Phase space distributions in quantum many-body systems

Discuss phase space description of QM due to Wigner [E.P. ~ 1902-1995]
$\leadsto$ reveals more directly the similarities between dynamics class $\leftrightarrow$ QM.

Description of a single particle in Wigner-Weyl formalism

[H. Weyl 1885-1955]

1 dof, no int. structure (e.g. spin), with

$$\mathbb{1} = \underbrace{\int d^d x \, |\vec{x}\rangle\langle\vec{x}|}_{\int_{\vec{x}}} = \underbrace{\int \frac{d^d p}{(2\pi\hbar)^d} \, |\vec{p}\rangle\langle\vec{p}|}_{\int_{\vec{p}}}$$

with $|\vec{p}\rangle = \int_x e^{i\vec{p}\vec{x}/\hbar} |\vec{x}\rangle$

$$\langle\vec{x}|\vec{x}'\rangle = \delta^{(d)}(\vec{x}-\vec{x}') \qquad \langle\vec{p}|\vec{p}'\rangle = (2\pi\hbar)^d \, \delta^{(d)}(\vec{p}-\vec{p}')$$

The problem in defining a phase-space distribution is

$$[x^i, p^j] = i\hbar \, \delta^{ij}$$

$\rightarrow$ cannot measure precise position & momentum at the same time.

To retain as much info as possible, define for any hermitean operator $\hat{O}$ the Wigner-Weyl-transform O_W as

$$O_W(\vec{x},\vec{p}) := \int_{\vec{s}} e^{i\vec{p}\vec{s}/\hbar} \langle \vec{x} - \tfrac{\vec{s}}{2} | \hat{O} | \vec{x} + \tfrac{\vec{s}}{2} \rangle$$

[or equivalently

$$O_W(\vec{x},\vec{p}) := \int_{\vec{q}} e^{-i\vec{q}\vec{x}/\hbar} \langle \vec{p} - \tfrac{\vec{q}}{2} | \hat{O} | \vec{p} + \tfrac{\vec{q}}{2} \rangle$$
]

In the case $\hat{O} = \hat{\rho}(t)$, we call ρ_W the Wigner function or Wigner distribution.

Idea: Hope that after 'marginalizing' = integrating over pos./mom., we obtain the corresponding mom./pos. distribution.

Indeed:

$$\int_{\vec{p}} \rho_W(t,\vec{x},\vec{p}) = \underbrace{\underbrace{\int_{\vec{p}}}\int_{\vec{s}} e^{i\vec{p}\vec{s}/\hbar}}_{\delta^{(d)}(\vec{s})} \langle \vec{x} - \tfrac{\vec{s}}{2} | \hat{\rho}(t) | \vec{x} + \tfrac{\vec{s}}{2} \rangle$$

$$= \langle \vec{x} | \hat{\rho}(t) | \vec{x} \rangle$$

$$\left(\boxed{\int_{\vec{x}} \rho_W(t,\vec{x},\vec{p})} = \int_{\vec{x}} \int_{\vec{s}} e^{i\vec{p}\vec{s}/\hbar} \langle \vec{x} - \tfrac{\vec{s}}{2} | \hat{\rho}(t) | \vec{x} + \tfrac{\vec{s}}{2} \rangle \right.$$

$$\vec{x}_\pm = \vec{x} \pm \tfrac{\vec{s}}{2}$$

$$\frac{\partial(\vec{x}_+, \vec{x}_-)}{\partial(\vec{x}, \vec{s})} = \begin{vmatrix} 1 & \frac{1}{2} \\ 1 & -\frac{1}{2} \end{vmatrix} = 1$$

$$e^{i\vec{p}\vec{s}/\hbar} = e^{i\vec{p}\frac{\vec{s}}{2}/\hbar} e^{i\vec{p}\frac{\vec{s}}{2}/\hbar} = e^{-i\vec{p}(\vec{x}-\frac{\vec{s}}{2})/\hbar} e^{i\vec{p}(\vec{x}+\frac{\vec{s}}{2})/\hbar}$$

$$= \left(\int_{\vec{x}_-} e^{-i\vec{p}\vec{x}_-/\hbar} \langle x_- | \right) \rho(t) \left(\int_{\vec{x}_+} e^{i\vec{p}\vec{x}_+/\hbar} | \vec{x}_+ \rangle \right)$$

$$\left. = \boxed{\langle \vec{p} | \rho(t) | \vec{p} \rangle} \right)$$

The Wigner-Weyl transform can be inverted:

