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

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- QM has many representations

  — coordinate rep, momentum rep, Bargmann rep, Zak's kq – rep, . . .

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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 *et al.*, Shirokov, . . .

Our treatment will necessarily be very selective . . .

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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 $\int |x\rangle\langle x|\, dx = \hat{I}$

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- Define a unitary mapping

$$\mathcal{H} \xrightarrow{u} \mathcal{H}' = L_2(C, dx)\,, \qquad |\varphi\rangle \xrightarrow{u} \varphi = u|\varphi\rangle$$

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 — $u^{-1} = u^{\dagger}$:

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

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- In the same way we can form the momentum rep:–

$$\hat{p}|p\rangle = p|p\rangle$$

$$\tilde{\varphi} = v|\varphi\rangle \in L_2(C, dp)\,, \qquad \tilde{\varphi}(p) = \langle p|\varphi\rangle$$

$$v^{\dagger}\tilde{\varphi} = |\varphi\rangle = \int |p\rangle\tilde{\varphi}(p)\, dp$$

- Then the coordinate and momentum reps are also related by a unitary transformation:

$$\varphi = u|\varphi\rangle = uv^\dagger\tilde{\varphi}$$

$$\varphi(x) = \int \langle x|p\rangle\tilde{\varphi}(p)\,dp$$

— 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:

$$\hat{a} \longrightarrow \hat{a}' = u\,\hat{a}\,u^\dagger$$

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

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

Note that

$$\hat{a}\,\hat{b} \longrightarrow u\,\hat{a}\,\hat{b}\,u^\dagger = u\,\hat{a}\,u^\dagger\,u\,\hat{b}\,u^\dagger = \hat{a}'\,\hat{b}'$$

— 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.*

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

— Hilbert-Schmidt operators

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- The importance of $\mathcal{T}$ stems from the fact that it contains the *density operator* (matrix)

$$\hat{\rho}(t) = \begin{cases} |\psi(t)\rangle\langle\psi(t)| \quad \text{pure state} \\ \\ \sum_r p_r|\psi_r(t)\rangle\langle\psi_r(t)| \quad \text{mixed state} \\ p_r > 0\,, \quad \sum_r p_r = 1 \end{cases}$$

$$\hat{\rho}(t)^\dagger = \hat{\rho}(t)\,, \qquad \hat{\rho}(t) \geq 0\,, \qquad \mathrm{Tr}(\hat{\rho}(t)) = 1$$

In fact

$$((\hat{\rho}(t), \hat{\rho}(t))) \equiv \mathrm{Tr}(\hat{\rho}(t)^2) \leq 1\,,$$

so $\hat{\rho}(t)$ is in $\mathcal{T}$.

Furthermore, we can calculate the *expectation value of any observable* $\hat{a} \in \mathcal{T}$ as

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

Unfortunately, $\mathcal{T}$ does not contain $\hat{I}\,,\ \ \hat{q}\,,\ \ \hat{p}\,,\ldots$

- We overcome this by 'rigging' $\mathcal{T}$:

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

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

or, with an abuse of notation,

$$\mathcal{S} \subset \mathcal{T} \subset \mathcal{S}^* \quad \text{Gel'fand triple}$$

Choosing *e.g.*

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

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

We can extend the definition of $((.,.))$ to $\mathcal{S}^*$ 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 $\mathcal{S}^*$)?

(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 $\mathcal{H}$:

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

$$((\hat{a}', \hat{b}'))_{\mathcal{T}'} = ((U(\hat{a}), U(\hat{b})))_{\mathcal{T}'} = ((\hat{a}, \hat{b}))_{\mathcal{T}} \,.$$

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• The previously-defined transformations of operators, induced by transformations of vectors in $\mathcal{H}$, provide examples:

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

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

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 *á priori* a well-defined product of $U(\hat{a})$ and $U(\hat{b})$ in $\mathcal{T}'$!

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- To recover the situation, we have to *define a product* in $\mathcal{T}'$:

$$U(\hat{a}) \star U(\hat{b}) \stackrel{\text{def}}{=} U(\hat{a}\hat{b})$$

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* (Stratonovich, 1957)

$$\hat{\Delta}(q,p) = 2\hat{P}\, e^{2i(q\hat{p}-p\hat{q})/\hbar} = 2e^{-2iqp/\hbar}\,\hat{P}\, e^{-2ip\hat{q}/\hbar}\, e^{2iq\hat{p}/\hbar} = 2e^{2iqp/\hbar}\,\hat{P}\, e^{2iq\hat{p}/\hbar}\, e^{-2ip\hat{q}/\hbar}$$

