Quantum Mechanics II

Review of quantum mechanics:

The quantum realm is characterized by Planck's constant h. Its value is given by

$$\hbar = \frac{h}{2\pi} = 1.05457182 \times 10^{-34} \; m^2\text{-}kg/s$$

Comments:

1. $\hbar$ is called 'h-bar', 'h cut' or 'Dirac's h'.

2. Dimension of $\hbar$ is same as angular momentum

$$\vec{J} = \vec{r} \times \vec{p}$$

Thus $[\vec{J}] = [\vec{r}] \cdot [\vec{p}] = L \cdot M \cdot L/T = L^2 M/T$

In SI units this translates to $m^2\text{-}kg/sec$.

3. In classical systems the action S functional characterizes a system. Newton's laws or any other classical system can be formulated as in terms of generalized coordinates $q_i(t)$ st for the physical path in configuration space the functional $S[q_i(t), \dot{q}_i(t)]$ is extremized. I.e.

$$\delta S[q_i]\Big|_{q_i = q_i^{\text{Physical}}} = 0 \iff \text{E.L. eqn} \quad \frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0$$

Roughly speaking we may say that a system for which $S \sim O(\hbar)$ then it is a system that follows the laws of quantum mechanics. For $S \gg \hbar$, we expect classical mechanics to hold. This is a rule of thumb, not an exact statement. The transition from quantum to classical is an unsolved problem.

4. For periodic systems the action-angle integral

$$\sum_i \oint p_i \, dq_i \sim n\hbar$$

This leads to angular momentum being quantized. $J \sim n\hbar$.
For large n J seems continuous and hence classical.

Review of QM:

There are many different formulations and iterpretations of quantum mechanics:

1. Copenhagen/Hilbert space interpretation
2. The many-Worlds interpretation due to Everette & Wheeler
3. The Path-Integral (or Sum over histories) formulation by Feynman
4. Non-local hidden variable approach by de Broglie & Bohm.

Within each school there are subschools.

In this course we follow approach 1. In QM III, an introduction approach 3 is given. Feynman's approach is useful for generalization to QFTs, especially gauge theories. E & M is an example of a gauge theory: $\vec{A} \longrightarrow \vec{A} + \vec{\nabla}\chi$, $\phi \longrightarrow \phi + \frac{\partial \chi}{\partial t}$ leaves Maxwell's eqns invariant. Other examples of Gauge theories: Yang-Mills theory & GR.

Postulates of QM

We shall begin our review of quantum mechanics by reviewing its postulates. No effort will be given to make the postulates completely independent of each other.

Postulate 1:

"All the distinct physical states of a quantum system are described by rays in a Hilbert Space $\mathcal{H}$.

A Hilbert space $\mathcal{H}$ is a complete vector space equipped with an inner product:

$$(\ ,\ ): \mathcal{H} \times \mathcal{H} \longrightarrow \mathbb{C} \quad \text{s.t.}$$

$\forall\ |\chi\rangle, |\phi\rangle, |\psi\rangle \in \mathcal{H}$ we have:

1) $(\psi, \phi) = (\phi, \psi)^*$

2) $(\psi, \psi) \geq 0$ with equality holding iff $|\psi\rangle = 0$.

3) $(\chi, \phi + a\psi) = (\chi, \phi) + a(\chi, \psi)$ where $a \in \mathbb{C}$.

Comment: Note that 1) + 3) imply $(\chi + a\psi, \phi) = (\chi, \phi) + a^* (\chi, \phi)$.

By a ray in $\mathbb{H}$ we mean an equivalence class of vectors:

$$|\psi\rangle \sim a|\psi\rangle \quad \forall\, a \in \mathbb{C}/\{0\}$$

In other words, the space is a projective vector space.

Comment: This above fact implies that we don't care about the normalization of state vectors in general. However, as we shall see there are two types of vectors — normalizable and non-normalizable. Both types of vectors play important roles in quantum mechanics.

Dimensionality of $\mathbb{H}$: Depending on the system the dimensionality of $\mathbb{H}$ can either finite or infinite.

