I. Introduction

I.1 Why phase space?

There are very many good reasons to look at quantum mechanics in phase space:

(i) a third way of quantization
(ii) understanding quantum phenomena in terms of classical concepts
(iii) approximation methods to solve quantum many-body problems close to the classical limit

$\boxed{\text{classical mechanics}}$

Poisson algebra

$\{A, B\}$

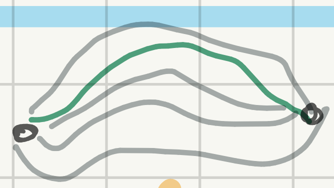
Heisenberg algebra

$-\frac{i}{\hbar}[\hat{A}, \hat{B}]$

minimum action

$\delta S = \delta \int_{t_1}^{t_2} dt\, L(q, \dot{q})$

path integrals



Liouville equation

$\frac{\partial}{\partial t} f(p, q) = -\{f, H\}$

Wigner-Weyl correspondence

$\frac{\partial}{\partial t} W = -\{\{W, H\}\}$

$\boxed{\text{quantum mechanics}}$

quantum mechanics $\overset{?}{\longleftrightarrow}$ classical mechanics with uncertainties

Ehrenfest equations

$$(1)\qquad \frac{d}{dt}\langle\hat{x}\rangle = \frac{1}{m}\langle\hat{p}\rangle$$

$$\frac{d}{dt}\langle\hat{p}\rangle = -\langle\vec{\nabla}V(\hat{x})\rangle = \langle F(\hat{x})\rangle$$

- classical limit

Newton eqs. for $\langle\hat{x}\rangle, \langle\hat{p}\rangle$

$$\langle F(\hat{x})\rangle \simeq F(\langle\hat{x}\rangle) + F'(\langle\hat{x}\rangle)\underbrace{\langle(\hat{x}-\langle\hat{x}\rangle)\rangle}_{=0}$$

$$+\frac{1}{2}F''(\langle\hat{x}\rangle)\,\Delta x^2 + \dots$$

Heisenberg uncertainty

$$(2)\qquad [\hat{x},\hat{p}] = i\hbar \qquad \Delta x^2 \Delta p^2 \geq \frac{\hbar^2}{4}$$