$$\int_{\vec{p}} e^{-i\vec{p}\vec{s}/\hbar} O_W(\vec{x},\vec{p}) = \underbrace{\underbrace{\int_{\vec{p}}}\int_{\vec{s}'} e^{-i\vec{p}\vec{s}/\hbar} e^{i\vec{p}\vec{s}'/\hbar}}_{\delta^{(d)}(\vec{s}-\vec{s}')} \langle \vec{x} - \tfrac{\vec{s}'}{2} | \hat{O} | \vec{x} + \tfrac{\vec{s}'}{2} \rangle$$

$$= \langle \vec{x} - \tfrac{\vec{s}}{2} | \hat{O} | \vec{x} + \tfrac{\vec{s}}{2} \rangle$$

[or equivalently

$$\int_{\vec{x}} e^{i\vec{q}\vec{x}/\hbar} O_W(\vec{x},\vec{p}) = \langle \vec{p} - \vec{q}/2 | \hat{O} | \vec{p} + \vec{q}/2 \rangle$$

],

Hence: it contains all possible operator matrix elements
→ it contains all info about the action of the Schrödinger operator on the Hilbert space ⇒ fully equiv. to op. formulation!

Expectation values

We can use this formalism to compute expectation values of hermitean operator $\hat{O}$. Schrödinger picture:

$$\langle \hat{O}(t) \rangle = \mathrm{tr}\left(\hat{O} \hat{\rho}(t) \right)$$

Evaluate in position space

$$\langle \hat{O}(t)\rangle = \int_{\vec{y}\,\vec{z}} \langle \vec{y} | \hat{O} | \vec{z} \rangle \langle \vec{z} | \hat{\rho}(t) | \vec{y} \rangle$$

(Jacobi = 1)

$$= \int_{\vec{x},\vec{s}} \underbrace{\left\langle \vec{x} - \tfrac{\vec{s}}{2} \right| \hat{O} \left| \vec{x} + \tfrac{\vec{s}}{2} \right\rangle}_{\int_{\vec{p}} e^{-i\vec{p}\vec{s}/\hbar} O_W(\vec{x},\vec{p})} \underbrace{\left\langle \vec{x} + \tfrac{\vec{s}}{2} \right| \hat{\rho}(t) \left| \vec{x} - \tfrac{\vec{s}}{2} \right\rangle}_{\int_{\vec{p}'} e^{+i\vec{p}'\vec{s}/\hbar} \rho_W(t,\vec{x},\vec{p}')}$$

$\int_{\vec{s}} \to \delta$

$$= \int_{\vec{x}\,\vec{p}} O_W(\vec{x},\vec{p})\, \rho_W(t,\vec{x},\vec{p})$$

analogous to the expression in the <u>classical ensemble</u>!

WOW! How can a "classical" object like ρ_W describe a quantum system? Well, ρ_W can be negative...

$\to$ interpretation as a probability density is <u>not</u> possible!

Evolution of the Wigner function

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

[von-Neumann equation
J. v. N. 1903–1957]

$$\Leftrightarrow \quad i\hbar\, \partial_t \rho_W(t,\vec{x},\vec{p}) = \int_{\vec{s}} \left\langle \vec{x} - \tfrac{\vec{s}}{2} \right| [\hat{H}, \hat{\rho}(t)] \left| \vec{x} + \tfrac{\vec{s}}{2} \right\rangle$$

insert $\mathbb{1} = 2^{-d} \int_{\vec{s}'} |\vec{x} + \tfrac{\vec{s}'}{2}\rangle\langle x + \tfrac{\vec{s}'}{2}|$

$$= 2^{-d} \int_{\vec{s}\,\vec{s}'} e^{i\vec{p}\vec{s}/\hbar} \left[\left\langle \vec{x} - \tfrac{\vec{s}}{2} \right| \hat{H} \left| \vec{x} + \tfrac{\vec{s}}{2} \right\rangle \left\langle \vec{x} + \tfrac{\vec{s}'}{2} \right| \hat{\rho}(t) \left| \vec{x} + \tfrac{\vec{s}}{2} \right\rangle - (\hat{H} \leftrightarrow \hat{\rho}) \right]$$

* change variables: $\vec{x}' = \frac{\vec{s}' - \vec{s}}{4}$ $\quad \vec{x}'' = \frac{\vec{s}' + \vec{s}}{4}$ $\quad \left| \begin{array}{l} \vec{s} = 2(\vec{x}'' - \vec{x}') \\ \vec{s}' = 2(\vec{x}' + \vec{x}'') \end{array} \right.$

$$\text{Jac. det} = \begin{vmatrix} \left(\frac{1}{4}\right) & \left(-\frac{1}{4}\right) \\ \left(\frac{1}{4}\right) & \left(\frac{1}{4}\right) \end{vmatrix}^d = \frac{1}{8^d}$$