Eg: $\mathbb{C}^2$ with inner product $\xi_1^\dagger \xi_2$

Verify that if $\xi = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$ with $z_i = x_i + i y_i$, $i=1,2$ complex numbers then $\mathbb{C}^2$ is a Hilbert space over $\mathbb{C}$

Aside:

The representation of an element of $\mathbb{H}$ as $|\psi\rangle$ is part of the Dirac notation. In the Dirac notation the inner product (ψ, ϕ) between two vectors $|\psi\rangle$ & $|\phi\rangle$ is represented as $\langle\psi|\phi\rangle$. However $\langle\psi|$ is not an element of $\mathbb{H}$ but its dual $\mathbb{H}^*$.

To define a dual vector space let us first begin with an orthonormal basis $\{e_i\}$ of a Hilbert space. This implies:

$$(e_i, e_j) = \delta_{ij}$$

This implies $\dim \mathbb{H}$ linear maps

$$(e_i, \;) : \mathbb{H} \to \mathbb{C}$$

The space of all these linear maps over $\mathbb{C}$ themselves form a vector space which is the dual vector space.

In the Dirac notation these linear maps are denoted by bra vectors $\langle e_i| : \mathbb{H} \to \mathbb{C}$.

Using the isomorphism $(e_i, e_j) = \delta_{ij}$ we write

$$(\psi, \phi) = \langle\psi|\phi\rangle.$$

Operators on Hilbert Spaces

Every system has associated with it a list of observables. Observables are Hermitian and Self-adjoint linear / anti-linear operators on the Hilbert space.

A linear operator $\hat{A}$ is a map from $\mathcal{H}$ to $\mathcal{H}$: $\hat{A} : \mathcal{H} \to \mathcal{H}$.

The Adjoint of $\hat{A}$ is denoted by $\hat{A}^{\dagger}$ and it is defined by $(\phi, \hat{A}^{\dagger}\psi) = (\psi, A\phi)^{*}$ $\forall$ $|\psi\rangle$ & $|\phi\rangle$

Comment: The definition of $A^{\dagger}$ implies $(\hat{A}\phi, \psi) = (\phi, \hat{A}^{\dagger}\psi)$.

A self-adjoint operator: A self-adjoint operator is one for which $(\phi, \hat{A}^{\dagger}\psi) = (\phi, \hat{A}\psi)$ $\forall$ $|\psi\rangle$ & $|\phi\rangle$.

In the Dirac notation: $(\phi, \hat{A}^{\dagger}\psi) = \langle\phi|\hat{A}^{\dagger}\psi\rangle = \langle\phi|\hat{A}\psi\rangle = \langle\hat{A}\phi|\psi\rangle \equiv \langle\phi|A|\psi\rangle$. $\Rightarrow$ $\hat{A}^{\dagger} = \hat{A}$

$= \langle\phi|\hat{A}^{\dagger}|\psi\rangle$

Theorem: The eigenvalues of self-adjoint operators are real numbers.

Proof: $\hat{A} \to$ Self adjoint operator.

$$\hat{A}\,|a\rangle = \underbrace{a}_{\text{eigenvalue}}\,\overbrace{|a\rangle}^{\text{eigenvector.}} \quad \text{——— ①}$$

$$\Rightarrow \quad \langle a|\hat{A}|a\rangle = a\langle a|a\rangle \quad \text{——— ②}$$

$$\text{①} \Rightarrow \quad \langle a|\hat{A}^{\dagger} = \langle a|\, a^{*} \quad \Rightarrow \quad \langle a|\hat{A} = a^{*}\langle a|$$

$$\Rightarrow \quad \langle a|\hat{A}|a\rangle = a^{*}\langle a|a\rangle \quad \text{— ③}$$

② − ③ :

$$0 = (a - a^{*})\langle a|a\rangle$$

If we assume $|a\rangle \neq 0$ Then $a = a^{*}$ ■

Postulate 2:

The result of an observation of the observable $\hat{A}$ of a system in state $|\psi\rangle$ is an eigenvalue of the observable $\hat{A}$.