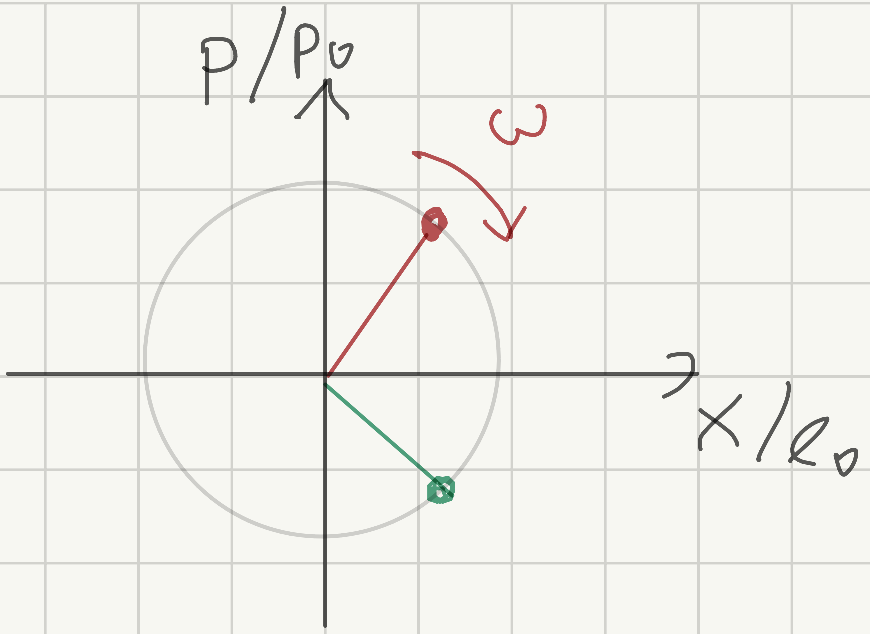
example: harmonic oscillator

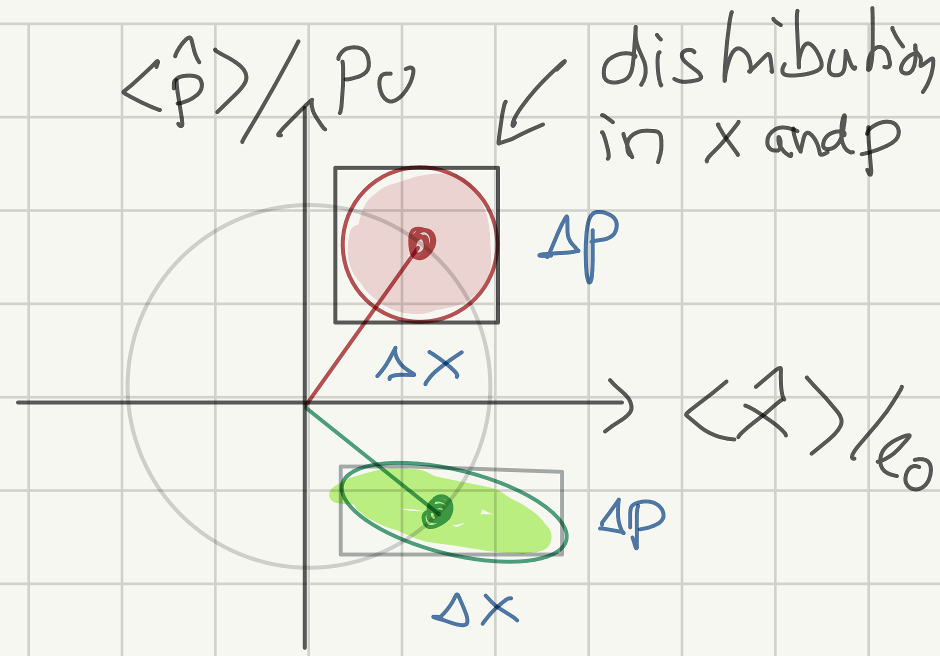
$$H = \frac{1}{2m}\hat{p}^2 + \frac{m}{2}\omega^2\hat{x}^2 \qquad F(\hat{x}) = -m\omega\hat{x}$$

$$F''(\langle\hat{x}\rangle) = F'''(\langle\hat{x}\rangle) = \dots = 0$$

$\Rightarrow$ equations of motion classical!

but to fulfill (2) $\Rightarrow$ uncertainty similar to Liouville dynamics





I.2 The Wigner-Weyl distribution of a single quantum particle

As one example for a (quasi) probability distribution we will now discuss the Wigner distribution of a single quantum particle.

<u>classical phase-space distribution</u> (Liouville)

(3) $$P_{cl}(q,p) \qquad q,p \in \mathbb{R}$$

expected values

(4) $$\langle A \rangle_{cl} = \int dq \int dp \, P_{cl}(q,p)\, A(q,p)$$

Liouville equation

(5) $$\frac{d}{dt} P_{cl}(q,p) = -\{P_{cl}, H\}$$

where $\{\cdot,\cdot\}$ is the Poisson bracket

(6) $$\{A,B\} = \frac{\partial A}{\partial q}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial q}$$

quantum phase-space distribution

(7) $$P(q,p) \qquad q,p \in \mathbb{R}$$

$f(q,p)$ should have the following property

(8) $$\langle A(\hat{q},\hat{p})\rangle = \mathrm{Tr}\{A(\hat{q},\hat{p})\,\rho\} \overset{!}{=} \int dq \int dp\, \mathcal{A}(q,p)\, P(q,p)$$

question:

$$\boxed{\begin{aligned} \mathcal{A}(q,p) &= ? \\ P(q,p) &= ? \end{aligned}}$$

Weyl transform

quasi-probability

to construct $P(q,p)$ lets consider the <u>marginals</u>

(9)
$$P_{pos}(q) \equiv \int dp\, P(q,p) = \mathrm{Tr}\{\rho\, \delta(\hat{q}-q)\}$$
$$P_{mom}(p) \equiv \int dq\, P(q,p) = \mathrm{Tr}\{\rho\, \delta(\hat{p}-p)\}$$

The position and momentum distributions can easily be constructed

$$\delta(q-\hat{q}) = |q\rangle\langle q| \qquad \delta(p-\hat{p}) = |p\rangle\langle p|$$

(10) $$P_{pos}(q) = \langle q|\hat{\varrho}|q\rangle = \varrho(q,q)$$

$$P_{mom}(p) = \langle p|\hat{\varrho}|p\rangle =$$

(11) $$= \int dq \int dq' \langle p|q\rangle\langle q|\hat{\varrho}|q'\rangle\langle q'|p\rangle$$

$$= \frac{1}{2\pi\hbar}\int dq \int dq' \, \varrho(q,q') \, e^{\frac{ip(q-q')}{\hbar}}$$

alternatively one can use $\langle p|\hat{\varrho}|p'\rangle$.

