II.2 Statistical description of quantum systems

While a microscopic realization of a classical system is described by phase space variables $\{q_i\}, \{p_i\}$ in QM the microscopic realization is described by a quantum state

__pure state:__ wave-function $|\psi\rangle$

__mixed state:__ density matrix $\hat{\rho}$

Generally for a pure state $|\psi\rangle$ the wavefunction can be characterized by a __complete set of commuting operators__ (CSCO) who's eigenstates $\{|\phi_n\rangle\}$ form an orthonormal basis of the Hilbert space $\mathcal{H}$

General form of a pure state is a superposition of basis states $\{|\phi_n\rangle\}$

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle \qquad \sum_n |c_n|^2 = 1$$

and the expectation value of an observable $\hat{O}$ which is represented by a self-adjoint/hermitian operator is given by

$$\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle = \sum_{n,m} \langle \phi_n | \hat{O} | \phi_m \rangle c_n^* c_m$$

Note that a single measurement of $\hat{O}$ will always project onto one of the eigenvalues of $\hat{O}$ and one needs to repeat the measurement to obtain expectation value

Now in reality it is hardly possible to measure or prepare an exact quantum state of a system, and instead one will be dealing with statistical mixtures of states $\{|\phi_i\rangle\}$ where with a probability $p_i \geq 0$ the system is in the state $|\phi_i\rangle$

Characterized by density matrix

$$\hat{\rho} = \sum_i \underbrace{p_i}_{\text{probability}} \underbrace{|\phi_i\rangle\langle\phi_i|}_{\text{projection onto state } |\phi_i\rangle}$$

which describes a statistical superposition analogous to the phase space density of classical mechanics

$\hat{\rho}$ is Hermitian $\quad \hat{\rho}^\dagger = \hat{\rho}$

$\hat{\rho}$ is normalized

$$\text{tr}[\hat{\rho}] = \sum_n \langle\phi_n|\hat{\rho}|\phi_n\rangle$$

$$= \sum_{ni} p_i \langle\phi_n|\phi_i\rangle\langle\phi_i|\phi_n\rangle$$

$$= \sum_{ni} p_i |c_{ni}|^2 = \sum_i p_i = 1$$

$\hat{\rho}$ is positive semi-definite $\quad \langle \phi | \hat{\rho} | \phi \rangle \geq 0$

$$\langle \phi_n | \hat{\rho} | \phi_n \rangle = \sum_i p_i |c_{ni}|^2 \geq 0$$

Expectation values of observables are then given by

$$\langle \hat{O} \rangle = \sum_i p_i \langle \psi_i | \hat{O} | \psi_i \rangle = \mathrm{tr}[\hat{O}\hat{\rho}]$$

Evolution of quantum systems

Evolution of pure states in Schrödinger picture described by time dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} | \psi_i(t) \rangle = \hat{H} | \psi_i(t) \rangle$$

and likewise using $\hat{H}^\dagger = \hat{H}$

$$-i\hbar \frac{\partial}{\partial t} \langle \psi_i(t) | = \langle \psi_i(t) | \hat{H}$$

Since statistical probabilities p_i are time independent it follows

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = \sum_i p_i \, i\hbar \frac{\partial}{\partial t} |\psi_i(t)\rangle\langle\psi_i(t)|$$

$$= \sum_i p_i \left[\hat{H} |\psi_i(t)\rangle\langle\psi_i(t)| - |\psi_i(t)\rangle\langle\psi_i(t)| \hat{H} \right]$$

$$= [\hat{H}, \hat{\rho}]$$

$\Rightarrow$ <u>Liouville von-Neumann equation</u>

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

where analogous to the classical description we can define the Liouville operator

$$\mathcal{L} = \frac{1}{\hbar} [\hat{H}, \cdot]$$

with $i\hbar \{\cdot,\cdot\} \rightarrow [\cdot,\cdot]$

classical Poisson bracket → quantum commutator

as usual in canonical quantization

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Similar to the classical case, the evolution equation can be formally solved in terms of an evolution operator

<u>Schrödinger picture:</u> (time dependence carried by $|\psi\rangle, \hat{\rho}$)

Define $U(t,t_0)$ such that for any state

$$U(t,t_0)\,|\psi_i(t_0)\rangle = |\psi_i(t)\rangle$$
$$\langle\psi_i(t_0)|\,U^\dagger(t,t_0) = \langle\psi_i(t)|$$

then

$$i\hbar\frac{\partial}{\partial t}U(t,t_0)\,|\psi_i(t_0)\rangle = i\hbar\frac{\partial}{\partial t}|\psi_i(t)\rangle$$
$$= \hat{H}\,|\psi_i(t)\rangle$$
$$= \hat{H}\,U(t,t_0)\,|\psi_i(t_0)\rangle$$