The spectral decomposition theorem states that for a linear operator:

$$\hat{A} = \sum_i a_i |a_i\rangle (a_i, \,)$$
$$\cong \sum_i a_i |a_i\rangle\langle a_i|$$

Comments: 1. The spectral decomposition theorem for Hermitian operators is the just the statement that when we express a matrix in its eigenbasis the matrix is diagonal with the eigenvalues along its diagonal.

$$A = \begin{pmatrix} a_1 & & & \\ & a_2 & & \\ & & \ddots & \\ & & & a_n \end{pmatrix}$$

2. From now on we shall write $\hat{A} = \sum_i a_i |a_i\rangle\langle a_i|$ instead of $\hat{A} \cong \sum_i a_i |a_i\rangle\langle a_i|$.

3. For continuous eigenvalue spectra we could write $\hat{A} = \int da \; a \, |a\rangle\langle a|$ and for mixed cases $\hat{A} = \sum\!\!\!\!\!\!\int_i a_i |a_i\rangle\langle a_i|$.

But in general we shall write $\hat{A} = \sum_i a_i |a_i\rangle\langle a_i|$

4. $|a_i\rangle\langle a_i|$ are operators since they map $\mathcal{H} \to \mathcal{H}$. They are known as projection operators. Due to the fact that $\langle a_i|a_j\rangle = \delta_{ij}$ for an orthonormal eigenbasis of a operator $\hat{A}$ we have

$P_i = |a_i\rangle\langle a_i|$, $\quad P_i P_j = P_i \delta_{ij}$. i.e. $P_i^2 = P_i$ and $P_i P_j = 0$ if $i \neq j$.

This has simple geometrical interpretation. In 3D let $\vec{\psi}$ be a vector then $\vec{\psi} = \psi_x \hat{i} + \psi_y \hat{j} + \psi_z \hat{k}$

$P_{\hat{i}} = \hat{i}\,(\hat{i}\cdot\,)$, $\quad P_{\hat{j}} = \hat{j}\,(\hat{j}\cdot\,)$, $\quad P_{\hat{k}} = \hat{k}\,(\hat{k}\cdot\,)$

Then $\quad P_{\hat{a}} \vec{\psi} = \hat{a}\,(\hat{a}\cdot\vec{\psi}) \quad = \hat{a}\,\psi_a$

If $\quad P_{\hat{a}} P_{\hat{a}} = \hat{a}\,(\hat{a}\cdot\hat{a}\,\psi_a) \quad = \hat{a}\,\hat{a}\cdot\hat{a}\,\psi_a = \hat{a}\,\psi_a$

If $\quad P_{\hat{b}} P_{\hat{a}} \vec{\psi} = \hat{b}\,(\hat{b}\cdot\hat{a}\,\psi_a) \quad = 0$ if $\hat{a} \neq \hat{b}$.

5. A special but important special case is $\hat{1} = \sum_i |i\rangle\langle i|$ in any eigenbasis $\{|i\rangle\}$. This is known as the decomposition of the identity.

Commutation Relationships

Operators on a Hilbert space do not necessarily commute. If $\hat{A}$ & $\hat{B}$ are two linear operators such that

$\hat{A}\hat{B}|\psi\rangle = \hat{B}\hat{A}|\psi\rangle$ does not hold for all $|\psi\rangle \in \mathcal{H}$ then we say $\hat{A}$ & $\hat{B}$ does not commute. In general, $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = \hat{C} \neq 0$.

Let $\hat{A}$ be a hermitian operator and $\{|a_i\rangle\}$ be its orthonormal eigenbasis. Then if $\hat{B}$ is another operator then $\hat{B}$ is said to have the following representation in the eigenbasis $\{|a_i\rangle\}$ of $\hat{A}$:

$$\hat{B}_{ij} = \langle a_i|\hat{B}|a_j\rangle.$$

There are two possibilities:

(i) $\hat{A}$ & $\hat{B}$ commute: $[\hat{A},\hat{B}]=0$ { We assume that both $\hat{A}$ & $\hat{B}$ are hermitian.}

Then if $|a\rangle$ is an eigenvector of $\hat{A}$ then it is also eigenvector of $\hat{B}$:

$$\hat{A}|a\rangle = a|a\rangle$$

$$[\hat{A},\hat{B}]|a\rangle = 0$$

$$\Rightarrow \hat{A}\hat{B}|a\rangle = a\,\hat{B}|a\rangle$$

$$\Rightarrow \hat{B}|a\rangle \propto |a\rangle \quad \{\text{assuming no degeneracy}\}$$

$$\Rightarrow \hat{B}|a\rangle = b|a\rangle$$

Thus $\hat{B} = \sum_i b_i |a_i\rangle\langle a_i|$

(ii) $\hat{A}$ & $\hat{B}$ do not commute { both hermitian} then in $\{a_i\}$ basis

$$\hat{B} = \sum_{i,j} \hat{B}_{ij} |a_i\rangle\langle a_j| \quad \text{s.t.}$$

$$\hat{B}^*_{ij} = \hat{B}_{ji}$$

so that $\hat{B}^\dagger = \hat{B}$.