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

Orthonormal:

$$((\hat{\Delta}(q,p), \hat{\Delta}(q',p'))) = \mathrm{Tr}(\hat{\Delta}(q,p)^\dagger \hat{\Delta}(q',p')) = 2\pi\hbar\delta(q-q')\delta(p-p')\,.$$

Complete:

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

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- *cf.* $\langle x|y\rangle = \delta(x-y)\,, \qquad \int |x\rangle\langle x|\varphi\rangle\, dx = |\varphi\rangle \qquad \forall|\varphi\rangle \in \mathcal{H}\,.$

- We now define the phase space rep by setting

$$A(q,p) = ((\hat{\Delta}(q,p), \hat{a})) = \mathrm{Tr}(\hat{\Delta}(q,p)^\dagger \hat{a})$$

— symbolically, $A = \mathcal{W}(\hat{a})$ $\mathcal{W}$ = Weyl-Wigner transform.

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- Then

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

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- 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 $\mathcal{T}' = \mathcal{K}$, 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

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

$$(A \star B)(q,p) = ((\hat{\Delta}(q,p), \hat{a}\hat{b}))\,.$$

In particular, we have to use the star product to describe

- Quantum Dynamics:

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

$$\xrightarrow{\mathcal{W}} \qquad i\hbar \frac{\partial W(q,p,t)}{\partial t} = H(q,p) \star W(q,p,t) - W(q,p,t) \star H(q,p)$$

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

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- Quantum symmetries:

$$\hat{a}' = \hat{u}_g \, \hat{a} \, \hat{u}_g^\dagger$$

$$\xrightarrow{\mathcal{W}} \qquad U_g(q,p) \star A(q,p) \star U_g(q,p)^*$$

$$\hat{u}_g \, \hat{u}_g^\dagger = \hat{u}_g^\dagger \, \hat{u}_g = \hat{I}\,, \qquad \xrightarrow{\mathcal{W}} \qquad U_g \star U_g^* = U_g^* \star U_g = 1\,.$$

— star-unitary representations of groups on phase space. (Fronsdal, 1978)

- To get $A(q,p)$ more explicitly, make use of the coordinate rep:–

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

$$\begin{aligned}
\Delta_K(x,y) = \langle x|\hat{\Delta}(q,p)|y\rangle &= 2e^{2iqp\hbar}\,\langle x|\hat{P}\,e^{2iq\hat{p}/\hbar}\,e^{-2ip\hat{q}/\hbar}|y\rangle \\
&= 2e^{2iqp\hbar}\,e^{2ipy/\hbar}\,\langle -x|e^{2iq\hat{p}/\hbar}|y\rangle \\
&= e^{2ip(q-y)/\hbar}\,\delta\big(\tfrac{x+y}{2} - q\big)\,.
\end{aligned}$$

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\end{aligned}$$

- Then

$$\begin{aligned}
\mathrm{Tr}(\hat{\Delta}(q,p)\hat{a}) &= \int \langle x|\hat{\Delta}(q,p)|y\rangle\langle y|\hat{a}|x\rangle\,dx\,dy \\
&= \int e^{2ip(q-y)/\hbar}\,\delta(\tfrac{x+y}{2}-q)a_K(y,x)\,dx\,dy \\
i.e. \qquad A(q,p) &= \int a_K(q-y/2,q+y/2)\,e^{ipy/\hbar}\,dy
\end{aligned}$$

- $$
\begin{aligned}
a_K(x,y) &= \frac{1}{2\pi\hbar}\int \langle x|\hat{\Delta}(q,p)|y\rangle A(q,p)\,dq\,dp \\
&= \frac{1}{2\pi\hbar}\int e^{2ip(q-y)/\hbar}\,\delta(\tfrac{x+y}{2}-q)A(q,p)\,dq\,dp \\
&= \frac{1}{2\pi\hbar}\int A(\tfrac{x+y}{2},p)\,e^{ip(x-y)/\hbar}\,dp\,.
\end{aligned}
$$

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

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

$$A = \mathcal{W}(\hat{a}) \qquad \hat{a} = \mathcal{W}^{-1}(A)$$

$$\mathcal{T} \xrightarrow{\mathcal{W}} \mathcal{K} \qquad \mathcal{K} \xrightarrow{\mathcal{W}^{-1}} \mathcal{T}$$

In $\mathcal{T}$: $((\hat{a}, \hat{b})) = \mathrm{Tr}(\hat{a}^\dagger \hat{b})$. In $\mathcal{K}$: $(A, B) = \frac{1}{2\pi\hbar} \int A(q,p)^* B(q,p)\, dq\, dp\,.$

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

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

$$\boxed{a_K(x,y) = \frac{1}{2\pi\hbar} \int A(\tfrac{x+y}{2}, p)\, e^{ip(x-y)/\hbar}\, dp}$$