* express

$$\left\langle \vec{x} - \frac{\vec{s}}{2} \right| \hat{H} \left| \vec{x} + \frac{\vec{s}'}{2} \right\rangle = \left\langle \vec{x} + \vec{x}' - \vec{x}'' \right| \hat{H} \left| \vec{x} + \vec{x}' + \vec{x}'' \right\rangle$$

$$= \left\langle (\vec{x} + \vec{x}') - \frac{2\vec{x}''}{2} \right| \hat{H} \left| (\vec{x} + \vec{x}') + \frac{2\vec{x}''}{2} \right\rangle$$

$$= \int_{\vec{p}'} e^{-i\vec{p}' 2\vec{x}''/\hbar} H_W(\vec{x} + \vec{x}', \vec{p}')$$

$$\overset{\text{shift}}{=} \int_{\vec{p}'} e^{-2i(\vec{p} + \vec{p}')/\hbar} H_W(\vec{x} + \vec{x}', \vec{p} + \vec{p}')$$

& analogously

$$\left\langle \vec{x} + \frac{\vec{s}'}{2} \right| \hat{\rho}(t) \left| \vec{x} - \frac{\vec{s}}{2} \right\rangle = \int_{\vec{p}''} e^{2i(\vec{p} + \vec{p}'')/\hbar} \rho_W(t, \vec{x} + \vec{x}'', \vec{p} + \vec{p}'')$$

then we obtain:

$$i\hbar \partial_t \rho_W(t, \vec{x}, \vec{p}) = 4^d \int_{\vec{x}', \vec{x}'', \vec{p}', \vec{p}''} e^{2i\vec{p}(\vec{x}'' - \vec{x}')/\hbar} e^{-2i(\vec{p} + \vec{p}')\vec{x}''/\hbar} e^{2i(\vec{p} + \vec{p}'')\vec{x}'/\hbar} \Big[H_W(\vec{x} + \vec{x}', \vec{p} + \vec{p}') \rho_W(\vec{x} + \vec{x}'', \vec{p} + \vec{p}'')$$
$$- \rho_W(\vec{x} + \vec{x}', \vec{p} + \vec{p}') H_W(\vec{x} + \vec{x}'', \vec{p} + \vec{p}'') \Big]$$

$$= 4^d \int_{\vec{x}', \vec{x}'', \vec{p}', \vec{p}''} e^{2i(\vec{p}''\vec{x}' - \vec{p}'\vec{x}'')/\hbar} \left[H_W \rho_W - \rho_W H_W \right]$$

(+) here, change $(\vec{x}', \vec{p}') \leftrightarrow (\vec{x}'', \vec{p}'')$

$$\left(= 4^d \int_{\vec{x}', \vec{x}'', \vec{p}', \vec{p}''} H_W(\vec{x} + \vec{x}', \vec{p} + \vec{p}') \rho_W(\vec{x} + \vec{x}'', \vec{p} + \vec{p}'') \underbrace{\left[e^{2i(\vec{p}''\vec{x}' - \vec{p}'\vec{x}'')/\hbar} - e^{-2i(\vec{p}''\vec{x}' - \vec{p}'\vec{x}'')/\hbar} \right]}_{2i \sin\left(\frac{2(\vec{p}''\vec{x}' - \vec{p}'\vec{x}'')}{\hbar}\right)} \right)$$

We can write the Taylor series in a fancy way:

$$H_W(\vec{x}+\vec{x}', \vec{p}+\vec{p}') = e^{\left(\vec{x}'\cdot\frac{\partial}{\partial\vec{x}}\right)} e^{\left(\vec{p}'\cdot\frac{\partial}{\partial\vec{p}}\right)} H_W(\vec{x},\vec{p})$$