Postulate 3: Suppose we have a quantum system in a state $|\psi\rangle$. We can pick an observable $\hat{A}$ in whose eigenbasis we can write $|\psi\rangle = \sum_i c_i |a_i\rangle$ where c_i are complex coefficients.

Suppose we have normalized $|\psi\rangle$ then $\langle\psi|\psi\rangle = 1$.

But since $\langle a_i | a_j \rangle = \delta_{ij}$ we have $\sum_i |c_i|^2 = 1$.

Now, suppose we want to measure the observable $\hat{A}$ for the system in state $|\psi\rangle$. Then the Born rule tells that the probability of obtaining a_i (an eigenvalue of $\hat{A}$) in our measurement is $|c_i|^2$.

Quantum mechanics only makes predictions about the probabilities of results of observations.

The measurement of $\hat{A}$ and the observation of a_i as the result implies that the state vector describing the system right after the observation $|a_i\rangle$. $|\psi\rangle \xrightarrow[\text{yielding } a_i]{\text{observation}} |a_i\rangle$.

This is known as the collapse postulate. We say that measurement leads to collapse of the 'wave-function.'

Postulate 4: Let $|\psi(t_0)\rangle$ be the state of a quantum system at time t_0. If the quantal system is allowed to evolve without interference from any external systems then at time t it is, in general, represented by another state vector $|\psi(t)\rangle$.
For every quantal system there exists a unitary operator $U(t,t_0)$, known as the time evolution operator, which evolves the system from its state at time t_0 to time t:

$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle$$

with b.c. $\hat{U}(t,t) = \hat{\mathbb{1}}$.

$\hat{U}$ is unitary $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{\mathbb{1}} \Rightarrow \hat{U}^\dagger = \hat{U}^{-1}$.

This implies conservation of probability. $\langle\psi(t)|\psi(t)\rangle = \langle\psi(t_0)|U^\dagger U|\psi(t_0)\rangle$
$= \langle\psi(t_0)|\psi(t_0)\rangle$.

Comment: Information is preserved under unitary time evolution.

For uniform time evolution (i.e. time-translation invariant) $U(t,t_0) = U(t-t_0)$.

Now consider the fact that every unitary operator $\hat{U}(t)$ $(\equiv \hat{U}(t,0))$ can be expressed as

$\hat{U}(t) = e^{i\hat{X}t}$ where $\hat{X}^\dagger = \hat{X}$ [i.e. $\hat{X}$ is Hermitian]

Proof: $(\hat{U}(t))^\dagger = (e^{i\hat{X}t})^\dagger = \left(\sum_{n=0}^{\infty} \frac{(i\hat{X}t)^n}{n!}\right)^\dagger = \sum_{n=0}^{\infty} \frac{(-i\hat{X}^\dagger t)^n}{n!} = \sum_{n=0}^{\infty} \frac{(-i\hat{X}t)^n}{n!}$
$= e^{-i\hat{X}t}$.

Now using BCH formula: $e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\cdots}$

we see $e^{i\hat{X}t} e^{-i\hat{X}t} = e^0 = \hat{\mathbb{1}}$. ■

We define $\hat{H} = -\hbar\hat{X}$ as the Hamiltonian operator.

Now consider $|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(t_0)\rangle$

$$\frac{d|\psi(t)\rangle}{dt} = \frac{i}{\hbar}\hat{H}|\psi(t)\rangle$$

$$\boxed{i\hbar\frac{d|\psi(t)\rangle}{dt} = \hat{H}|\psi(t)\rangle}$$

This is the Schrödinger equation. $\hat{H}$ is known as the Hamiltonian operator and its eigenvalues represent energy eigenvalues.