Since this is valid for each state it follows that

$$\boxed{i\hbar\frac{\partial}{\partial t}U(t,t_0) = \hat{H}\,U(t,t_0)}$$

Solution is formally given by

$$U(t,t_0) = \underset{\text{time ordering}}{T} \exp\left(\frac{-i}{\hbar} \int_{t_0}^{t} dt' \, \hat{H}(t')\right)$$

which for $\hat{H}(t') = \hat{H}$ (time independent

$$= \exp\left(\frac{-i}{\hbar} \hat{H}(t-t_0)\right)$$

$U^\dagger U = 1\!\!1$ unitarity

Similarly for the density matrix it follows that

$$\hat{\rho}(t) = U(t,t_0)\, \hat{\rho}(t_0)\, U^\dagger(t,t_0)$$

with $U(t,t_0)\, U^\dagger(t,t_0) = 1\!\!1$

Evolution of observables in Schrödinger picture

$$\langle \hat{O}(t) \rangle = \mathrm{Tr}\left[\hat{\rho}(t)\, \hat{O}_S\right]$$

$$= \mathrm{Tr}\left[U(t,t_0)\, \hat{\rho}(t_0)\, U^\dagger(t,t_0)\, \hat{O}_S\right]$$

Due to cyclicity of the trace we can also write this as

$$\langle \hat{O}(t) \rangle = \mathrm{Tr}\left[\underbrace{\hat{\rho}(t_0)}_{\text{time independent}} \underbrace{U^\dagger(t,t_0)\, \hat{O}_S\, U(t,t_0)}_{\text{time dependent}} \right]$$

Heisenberg picture (time dependence carried by operators)

$$\hat{\rho}_H(t) = \hat{\rho}_H(t_0) = \hat{\rho}_S(t_0)$$

$$\hat{O}_H(t) = U^\dagger(t,t_0)\, \hat{O}_S\, U(t,t_0)$$

Differentiating $\hat{O}_H(t)$ with respect to time we find

$$i\hbar \frac{d}{dt} \hat{O}_H(t) = \left(i\hbar \frac{d}{dt} U^\dagger(t,t_0) \right) \hat{O}_S\, U(t,t_0) + U^\dagger(t,t_0)\, \hat{O}_S \left(i\hbar \frac{d}{dt} U(t,t_0) \right)$$

$$= - U^\dagger(t,t_0)\, \hat{H}\, \hat{O}_S\, U(t,t_0) + U^\dagger(t,t_0)\, \hat{O}_S\, \hat{H}\, U(t,t_0)$$

Now if $\hat{H}$ is time independent $[\hat{H}, \hat{U}] = 0$

Heisenberg equation:

$$\frac{d}{dt}\hat{O}_H(t) = \frac{1}{i\hbar}\left[\hat{O}_H(t), \hat{H}\right]$$

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Now irrespective of the picture we can investigate the evolution of expectation values

$$\frac{d}{dt}\langle\hat{O}(t)\rangle = \frac{1}{i\hbar}\left\langle\left[\hat{O},\hat{H}\right]\right\rangle$$

which is again analogous to the classical description with Poisson brackets replaced by $\frac{1}{i\hbar}$ times the commutator

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II.3 Phase space description of QM

Based on discussion of classical and quantum systems, we find analogous descriptions for phase space distribution f and density matrix $\hat{\rho}$, however they are formulated on different spaces phase-space vs. Hilbert space.

Will now discuss phase-space formulation of quantum mechanics

Wigner-Weyl formalism

more directly similarities and differences between classical and quantum dynamics

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Description of single particle in Wigner-Weyl formalism

We consider single particle w/o internal structure (spin, ...) such that

position states $|x\rangle$

momentum states $|p\rangle$

form a complete set of states on the Hilbert space

$$\int d^dx \, |x\rangle\langle x| = \int \frac{d^dp}{(2\pi\hbar)^d} \, |p\rangle\langle p| = \mathbb{1}$$

We remind ourselves that states are related by

$$|p\rangle = \int d^dx \; e^{ipx/\hbar} \, |x\rangle$$

and normalized such that

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

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Now the challenge in describing the system in phase-space is that we can not measure position $\hat{x}$ and momentum $\hat{p}$ simultaneously with arbitrary precision

