Chapter IV: The postulates of quantum mechanics

4.1 The postulates (here for motion in 1 dimension)

Classical Mechanics	Quantum Mechanics
I. A state of a particle at time t is $(x(t), p(t))$ (2-d phase space)	I. The state of a particle at time t is $\|\psi(t)\rangle$ (vector in Hilbert space)
II. Every dynamical variable ω is a fct. of x and p: $\omega(x,p)$	II. x and p are represented by Hermitean operators $\hat{X}$ and $\hat{P} = \hbar\hat{K}$ with the following matrix elements in the $\hat{X}$-eigenbasis: $\langle x\|\hat{X}\|x'\rangle = x\,\delta(x-x')$, $\langle x\|\hat{P}\|x'\rangle = -i\hbar\,\delta'(x-x')$. Operators corresponding to classical observables $\omega(x,p)$ are given by $\hat{\Omega}(\hat{X},\hat{P})$, where the functional dependence of $\hat{\Omega}$ on $\hat{X}$ and $\hat{P}$ is the same as that of ω on x and p.
III. If particle is in state (x,p), then a measurement of ω gives $\omega(x,p)$. The state remains unaffected.	III. If particle is in state $\|\psi\rangle$, measuring the observable represented by $\hat{\Omega}$ yields one of the eigenvalues ω with probability $P(\omega) \sim \|\langle\omega\|\psi\rangle\|^2$. As a result of the measurement, the state of the particle changes from $\|\psi\rangle$ to $\|\omega\rangle$.

Time evolution:

Classical Mechanics	Quantum Mechanics
IV. The state variables change with time according to $\dot{x} = \frac{\partial H}{\partial p}$, $\dot{p} = -\frac{\partial H}{\partial x}$; $H(x,p)$ = Hamiltonian	IV. The state vector $\|\psi(t)\rangle$ evolves according to the Schrödinger equation $i\hbar\frac{d}{dt}\|\psi(t)\rangle = \hat{H}\|\psi(t)\rangle$ where $\hat{H}(\hat{X},\hat{P}) \leftrightarrow H(x,p)$ is the Hamilton operator, obtained by substituting in the classical Hamiltonian $x \mapsto \hat{X}$, $p \mapsto \hat{P}$.

4.2 Discussion

- The state vector $|\psi\rangle$ can be a proper vector (normalizable as $\langle\psi|\psi\rangle = 1$) or an improper vector (normalizable to δ-functions, see later). Usually the Hilbert space describing realistic physical systems contains both types of vectors (corresponding to localized bound states and delocalized unbound states).

- The Hilbert space for $|\psi\rangle$ is infinite dimensional (i.e. the state of a particle has an infinite number of degrees of freedom), since it represents the distribution $\psi(x)$ ("wave function") of the particle in position space. Contrary to classical mechanics, where in a given state the particle is localized at a fixed point x, in quantum mechanics the probability distribution $|\psi(x)|^2$ (see later) is usually spread out over all x-space.

- Superposition principle: if $|\psi\rangle$ and $|\psi'\rangle$ represent possible states of the system, then $\alpha|\psi\rangle + \beta|\psi'\rangle$ $(\alpha, \beta \in \mathbb{C})$ also represents a possible state of the system.
  (Think of a string with displacement functions $f(x)$ or $g(x)$ $\rightarrow \alpha f(x) + \beta g(x)$ $(\alpha, \beta \in \mathbb{R})$ is then another possible displacement fct.)
  The implication of such a linear superposition for measurements of an observable is, however, quite different in QM than in classical mechanics:

Measurement of an observable $\omega(x,p)$ in QM:

① Construct $\hat{\Omega}(\hat{X},\hat{P})$ by letting $x \mapsto \hat{X}$, $p \mapsto \hat{P}$ in $\omega(x,p)$.

② Find eigenvalues ω_i (all real since $\hat{\Omega} = \hat{\Omega}^+$) and orthonormal eigenvector $|\omega_i\rangle$ of $\hat{\Omega}$.