Comment on Linearity of the Schrödinger Equation

The Schrödinger equation is a linear differential equation. So if ϕ_1 & ϕ_2 are two solutions to the equation then so is the arbitrary linear combination $\phi = c_1\phi_1 + c_2\phi_2$ for c_1 & c_2 complex constants.

The linearity of the Schrödinger equation has far-reaching consequences, but, as we shall see it puts the energy eigenstates in a very important and central position. The assumption of linearity of the observables also imply that we can use the eigenbasis of any observable as the basis in which we can express any state.

Discussion on Postulates

The state vector $|\psi(t)\rangle$ representing the state of a system is an abstract vector in an abstract vector space $\mathcal{H}$. But for physical applications it is convenient to represent $|\psi(t)\rangle$ in the eigenbasis of a particular observable. Important among them are:

1. The position basis
2. The momentum basis

The Position Basis:

The position of a quantum particle is an important observable. Let us consider a one dimensional system and the position operator is then represented by $\hat{X}$. Let us assume that the system lives on $\mathbb{R}^1$. Then $\hat{X}|x\rangle = x|x\rangle$ with $x \in \mathbb{R}$.

Then the orthonormality condition becomes

$$\langle x|x'\rangle = \delta(x-x')$$

where $\delta(x-x')$ is the Dirac delta 'function' (In reality, it is a distribution).

In this basis, the position operator is diagonal:

$$\boxed{\langle x'|\hat{X}|x\rangle = x\,\delta(x-x')}$$

$\delta(x-x')$ is of course the continuous version of δ_{ij}. A finite dimensional diagonal matrix has the form: $A_{ij} = a_i \delta_{ij}$ [no sum over repeated indices].

The state vector $|\psi(t)\rangle$ in this basis is called the position space wave-function, or just the wavefunction:

$$\boxed{\psi(x,t) \equiv \langle x|\psi(t)\rangle}$$

For an arbitrary equation:

$\hat{O}|\psi\rangle = |\phi\rangle$ we use the decomposition of identity $\hat{\mathbb{1}} = \int dx\, |x\rangle\langle x|$

to write

$$\phi(x) = \langle x|\phi\rangle = \langle x|\hat{O}|\psi\rangle$$ [Suppressing any time-dependence for the moment.]

$$= \int dx' \langle x|\hat{O}|x'\rangle\langle x'|\psi\rangle$$

$$\equiv \int dx' \; \hat{O}_{xx'} \; \psi(x')$$

or

$$\boxed{\int dx' \; \hat{O}_{xx'} \; \psi(x') = \phi(x)} \quad \text{———} \quad (\dagger)$$

where we have defined $\hat{O}_{xx'} \equiv \langle x|\hat{O}|x'\rangle$.

$(\dagger)$ is of course the continuum version of the matrix equation

$$\sum_j A_{ij} \psi_j = \phi_i$$

$\hat{O}_{xx'}$ is known as the integral kernel of the operator $\hat{O}$.

For quantum mechanics the Dirac delta function and other close relatives allow us to work out the integral kernels of important operators.

Review of Important Dirac Delta Function Relations:

Definition: $\int_{-\infty}^{+\infty} f(x)\,\delta(x-x')\,dx = f(x')$ $\forall$ any differentiable functions.

The following properties are assumed to hold under the integral sign:

1. $\delta(-x) = \delta(x)$

2. $f(x)\dfrac{d}{dx}\delta(x-x') = -\left(\dfrac{d f(x)}{dx}\right)\delta(x-x')$

3. $\dfrac{d\,\delta(x-x')}{dx} = -\dfrac{d}{dx'}\delta(x-x')$

4. $\delta(ax) = \dfrac{\delta(x)}{|a|}$

5. $\delta(f(x)) = \sum_i \dfrac{\delta(x-x_i)}{\left|\dfrac{\partial f}{\partial x}\right|_{x=x_i}}$ $\sim$ the zeros of $f(x)$

6. $\int_{-\infty}^{+\infty} \delta(x-x')\,\delta(x'-x'')\,dx' = \delta(x-x'')$

Important Representation of the Delta Function:

$$\int_{-\infty}^{+\infty} e^{ix(k-k')}\,dx = 2\pi\,\delta(k-k')$$

This formula generalizes $\int_0^{2\pi} e^{imx}\,e^{-inx}\,dx = 2\pi\,\delta_{mn}$

The Fundamental Commutation Relationship (Postulate 5?)