(12) $$P_{mom}(p) = \langle p|\hat{\varrho}|p\rangle = \varrho(p,p)$$

(13) $$P_{pos}(q) = \langle q|\hat{\varrho}|q\rangle$$

$$= \int dp \int dp' \langle q|p\rangle\langle p|\hat{\varrho}|p'\rangle\langle p'|q\rangle$$

$$= \frac{1}{2\pi\hbar}\int dp \int dp' \, \varrho(p,p') \, e^{+\frac{iq(p-p')}{\hbar}}$$

From this one could define the full distribution as

(14) $$P_1(q,p) = \mathrm{Tr}\{\varrho \, \delta(q-\hat{q}) \, \delta(p-\hat{p})\}$$

$$\cancel{\#} \quad [\hat{q},\hat{p}] = i\hbar \neq 0$$

or

(15) $$P_2(q,p) = \mathrm{Tr}\{\varrho \, \delta(p-\hat{p}) \, \delta(q-\hat{q})\}$$

We see: The definition of a quantum mechanical phase space distribution is not unique due to the ambiguity in operator ordering

Depending on the chosen order, the correspondence

$$\hat{A}(\hat{q},\hat{p}) \Leftrightarrow \mathcal{A}(q,p) \tag{16}$$

will be different!

- Neither $P_1(q,p)$ nor $P_2(q,p)$ are suitable as they are in general not real

Wigner-function

$$\boxed{\begin{aligned} W(q,p) &= \frac{1}{2\pi\hbar}\int dy\ \varrho\left(q-\frac{y}{2}, q+\frac{y}{2}\right) e^{ipy/\hbar} \\ &= \frac{1}{2\pi\hbar}\int dy\ \left\langle q-\frac{y}{2}\right|\hat{\varrho}\left|q+\frac{y}{2}\right\rangle e^{ipy/\hbar} \end{aligned}} \tag{17}$$

note that

$$W(q,p)^* = W(q,p) \qquad \text{real!}$$

corresponding Weyl transform

(18) $$\boxed{\mathcal{A}(q,p) = \int dz\, e^{ipz/\hbar} \langle q - \tfrac{1}{2}z | \hat{A} | q + \tfrac{1}{2}z \rangle}$$

such that for expectation values we find

(19) $$\boxed{\langle \hat{A}(\hat{q},\hat{p}) \rangle = \mathrm{Tr}\{\hat{\varrho}\hat{A}\} = \int dq \int dp\, W(q,p)\, \mathcal{A}(q,p)}$$

An interesting property of W becomes visible if we consider

(20) $$\begin{aligned} |\langle \psi | \theta \rangle|^2 &= \mathrm{Tr}\{ |\psi\rangle\langle\psi|\theta\rangle\langle\theta| \} \\ &= 2\pi\hbar \int dq \int dp\, W_\psi(q,p)\, W_\theta(q,p) \end{aligned}$$

(20) shows that $W(q,p)$ cannot be positive for all states as for orthogonal states $\langle \psi | \phi \rangle = 0$

▶ Can we give a simpler recipe for obtaining the Weyl transform and thus expectation values?

$\Rightarrow$ yes

Wigner operator ordering

consider ($\hbar = 1$)

$$\hat{A}(\hat{q},\hat{p}) = \int d\sigma \int d\tau \, \alpha(\sigma,\tau)\, e^{i(\sigma\hat{q}+\tau\hat{p})} \tag{21}$$

then

$$A(q,p) = \int dz \int d\sigma \int dz \, \alpha(\sigma,\tau)\, e^{ipz} \cdot \langle q - \tfrac{1}{2}z |\, \underbrace{e^{i(\sigma\hat{q}+\tau\hat{p})}}_{e^{i\sigma\hat{q}}\, e^{i\tau\hat{p}}\, e^{i\sigma\tau/2}} \,| q + \tfrac{1}{2}z \rangle$$