③ Expand $|\psi\rangle$ in this basis:

$$|\psi\rangle = \sum\!\!\!\!\!\!\int_i |\omega_i\rangle\langle\omega_i|\psi\rangle$$

($\sum\!\!\!\!\!\!\int_i$ indicates a sum over discrete and an integral over continuous eigenvalues)

④ $P(\omega) \sim |\langle\omega|\psi\rangle|^2$ (probability for result of measurement yielding the specific eigenvalue ω).

$P(\omega) = 0$ for any ω that is not an eigenvalue of $\hat{\Omega}$!

Can write this as

$$P(\omega) \sim \langle\psi|\omega\rangle\langle\omega|\psi\rangle = \langle\psi|\hat{\mathbb{P}}_\omega|\psi\rangle = \langle\psi|\hat{\mathbb{P}}_\omega\hat{\mathbb{P}}_\omega|\psi\rangle$$
$$= \langle\hat{\mathbb{P}}_\omega\psi|\hat{\mathbb{P}}_\omega\psi\rangle$$

The probability should be normalized to 100%:

$$\sum\!\!\!\!\!\!\int_i P(\omega_i) = 1 = \sum\!\!\!\!\!\!\int_i |\langle\omega_i|\psi\rangle|^2 = \langle\psi|\underbrace{\left(\sum\!\!\!\!\!\!\int_i |\omega_i\rangle\langle\omega_i|\right)}_{\hat{I}}|\psi\rangle = \langle\psi|\psi\rangle$$

(This makes sense only for proper Hilbert space vectors, since for improper vectors $\langle\psi|\psi\rangle = \infty$. We'll explain below how to interpret postulate III for improper state vectors.)

The normalized probability is then

$$\boxed{P(\omega_i) = \frac{|\langle\omega_i|\psi\rangle|^2}{\langle\psi|\psi\rangle} \xrightarrow[|\psi\rangle\,\text{normalized}]{} |\langle\omega_i|\psi\rangle|^2}$$

- State vectors $\alpha|\psi\rangle$ with the same "direction" as $|\psi\rangle$ give the same normalized probability

  $\Rightarrow$ state is represented by a ray $\alpha|\psi\rangle, \alpha \in \mathbb{C}$ in Hilbert space; this ray is represented by the normalized unit vector $|\psi\rangle$, which we will usually employ. Even the unit vector is ambiguous, since $|\psi\rangle$ and $e^{i\theta}|\psi\rangle$ both have unit norm. ($\theta \in \mathbb{R}$)

  This freedom can be used to make the component of $|\psi\rangle$ come out real in some basis.

- If $|\psi\rangle$ is an eigenstate $|\omega_i\rangle$, the measurement of $\hat{\Omega}$ yields the eigenvalue ω_i with 100% probability (i.e. with certainty). (This is like in a classical measurement.)

- If $|\psi\rangle$ is a (normalized) superposition of two $\hat{\Omega}$-eigenstates,

$$|\psi\rangle = \frac{\alpha|\omega_1\rangle + \beta|\omega_2\rangle}{\sqrt{\alpha^2+\beta^2}}$$

  the measurement of $\hat{\Omega}$ can yield ω_1 or ω_2, but no other value! This has no classical analog:

  If a string has displacement $\alpha f(x) + \beta g(x) = h(x)$, a measurement of a dynamical variable in state $h(x)$ doesn't give you the value measured in state $f(x)$ some times and the value corresponding to $g(x)$ at other times, but instead a unique value that is distinct from both. Similarly, $f(x)$ and $\alpha f(x)$ don't represent the same string state.

