

# Phase Space Formulation of Quantum Mechanics

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SMFT07, Melbourne, January-February 2007

## Lecture 1 A gentle 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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  - not equivalent to the above
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    - 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 *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

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

by setting

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

- Inverse

$$\begin{aligned} |\varphi\rangle &= u^{-1}\varphi = \int |x\rangle\langle x|\varphi\rangle dx \\ &= \int \varphi(x)|x\rangle dx. \end{aligned}$$

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:–

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

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

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

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

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

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

— 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.

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

— Hilbert-Schmidt operators

— scalar product

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

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

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

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  $\hat{I}$ ,  $\hat{q}$ ,  $\hat{p}$ , ...

- 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  $m, n = 0, 1, 2, \dots$ , it is easy to see that  $\mathcal{S}^*$  contains all polynomials in  $\hat{I}, \hat{q}, \hat{p}$ .

We can extend the definition of  $((\cdot, \cdot))$  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  $\mathcal{H}$ :

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

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

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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 *a 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)

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

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

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

Orthonormal:

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

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

- 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,  $A = \mathcal{W}(\hat{a})$      $\mathcal{W} =$  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

$$|\varphi\rangle = u^{-1}\varphi = \int |x\rangle\varphi(x) dx.$$

*Aside:*

The approach is similar if we wish to set up a phase space formulation of a spin system.

Find a suitable *kernel matrix*  $\Delta(\mathbf{n})$  in the Hilbert-Schmidt space  $\mathcal{T}$  of  $(2s+1) \times (2s+1)$  spin matrices, depending on a unit vector  $\mathbf{n}$ , and map matrices to functions on the unit sphere using

$$\hat{S} \longrightarrow S(\mathbf{n}) = ((\Delta(\mathbf{n}), \hat{S}))_{\mathcal{T}}.$$

Then, for example, we will get

$$(S_i \star S_j)(\mathbf{n}) - (S_j \star S_i)(\mathbf{n}) = i\hbar \epsilon_{ijk} S_k(\mathbf{n}).$$

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

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

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

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

- Quantum Dynamics:

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

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

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

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- Quantum symmetries:

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

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

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

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

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

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

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

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- Then

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

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

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

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:

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

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

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

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

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

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

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

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