[will look more classical later]

to rewrite (†) as:

$$4^d \int_{\vec{x}',\vec{x}'',\vec{p}',\vec{p}''} H_W(\vec{x},\vec{p})\, e^{\vec{x}'\cdot\overleftarrow{\partial}_{\vec{x}}}\, e^{\vec{p}'\cdot\overleftarrow{\partial}_{\vec{p}}}\, e^{\vec{x}''\cdot\overrightarrow{\partial}_{x}}\, e^{\vec{p}''\cdot\overrightarrow{\partial}_{\vec{p}}}\, e^{2i(\vec{p}''\cdot\vec{x}'-\vec{p}'\cdot\vec{x}'')/\hbar}\, \rho_W(\vec{x},\vec{p})$$

$$= 4^d \int_{\vec{x}',\vec{x}'',\vec{p}',\vec{p}''} H_W(\vec{x},\vec{p})\, e^{\frac{2i}{\hbar}\vec{x}'\cdot\left(\vec{p}''-\frac{i\hbar}{2}\overleftarrow{\partial}_{\vec{x}}\right)}\, e^{-\frac{2i}{\hbar}\vec{x}''\cdot\left(\vec{p}'+\frac{i\hbar}{2}\overrightarrow{\partial}_{\vec{x}}\right)}\, e^{\vec{p}'\cdot\overleftarrow{\partial}_{\vec{p}}}\, e^{\vec{p}''\cdot\overrightarrow{\partial}_{\vec{p}}}\, \rho_W(\vec{x},\vec{p})$$

$$\int_{\vec{x}'} \to (2\pi)^d\, \delta^{(d)}\left[\frac{2}{\hbar}\left(\vec{p}''-\frac{i\hbar}{2}\overleftarrow{\partial}_{\vec{x}}\right)\right] = \frac{1}{2^d}(2\pi\hbar)^d\, \delta\left[\vec{p}''-\frac{i\hbar}{2}\overleftarrow{\partial}_{\vec{x}}\right]$$

$$\int_{\vec{x}''} \to (2\pi)^d\, \delta^{(d)}\left[-\frac{2}{\hbar}\left(\vec{p}'+\frac{i\hbar}{2}\overrightarrow{\partial}_{\vec{x}}\right)\right] = \frac{1}{2^d}(2\pi\hbar)^d\, \delta\left[\vec{p}'+\frac{i\hbar}{2}\overrightarrow{\partial}_{\vec{x}}\right]$$

($i\partial_{\vec{x}}$ has real eigenvalues)

$$= H_W(\vec{x},\vec{p})\, e^{-\frac{i\hbar}{2}\overrightarrow{\partial}_{\vec{x}}\cdot\overleftarrow{\partial}_{\vec{p}}}\, e^{\frac{i\hbar}{2}\overleftarrow{\partial}_{\vec{x}}\cdot\overrightarrow{\partial}_{\vec{p}}}\, \rho(\vec{x},\vec{p})$$

$$= H_W(\vec{x},\vec{p}) \exp\left\{\frac{i\hbar}{2}\left[\overleftarrow{\partial}_{\vec{x}}\cdot\overrightarrow{\partial}_{\vec{p}} - \overrightarrow{\partial}_{\vec{x}}\cdot\overleftarrow{\partial}_{\vec{p}}\right]\right\} \rho(\vec{x},\vec{p})$$

Do the same for the second term on p.4, to obtain

$$\partial_t \rho_W(t,\vec{x},\vec{p}) = H_W(\vec{x},\vec{p})\, \frac{2}{\hbar} \sin\left\{\frac{\hbar}{2}\left[\overleftarrow{\partial}_{\vec{x}}\cdot\overrightarrow{\partial}_{\vec{p}} - \overrightarrow{\partial}_{\vec{x}}\cdot\overleftarrow{\partial}_{\vec{p}}\right]\right\} \rho_W(t,\vec{x},\vec{p})$$

More generally, and in analogy to classical mechanics, define the *Moyal bracket* as:

$$\{\{f,g\}\} := f(\vec{x},\vec{p})\, \frac{2}{\hbar} \sin\left\{\frac{\hbar}{2}\left[\overleftarrow{\partial}_{\vec{x}}\cdot\overrightarrow{\partial}_{\vec{p}} - \overrightarrow{\partial}_{\vec{x}}\cdot\overleftarrow{\partial}_{\vec{p}}\right]\right\} g(\vec{x},\vec{p})$$

Then in analogy to classical eom for phase space density, the eom for the Wigner function reads:

$$\partial_t \rho_W(t, \vec{x}, \vec{p}) = \{\{H_W, \rho_W\}\}$$

classical: Poisson bracket ⟶ QM: Moyal bracket

Note: $\{\{f, g\}\} = \underbrace{\{f, g\}}_{\text{classical}} + \underbrace{O(\hbar^2)}_{\text{quantum corrections}}$

Remark: There are some settings in which all higher order (in $\hbar$) terms than the Poisson bracket vanish ⟶ The QM phase space dynamics are then described exactly by the classical eom. (e.g. HO)