- Suppose we solved the eigenvalue for $\hat{\Omega}$, but now want to measure the observable $\hat{\Lambda}$ in state $|\psi\rangle$. The result will be one of the eigenvalue λ_j of $\hat{\Lambda}$. We can calculate the probability $P(\lambda_j)$ by starting from the matrix elements $\Lambda_{ij} = \langle\omega_i|\hat{\Lambda}|\omega_j\rangle$ in the $\hat{\Omega}$-eigenbasis, find the eigenvalues λ_i and eigenvectors $|\lambda_i\rangle$ (with components $\langle\omega_j|\lambda_i\rangle$ in the $\hat{\Omega}$-eigenbasis, arranged as column vectors with index j) of this matrix, and take the inner product in this basis:

$$\boxed{\langle\lambda_j|\psi\rangle = \sum_k \langle\lambda_j|\omega_k\rangle\langle\omega_k|\psi\rangle}$$

$$P(\lambda_i) = |\langle\lambda_i|\psi\rangle|^2 \quad (|\psi\rangle \text{ normalized})$$

So the entire calculation can be done in the $\hat{\Omega}$-eigenbasis, i.e. by working out vector components and matrix elements in that basis.

Example

Suppose $|\psi\rangle = \frac{1}{2}|\omega_1\rangle + \frac{1}{2}|\omega_2\rangle + \frac{1}{\sqrt{2}}|\omega_3\rangle$ $\left(\frac{1}{4}+\frac{1}{4}+\frac{1}{2}=1 \Rightarrow \text{normalized}\right)$

$P(\omega_1) = |\langle\omega_1|\psi\rangle|^2 = \frac{1}{4} = |\langle\omega_2|\psi\rangle|^2 = P(\omega_2)$

$P(\omega_3) = \frac{1}{2}$

Complications:

(A) The recipe $x \mapsto \hat{X}$, $p \mapsto \hat{P}$ is ambiguous: e.g. $\omega(x,p) = xp$

$\rightarrow \hat{\Omega} = \hat{X}\hat{P}$ or $\hat{\Omega} = \hat{P}\hat{X}$ or ?

Answer: $\hat{\Omega}$ must be Hermitean for measurements to produce real results

This resolves the ambiguity for terms of the type $x^m p^n$ as long as $m+n \leq 3$ $(m,n \geq 0)$:

$xp \mapsto \frac{1}{2}(\hat{X}\hat{P} + \hat{P}\hat{X})$

$x^2 p \mapsto \hat{X}\hat{P}\hat{X}$

$x p^2 \mapsto \hat{P}\hat{X}\hat{P}$

For higher powers experiment must decide the correct transcription rule.

(B) $\hat{\Omega}$ is degenerate:

Let $\omega_1 = \omega_2 = \omega$. What to take for $P(\omega)$?

Select orthonormal basis $|\omega,1\rangle$, $|\omega,2\rangle$ in the degenerate subspace:

$$P(\omega) = |\langle\omega,1|\psi\rangle|^2 + |\langle\omega,2|\psi\rangle|^2 = \langle\psi|\hat{\mathbb{P}}_\omega|\psi\rangle$$

where $\hat{\mathbb{P}}_\omega = |\omega,1\rangle\langle\omega,1| + |\omega,2\rangle\langle\omega,2|$

(generally: $\hat{\mathbb{P}}_\omega = \sum_\alpha |\omega,\alpha\rangle\langle\alpha,\omega|$ where α is a multiindex that uniquely labels each state in the ω-subspace)

(C) The eigenvalue spectrum of $\hat{\Omega}$ is continuous:

$$|\psi\rangle = \int d\omega \, |\omega\rangle\langle\omega|\psi\rangle$$

In this case $|\langle\omega|\psi\rangle|$ is the differential probability $\frac{dP}{d\omega}$ such that $dP = \frac{dP}{d\omega}d\omega$ is the probability of finding ω in the interval $[\omega, \omega+d\omega]$. (The probability for a single value ω is zero since this value has zero measure in the eigenvalue space.)

$$\rightarrow \int \frac{dP}{d\omega}d\omega = \int |\langle\omega|\psi\rangle|^2 d\omega = \int \langle\psi|\omega\rangle\langle\omega|\psi\rangle$$

$$= \langle\psi|\underbrace{\left(\int |\omega\rangle\langle\omega| d\omega\right)}_{\hat{I}}|\psi\rangle = \langle\psi|\psi\rangle = 1.$$

(For improper vectors $|\psi\rangle$ see later.)