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

Now to retain as much information as possible define for any hamilton operator $\hat{O}$ its Wigner-Weyl transform O_W

$$O_W(x,p) = \int d^d s \, e^{ips/\hbar} \langle x - \tfrac{s}{2} | \hat{O} | x + \tfrac{s}{2} \rangle$$

or equivalent

(inverse) Fourier transform

off-diagonal matrix elements in X/P space

$$O_W(x,p) = \int \frac{d^d q}{(2\pi\hbar)^d} e^{-iqx/\hbar} \langle p - \tfrac{q}{2} | \hat{O} | p + \tfrac{q}{2} \rangle$$

which is a function of phase space variable x, p

Specifically for $\hat{O} = \hat{\rho}$ this object is called <u>Wigner function</u> or <u>Wigner distribution</u>

$$\rho_W(t, x, p) = \int d^d s \, e^{ips/\hbar} \langle x - \tfrac{s}{2} | \hat{\rho}(t) | x + \tfrac{s}{2} \rangle$$

Since we cannot measure x, p precisely at the same time the best we can hope is that upon marginalizing over p (or x) we retain the full information about x (or p) distribution

$$\int \frac{d^d p}{(2\pi\hbar)^d} \rho_W(t, x, p) = \langle x | \hat{\rho}(t) | x \rangle$$

$$\int d^dx \; \rho_W(t,x,p) = \langle p | \hat{\rho}(t) | p \rangle$$

Since the Wigner-Weyl transformation can be inverted

$$\int \frac{d^dp}{(2\pi\hbar)^d} e^{-ips/\hbar} O_W(x,p) = \langle x - \tfrac{s}{2} | \hat{O} | x + \tfrac{s}{2} \rangle$$

or equivalently

$$\int d^dx \; e^{iqx/\hbar} O_W(x,p) = \langle p - \tfrac{q}{2} | \hat{O} | p + \tfrac{q}{2} \rangle$$

we can recover all possible operator matrix elements from the Wigner-Weyl transform

$\Rightarrow$ Equivalent formulation of QM compared to usual operator formalism

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Expectation values of observables

Based on Wigner-Weyl formalism, the next thing to understand is how to compute observables

Operator formalism: $\langle \hat{O}(t) \rangle = \mathrm{tr}\left[\hat{O}\,\hat{\rho}(t)\right]$

Schrödinger picture

Evaluating trace in position space

$$\langle \hat{O}(t) \rangle = \int d^d\tilde{x}\, \langle \tilde{x} | \hat{O}\,\hat{\rho}(t) | \tilde{x} \rangle$$

$$= \int d^d\tilde{x}\, d^dx'\, \langle \tilde{x} | \hat{O} | x' \rangle \langle x' | \hat{\rho}(t) | \tilde{x} \rangle$$

change of variables

$$\tilde{x} = x - s/2 \qquad x' = x + s/2$$

$$= \int d^dx \int d^ds\, \langle x - \tfrac{s}{2} | \hat{O} | x + \tfrac{s}{2} \rangle \langle x + \tfrac{s}{2} | \hat{\rho} | x - \tfrac{s}{2} \rangle$$

now using the representation of matrix elements in terms of Wigner transform we get

$$= \int d^d x \int d^d s \int \frac{d^d p}{(2\pi\hbar)^d} O_W(x,p)\, e^{-ips/\hbar}$$

$$\int \frac{d^d p'}{(2\pi\hbar)^d} \rho_W(x,p)\, e^{+ip's/\hbar}$$

so performing s integral we get

$(2\pi\hbar)^d \delta^{(d)}(p-p')$

$$\langle \hat{O}(t) \rangle = \int d^d x \int \frac{d^d p}{(2\pi\hbar)^d} O_W(x,p)\, \rho_W(x,p)$$

which is analogous to expression in classical ensemble with O_{cl} and f replaced by O_W and ρ_W

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Now there are however two crucial differences, in that O_W is the Wigner transform of an operator and not necessarily the same as O_{cl} and most importantly

classically	quantum
$f \geq 0$	ρ_W
positive semi definite	generally not positive semi definite
→ probabilistic interpretation	→ no probabilistic interpretation

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Evolution of the Wigner function

We started to see analogies between classical and quantum descriptions in phase space

Now investigate how quantum dynamics is different from classical dynamics

Based on the von-Neumann equation for the density matrix

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

we can now derive evolution equation for Wigner function $\rho_W(x,p)$

$$i\hbar \frac{\partial}{\partial t} \rho_W(t,x,p) = \int d^d s \, e^{ips/\hbar} \langle x - \tfrac{s}{2} | [\hat{H}, \hat{\rho}(t)] | x + \tfrac{s}{2} \rangle$$

Spelling out $[\hat{H}, \hat{\rho}] = \hat{H}\hat{\rho} - \hat{\rho}\hat{H}$

we get two terms

$$\int d^d s \, e^{ips/\hbar} \left[\langle x - \tfrac{s}{2} | \hat{H} \hat{\rho} | x + \tfrac{s}{2} \rangle - (\hat{\rho} \leftrightarrow \hat{H}) \right]$$

will look at the first term as second term is analogous

① Insert $\mathbb{1} = \frac{1}{2^d} \int d^d s' \, | x + \tfrac{s'}{2} \rangle \langle x + \tfrac{s'}{2} |$ between $\hat{H}$ and $\hat{\rho}$

$$\frac{1}{2^d} \int d^d s \int d^d s' \, e^{ips/\hbar} \underbrace{\langle x - \tfrac{s}{2} | \hat{H} | x + \tfrac{s'}{2} \rangle}\, \underbrace{\langle x + \tfrac{s'}{2} | \hat{\rho} | x + \tfrac{s}{2} \rangle}$$

off-diagonal matrix elements of $\hat{H}$ and $\hat{\rho}$ which can be rewritten as integrals of H_W and ρ_W using

$$\int \frac{d^d p}{(2\pi\hbar)^d} e^{-ips/\hbar} O_W(x,p) = \langle x - \tfrac{s}{2} | \hat{O} | x + \tfrac{s}{2} \rangle$$

② Define

$$X_H = \frac{x - \frac{s}{2} + x + \frac{s'}{2}}{2} = x + \frac{s'-s}{4} \equiv x + x'$$

$$X_p = \frac{x + \frac{s'}{2} + x + \frac{s}{2}}{2} = x + \frac{s'+s}{4} = x + x''$$

$$S_H = x + \frac{s'}{2} - \left(x - \frac{s}{2}\right) = \frac{s'+s}{2} = +2x''$$

$$S_p = x + \frac{s}{2} - \left(x + \frac{s'}{2}\right) = \frac{s-s'}{2} = -2x'$$

so

$$\langle x - \tfrac{s}{2} | \hat{H} | x + \tfrac{s'}{2} \rangle = \int \frac{d^d p_H}{(2\pi\hbar)^d} \, e^{-i p_H S_H/\hbar} \, H_W(X_H, p_H)$$

$$= \int \frac{d^d p_H}{(2\pi\hbar)^d} \, e^{-2i p_H x''/\hbar} \, H_W(x + x', p_H)$$

$$\langle x + \tfrac{s'}{2} | \hat{\rho} | x + \tfrac{s}{2} \rangle = \int \frac{d p_\rho}{(2\pi\hbar)^d} e^{+2i p_\rho x'/\hbar} \rho_W(x + x'', p_\rho)$$

suggestive to set $p_H = p + p'$ and $p_\rho = p + p''$

$$i\hbar \frac{\partial}{\partial t} \rho_W(t, x, p) = \frac{1}{2^d} \int d^d s \, d^d s' \, e^{ips/\hbar} \int \frac{d^d p'}{(2\pi\hbar)^d} \int \frac{d^d p''}{(2\pi\hbar)^d}$$

$$e^{-2i(p+p')x''/\hbar} e^{+2i(p+p'')x'/\hbar}$$

$$\Big[H_W(x+x', p+p') \rho_W(x+x'', p+p'') - \rho_W(x+x', p+p') H_W(x+x'', p+p'') \Big]$$

where $x' = \frac{s'-s}{4}$ and $x'' = \frac{s'+s}{4}$

and $s' = 2(x' + x'')$ || $s = 2(x'' - x')$

③ Change integration variables from (s, s') to (x', x'') with $\det\left(\frac{\partial(x', x'')}{\partial(s, s')} \right) = \frac{1}{8^d}$

$$i\hbar \frac{\partial}{\partial t} \rho_W(t,x,p) = 4^d \int d^dx' \int d^dx'' \int \frac{d^dp'}{(2\pi\hbar)^d} \int \frac{d^dp''}{(2\pi\hbar)^d}$$

$$e^{2ip(x''-x')} \quad e^{-2i(p+p')x''/\hbar} e^{+2i(p+p'')x'/\hbar}$$

$$\left[H_W(x+x', p+p') \rho_W(x+x'', p+p'') - \rho_W(x+x', p+p') H_W(x+x'', p+p'') \right]$$

Now terms proportional to p in the exponent $e^{i\ldots}$ cancel out and we can re-express the terms in [ ] by changing x' and x'' changing the exponential factor to

$$e^{-2ip'x''/\hbar} e^{2ip''x'/\hbar} - e^{-2ip''x'/\hbar} e^{2ip'x''/\hbar}$$

$$= 2i \sin\left(\frac{2}{\hbar} (p''x' - p'x'') \right)$$

Dividing by $i\hbar$

$$\frac{\partial}{\partial t} \rho_W(t,x,p) = 4^d \int d^dx' \int d^dx'' \int \frac{d^dp'}{(2\pi\hbar)^d} \int \frac{d^dp''}{(2\pi\hbar)^d}$$

$$\frac{2}{\hbar} \sin\left(\frac{2}{\hbar} (p''x' - p'x'') \right) H_W(x+x', p+p') \rho_W(x+x'', p+p'')$$

Now to make this expression look more classical, it is good to realize

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

such that

$$\frac{\partial}{\partial t} \rho_W(t,x,p) = 4^d \int d^dx' \int d^dx'' \int \frac{d^dp'}{(2\pi\hbar)^d} \int \frac{d^dp''}{(2\pi\hbar)^d}$$

$$H_W(x,p)\, e^{x'\overleftarrow{\frac{\partial}{\partial x}}} e^{p'\overleftarrow{\frac{\partial}{\partial p}}} \left[\frac{2}{\hbar} \frac{e^{\frac{2i}{\hbar}(p''x' - p'x'')} - e^{-\frac{2i}{\hbar}(p''x' - p'x'')}}{2i} \right] e^{x''\overrightarrow{\frac{\partial}{\partial x}}} e^{p''\frac{\partial}{\partial p}} \rho_W(x,p)$$

Now grouping the exponential factors

$$4^d \int d^dx' \int d^dx'' \int \frac{d^dp'}{(2\pi\hbar)^d} \int \frac{d^dp''}{(2\pi\hbar)^d} e^{\frac{2i}{\hbar}\left(p'' - \frac{i\hbar}{2}\overleftarrow{\frac{\partial}{\partial x}}\right)x'} \; e^{-\frac{2i}{\hbar}\left(x'' + \frac{i\hbar}{2}\overleftarrow{\frac{\partial}{\partial p}}\right)p'} \; e^{x''\overrightarrow{\frac{\partial}{\partial x}}} e^{p''\overrightarrow{\frac{\partial}{\partial p}}}$$

$$= e^{\frac{i\hbar}{2}\overleftarrow{\frac{\partial}{\partial x}}\overrightarrow{\frac{\partial}{\partial p}}} \; e^{-\frac{i\hbar}{2}\overleftarrow{\frac{\partial}{\partial p}}\overrightarrow{\frac{\partial}{\partial x}}}$$

$$= \exp\left(\frac{i\hbar}{2}\left(\overleftarrow{\frac{\partial}{\partial x}}\overrightarrow{\frac{\partial}{\partial p}} - \overrightarrow{\frac{\partial}{\partial x}}\overleftarrow{\frac{\partial}{\partial p}}\right)\right)$$

and similarly for the other term of the sum.

So collecting everything we finally get

$$\frac{\partial}{\partial t}\rho_W(t,x,p) =$$

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

which is compactly expressed as

$$\frac{\partial}{\partial t}\rho_W(t,x,p) = \{\{H_W, \rho_W\}\}$$

Moyal bracket

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Now the result can be used to compare classical and quantum dynamics

$$\frac{\partial}{\partial t} \rho_w(t,x,p) = H_w(x,p) \, \frac{2}{\hbar} \sin\left(\frac{\hbar}{2} \left(\frac{\overleftarrow{\partial}}{\partial x} \frac{\overrightarrow{\partial}}{\partial p} - \frac{\overrightarrow{\partial}}{\partial x} \frac{\overleftarrow{\partial}}{\partial p} \right) \right) \rho_w(t,x,p)$$

$$= \underbrace{\left(\frac{\partial H_w}{\partial x} \frac{\partial \rho_w}{\partial p} - \frac{\partial H_w}{\partial p} \frac{\partial \rho_w}{\partial x} \right)}_{= \{H_w, \rho_w\}} + O(\hbar^2)$$

Poisson Bracket

so quantum system follow classical trajectory to leading order in $\hbar$, while in a certain sense higher order terms describe fluctuations around classical path.

Note that if $H_W(x,p)$ is quadratic in x,p (c.f. exercises) then classical dynamics is exact. However even in this case P_W can still carry $\hbar^2$ corrections and does not have to be positive definite