For spinless quantum mechanical particles the position operator $\hat{x}$ & the momentum operator $\hat{p}$ are of fundamental importance. But operators on Hilbert space do not commute. So we need to specify their commutation relationship or their algebra.

So if $\{\theta_i\}$ is the complete set of operators we have some kind of operator algebra:

$$\hat{\theta}_i\hat{\theta}_j = \sum_k c_{ijk}\,\hat{\theta}_k$$

From which we can find out $[\hat{\theta}_i, \hat{\theta}_j]$.

For the $\hat{x}$ & $\hat{p}$ operators the algebra is called the Heisenberg algebra:

$$[\hat{x}, \hat{p}] = i\hbar\,\hat{\mathbb{1}}$$

For three dimensional systems the position & momentum operators are 3-vector operators $\hat{\vec{x}} = (\hat{x}, \hat{y}, \hat{z})$ & $\hat{\vec{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$ and the Heisenberg algebra becomes

$$[\hat{x}_i, \hat{p}_j] = i\hbar\,\delta_{ij}\,\hat{\mathbb{1}}.$$

The Quantization of a classical system:

The Heisenberg algebra $[\hat{x}, \hat{p}] = i\hbar$ is the quantum analog of the Poisson bracket relation

$$\{x, p\} = 1$$

of classical Hamiltonian dynamics.

Given the Hamiltonian function (the energy function) $H(x,p)$ of a classical mechanical system we can specify the quantum Hamiltonian operator by by the replacement $x \longrightarrow \hat{X}$, $p \longrightarrow \hat{P}$ in $H(x,p)$ and thus obtain

$$H(x,p) \longrightarrow \hat{H}(\hat{x},\hat{p})$$

Comment:

1. If the classical Hamiltonian has terms which are a mixture of x & p then the quantal version is not unique as there may be operator ordering choices. $\exists$ various recipes for such cases. In this course we shall not deal with such Hamiltonians.

A typical classical Hamiltonian has the form:

$$H = \frac{p^2}{2m} + V(x)$$

And so we get their quantum analog as

$$\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{x})$$

To find the position representation of $\hat{H}$ we first need to find the position space representation of $\hat{P}$:

$$[\hat{X}, \hat{P}] = i\hbar$$

$$\langle x|[\hat{X},\hat{P}]|x'\rangle = i\hbar \; \delta(x-x')$$

$$\text{LHS} = \langle x|(\hat{X}\hat{P} - \hat{P}\hat{X})|x'\rangle = \int dx'' \{\langle x|\hat{X}|x''\rangle\langle x''|p|x'\rangle - \langle x|\hat{p}|x''\rangle\langle x''|\hat{X}|x'\rangle\}$$

$$= \int dx'' \{\delta(x-x'')\, x''\, \hat{P}_{x''x'} - \hat{P}_{xx''}\, x'\delta(x''-x')\}$$

$$= x\hat{P}_{xx'} - x'\hat{P}_{xx'} = (x-x')\hat{P}_{xx'}$$

Thus we have $(x-x')P_{xx'} = i\hbar\,\delta(x-x')$

Using the delta function identity $f(x)\frac{d\delta(x-x')}{dx} = -\frac{df(x)}{dx}.\delta(x-x')$

we see that if we set $P_{xx'} = -i\hbar\frac{\partial}{\partial x}\delta(x-x')$

Then $(x-x')P_{xx'} = -i\hbar(x-x')\frac{\partial}{\partial x}\delta(x-x') = i\hbar\,\delta(x-x')$.

So, we conclude:
$$\boxed{P_{xx'} = -i\hbar \frac{\partial}{\partial x} \delta(x-x')}$$

Dropping the delta function:

When we have an equation such as
$$\hat{P}|\psi\rangle = |\phi\rangle$$
we can write it as
$$\int dx'\, P_{xx'} \psi(x') = \phi(x)$$
$$\Rightarrow \int dx' \, -i\hbar \frac{\partial}{\partial x} \delta(x-x') \psi(x') = \phi(x)$$

Now using $\frac{d}{dx}\delta(x-x') = -\frac{d}{dx'}\delta(x-x')$ we get
$$\int dx' \, +i\hbar \frac{\partial}{\partial x'} \delta(x-x') \psi(x') = \phi(x)$$
$$\Rightarrow -i\hbar \int dx' \, \delta(x-x') \frac{\partial}{\partial x'} \psi(x') = \phi(x)$$
$$\Rightarrow -i\hbar \frac{\partial \psi(x)}{\partial x} = \phi(x)$$

This inspires us to conclude that in the position representation
$$\hat{X} \longrightarrow x$$
$$\hat{P} \longrightarrow -i\hbar \frac{\partial}{\partial x}$$

Thus $\hat{H} = \frac{\hat{P}^2}{2m} + V(\hat{X}) \longrightarrow \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

The schrödinger equation in position representation:

Using the above replacements in the abstract schrödinger equation we get in the position rep:
$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x)\psi(x,t)$$

In 3D:
$$\boxed{i\hbar \frac{\partial}{\partial t}\psi(\vec{x},t) = -\frac{\hbar^2}{2m}\nabla^2 \psi(\vec{x},t) + V(\vec{x})\psi(\vec{x},t)}$$

Hermitian and Self-Adjoint Operators

For finite dimensional Hilbert spaces there is no difference between Hermitian and self-adjoint operators. Following the finite dimensional case, we define for the infinite dimensional case $\hat{O}$ is hermitian if its integral kernel satisfies

$$\hat{O}_{xx'} = \underline{\hat{O}^{\dagger}_{xx'} \equiv \hat{O}^{*}_{x'x}}$$

Defines Hermitian adjoint of integral kernel

This is implied by the self-adjoint condition but not vice-versa:

Let $\hat{O}$ is self-adjoint. Then we have

$$\langle\psi|\hat{O}|\phi\rangle = \langle\psi|\hat{O}^{\dagger}|\phi\rangle.$$

Recall

$$P_{xx'} = -i\hbar \frac{\partial}{\partial x}\delta(x-x')$$

Let us take $\hat{O} = \hat{P}$ then we get:

$$\langle\psi|\hat{P}|\phi\rangle = \int_{-\infty}^{+\infty} dx\,dx' \langle\psi|x\rangle\langle x|\hat{P}|x'\rangle\langle x'|\phi\rangle$$

$$= \int_{-\infty}^{+\infty} dx\,dx'\, \psi^{*}(x)\left\{-i\hbar \frac{\partial}{\partial x}\delta(x-x')\right\}\phi(x')$$

$$= +i\hbar \int_{-\infty}^{+\infty} dx\,dx'\, \psi^{*}(x)\left\{\frac{\partial}{\partial x'}\delta(x-x')\right\}\phi(x')$$

$$= -i\hbar \int_{-\infty}^{+\infty} dx\,dx'\, \psi^{*}(x)\,\delta(x-x')\,\frac{\partial}{\partial x'}\phi(x')$$

$$= -i\hbar \int_{-\infty}^{+\infty} dx\, \psi^{*}(x)\,\frac{\partial\phi(x)}{\partial x}$$

$$= -i\hbar \int_{-\infty}^{+\infty} dx\, \frac{\partial}{\partial x}\left(\psi^{*}(x)\phi(x)\right) + i\hbar \int_{-\infty}^{+\infty} dx\, \frac{\partial\psi^{*}(x)}{\partial x}\,\phi(x)$$

$$\text{RHS} = \langle\psi|\hat{P}^{\dagger}|\phi\rangle = \int dx'\,dx\, \psi^{*}(x')\,\hat{P}^{\dagger}_{x'x}\,\phi(x)$$

$$= \int dx'\,dx\, \psi^{*}(x')\,\hat{P}^{*}_{xx'}\,\phi(x)$$

$$= \int dx'\,dx\, \psi^{*}(x')\left\{-i\hbar \frac{\partial}{\partial x}\delta(x-x')\right\}^{*}\phi(x)$$

$$= i\hbar \int dx'\,dx\ \psi^*(x') . \frac{\partial}{\partial x} \delta(x-x') . \ \phi(x)$$

$$= i\hbar \int dx\,dx' \ \frac{\partial}{\partial x'} \psi^*(x') . \delta(x-x')\, \phi(x)$$

$$= i\hbar \int dx \ \frac{\partial \psi^*(x)}{\partial x} . \ \phi(x)$$

Thus we see the $\langle \psi | \hat{P} | \phi \rangle = \langle \psi | \hat{p}^\dagger | \phi \rangle$ if, in addition to $\hat{P}^\dagger_{xx'} = \hat{P}_{xx'}$ we

we also have $i\hbar \int_{-\infty}^{+\infty} dx \ \frac{\partial}{\partial x} \left(\psi^*(x) \phi(x) \right) = 0$