Important example: $\hat{\Omega} = \hat{X}$ (has continuous spectrum).

$$\int \frac{dP}{dx}dx = \int \langle\psi|x\rangle\langle x|\psi\rangle dx = \int |\psi(x)|^2 dx = 1$$

$\Rightarrow |\psi(x)|^2 =$ probability density for finding the particle at x.

Similarly, $|\langle p|\psi\rangle|^2 = |\psi(p)|^2$ is probability density for the particle to be measured with momentum p when in state $|\psi\rangle$.

$$\psi(p) = \langle p|\psi\rangle = \int \langle p|x\rangle\langle x|\psi\rangle dx = \int \frac{dx}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}\psi(x)$$

(normalized to $\langle p|p'\rangle = \delta(p-p') = \frac{\delta(k-k')}{\hbar}$)

Ⓓ The quantum variable $\hat{\Omega}$ has no classical counterpart:

(for example, spin)

→ our postulates give no guidance how to describe it

→ use intuition, semi-classical analogies and <u>experiment</u>(!)

"Collapse" of the state vector

General decomposition in eigenstates of $\hat{\Omega}$ of the state vector $|\psi\rangle$ <u>before</u> "measuring $\hat{\Omega}$":

$$|\psi\rangle = \sum_{\omega} |\omega\rangle\langle\omega|\psi\rangle$$

Knowing $|\psi\rangle$ does not tell us the value of ω that we will find when measuring $\hat{\Omega}$; it only gives us the probabilities $P(\omega) \sim |\langle\omega|\psi\rangle|^2$ for each eigenvalue ω to be the actually measured value when performing the measurement.

However, after the measurement, we <u>know</u> that the system has the value $\omega_{measured}$ of the observable $\hat{\Omega}$. Assuming an "ideal measurement" (I'll explain below what that means), it doesn't change the value of ω. So we now <u>know</u> for sure that at the time of measurement the system was in an $\hat{\Omega}$-eigenstate with eigenvalue $\omega_{measured}$, and (at least directly after the measurement, before any other extraneous influences on the system might have caused it to change its state) it still is in that eigenstate. This "knowledge" established by the measurement has dramatically changed the probabilities for finding value ω for $\hat{\Omega}$ in the system: the probability $P(\omega_{measured})$ has shot up to $1 = 100\%$, while the probabilities for all other values $\omega \neq \omega_{measured}$ have all collapsed to $P(\omega) = 0$. The new state (after the measurement) is now (after normalization)

$$|\psi_{new}\rangle = |\omega_{measured}\rangle$$

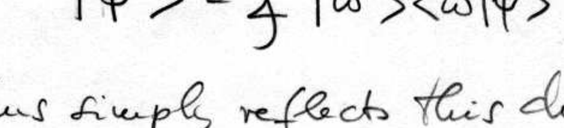
even if the measurement was ideal, i.e. it didn't change the system, it just "looked".

<u>The collapse of the wave function</u>

$$|\psi\rangle = \sum |\omega\rangle\langle\omega|\psi\rangle \xrightarrow[\text{ment of } \hat{\Omega}]{\text{measure-}} |\psi_{new}\rangle = |\omega_{measured}\rangle$$

thus simply reflects this change in our knowledge about the system, and not a change in the system itself!

What is an "ideal measurement"? Consider the following example: take an electron that somehow is constrained to move only along the x-direction (1-d motion). We want to measure its momentum by Compton scattering of light:



$$cp' = cp + \hbar(\omega + \omega')$$
$$E' = E + \hbar(\omega - \omega')$$

Can solve these to give p and p' as functions of observed photon frequency before and after: