\Delta}(q, p)\hat{a}) = \int \langle x | \hat{\Delta}(q, p) | y \rangle \langle y | \hat{a} | x \rangle\,dx\,dy = \int e^{2ip(q-y)/\hbar} \delta\left(\frac{x+y}{2} - q\right)a_K(y, x)\,dx\,dy$$

i.e.  

$$A(q, p) = \int a_K(q - y/2, q + y/2) e^{ipy/\hbar}\,dy$$
\[ a_K(x, y) = \frac{1}{2\pi\hbar} \int \langle x|\hat{\Delta}(q, p)|y\rangle A(q, p) \, dq \, dp \]

\[ = \frac{1}{2\pi\hbar} \int e^{2ip(q-y)/\hbar} \delta\left(\frac{x+y}{2} - q\right) A(q, p) \, dq \, dp \]

\[ = \frac{1}{2\pi\hbar} \int A\left(\frac{x+y}{2}, p\right) e^{ip(x-y)/\hbar} \, dp . \]

**Note:** If \( \hat{a}^\dagger = \hat{a} \), then \( A(q, p)^* = A(q, p) \)

***************
To summarize: The phase space rep is defined by the Weyl-Wigner transform:

\[ A = \mathcal{W}(\hat{a}) \quad \hat{a} = \mathcal{W}^{-1}(A) \]

\[ \mathcal{T} \xrightarrow{\mathcal{W}} \mathcal{K} \quad \mathcal{K} \xrightarrow{\mathcal{W}^{-1}} \mathcal{T} \]

In $\mathcal{T}$: \((\hat{a}, \hat{b}) = \text{Tr}(\hat{a}^\dagger \hat{b})\).

In $\mathcal{K}$: \((A, B) = \frac{1}{2\pi \hbar} \int A(q, p)^* B(q, p) \, dq \, dp \).

\[ A \star B = \mathcal{W}(\hat{a}\hat{b}) \neq \mathcal{W}(\hat{b}\hat{a}) = B \star A \]

\[ A(q, p) = \int a_K(q - y/2, q + y/2) e^{ipy/\hbar} \, dy \]

\[ a_K(x, y) = \frac{1}{2\pi \hbar} \int A\left(\frac{x+y}{2}, p\right) e^{ip(x-y)/\hbar} \, dp \]