$$= \int dz \int d\sigma \int d\tau \, \alpha(\sigma,\tau)\, e^{ipz}\, e^{i\sigma(q-\frac{1}{2}z)}\, e^{i\sigma\frac{\tau}{2}}$$

$$\underbrace{\langle q - \tfrac{1}{2}z |\, \underbrace{e^{i\tau\hat{p}} \,| q + \tfrac{1}{2}z \rangle}_{= | q - \tau + \frac{1}{2}z \rangle}}_{\delta(q - \frac{1}{2}z - (q - \tau + \frac{1}{2}z)) = \delta(z-\tau)}$$

$$A(q,p) = \int d\sigma \int d\tau \, \alpha(\sigma,\tau)\, e^{i(\sigma q + \tau p)} \tag{22}$$

$\Rightarrow$ If we can represent an operator in the form (21) we immediately know its Weyl transform

We notice that the r.h.s. of (21) is symmetrically ordered in $\hat{q}, \hat{p}$

so

$$A(q,p) = q^n p^m \quad \longleftrightarrow \quad \hat{A}(\hat{q},\hat{p}) = \frac{1}{2^n} \sum_{r=0}^{n} \binom{n}{r} \hat{q}^{n-r} \hat{p}^m \hat{q}^r \tag{23}$$

e.g.

$$qp \quad \longleftrightarrow \quad \frac{1}{2}\left(\hat{q}\hat{p} + \hat{p}\hat{q}\right)$$

$$q^2 p \quad \longleftrightarrow \quad \frac{1}{4}\left(\hat{q}^2\hat{p} + 2\hat{q}\hat{p}\hat{q} + \hat{p}\hat{q}^2\right)$$

i.e. vice versa

$$\hat{q}\hat{p} \longrightarrow \hat{q}\hat{p} = \frac{1}{2}\left(\hat{q}\hat{p} + \hat{p}\hat{q} + [\hat{p},\hat{q}]\right)$$

$$= \underbrace{\frac{1}{2}\left(\hat{q}\hat{p} + \hat{p}\hat{q}\right)}_{\text{symmetrically ordered}} - \frac{i\hbar}{2}$$

$\Rightarrow$ recipe

(i) write $\hat{A}(\hat{q},\hat{p})$ into symmetrically ordered form

(ii) replace $\hat{q} \to q$ and $\hat{p} \to p$

Now what is the dynamical equation of motion of W?

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[H,\hat{\rho}] \longrightarrow \frac{dW}{dt} = ?$$

$$\frac{d}{dt}W = \frac{1}{2\pi\hbar}\int dy\, \langle q-\tfrac{y}{2}|\, \frac{d\hat{\rho}}{dt}\, |q+\tfrac{y}{2}\rangle\, e^{ipy/\hbar}$$

$$= -\frac{i}{2\pi\hbar^2}\int dy\, \langle q-\tfrac{y}{2}|\, H\rho - \rho H\, |q+\tfrac{y}{2}\rangle\, e^{ipy/\hbar}$$

for

(24) $$\boxed{\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q})}$$

One finds

Wigner EOM

(25) $$\boxed{\begin{aligned}\frac{\partial W}{\partial t} &= -\frac{p}{m}\frac{\partial W}{\partial q} \\ &+ \sum_{n=0}^{\infty} \frac{1}{(2n+1)!}\left(\frac{\hbar}{2i}\right)^{2n} \frac{\partial^{2n+1} V(q)}{\partial q^{2n+1}} \frac{\partial^{2n+1} W(q,p)}{\partial p^{2n+1}}\end{aligned}}$$

Compare this to the classical Liouville equation

(25) $$\boxed{\begin{aligned}\frac{\partial f}{\partial t} &= -\{f, H\} = -\frac{\partial f}{\partial q}\frac{\partial H}{\partial p} + \frac{\partial f}{\partial p}\frac{\partial H}{\partial q} \\ &= -\frac{p}{m}\frac{\partial f}{\partial q} + \frac{\partial V}{\partial q}\frac{\partial f}{\partial p}\end{aligned}}$$

this is eq. (25) truncated at $n = 0$

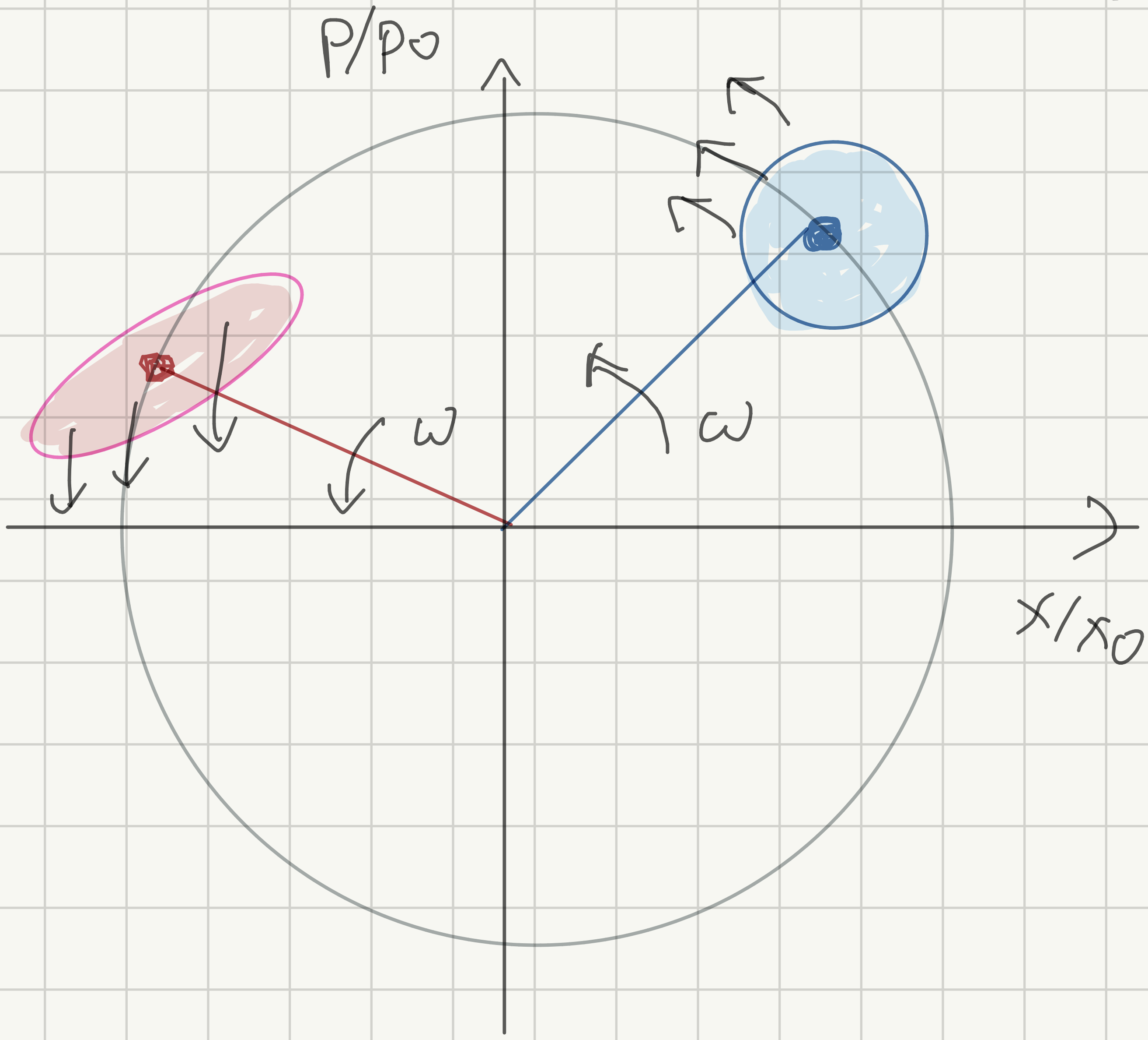
or in the limit

$$\hbar \to 0 \quad !$$

The EOM of the Wigner distribution becomes identical to the classical Liouville equation in the classical limit $\hbar \to 0$.

It is also identical if $V(q)$ is at most quadratic; i.e

free particle, linear potential, harmonic oscillator



scetch of time evolution of Wigner function for H.O. for different initial states

We have represented the time evolution of a quantum particle in terms of a close-to-classical quasi-probability concept. The time evolution of classical probabilty distribution can efficiently be simulated by Monte Carlo techniques!

$\Rightarrow$ Lets try to apply these ideas to quantum many-body systems