But this implies $\psi^*(x)\, \phi(x) \Big|_{-\infty}^{+\infty} = 0$

For normalizable states we then want the wave functions to go to zero sufficiently rapidly so that $\langle \psi | \psi \rangle = \int dx \ \psi^*(x)\, \psi(x)$ is finite.

In conclusion, the momentum operator is hermitian but it is only self-adjoint if we restrict its domain of operation on square-integrable functions.

<u>The L^2-norm:</u>

The norm $\langle \psi | \psi \rangle = \int dx \ |\psi(x)|^2$ is known as the L^2 norm. We use the L^2-norm to impose the vanishing of normalizable states because of the Born rule.

<u>The Momentum Eigenstates</u>

The eigenvalue equation for the momentum operator is:

$$\hat{P} |p\rangle = p |p\rangle \ , \quad p \in \mathbb{R}$$

We have seen that the momentum operator in the position basis is given by $\hat{P} = -i\hbar \frac{\partial}{\partial x}$

Thus the above equation in the position representation is

$$-i\hbar \frac{\partial}{\partial x} \psi_p(x) = p\, \psi_p(x) \quad \text{where} \quad \psi_p(x) = \langle x | p \rangle$$

The solution to this equation is $\psi_p(x) = c\, e^{ipx/\hbar}$

c is a constant. Since we expect $\langle p|p'\rangle = \delta(p-p')$ we can write

$$\langle p|p'\rangle = \int dx\, \psi_p^*(x)\, \psi_{p'}(x) = |c|^2 \int dx\, e^{+i(p'-p)x/\hbar}$$

But since $\int dx\, e^{i(p'-p)x} = 2\pi\, \delta(p-p')$

we get $\quad c = \dfrac{1}{\sqrt{2\pi\hbar}}$

And so $\psi_p(x) = \dfrac{1}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar}$ are the properly normalized momentum eigenstates.

<u>Stationary States:</u>

The eigenvectors of the Hamiltonian operator are known as stationary states. Because of the central role of $\hat{H}$ in the Schrödinger equation these states play a central role in quantum mechanics. In a sense, if one can find these eigenstates one has solved the problem.

Let E_m be the eigenvalues of $\hat{H}$. E_m may or may not be a continuous spectrum.

$$\hat{H}|\phi_m\rangle = E_m|\phi_m\rangle$$

Now suppose we know E_m & $|\phi_m\rangle$, i.e., we have diagonalized the Hamiltonian operator. Then we can express any state $|\psi(t_0)\rangle$ at time t_0 in terms of $|\phi_m\rangle$:

$$|\psi(t_0)\rangle = \sum_m c_m\, |\phi_m\rangle$$

where $c_m = \langle \phi_m|\psi(t_0)\rangle$

Now if I apply the time evolution operator $\hat{U}(t-t_0)$ on $|\psi(t_0)\rangle$ we get

$$|\psi(t)\rangle = U(t-t_0)\,|\psi(t_0)\rangle$$

$$= e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} \sum_m c_m\, |\phi_m\rangle$$

$$= \sum_m c_m e^{-\frac{i}{\hbar}\hat{H}(t-t_0)} |\phi_m\rangle$$

$$|\psi(t)\rangle = \sum_m c_m e^{-\frac{i}{\hbar}E_m(t-t_0)} |\phi_m\rangle$$

In the position representation $\psi(x,t) = \sum_m c_m e^{-\frac{i}{\hbar}E_m(t-t_0)} \phi_m(x)$

In particular $\phi_m(x,t) = e^{-\frac{i}{\hbar}E_m(t-t')} \phi_m(x)$ are the stationary states.

The time dependence of stationary states is particularly simple.

The Time-Independent Schrödinger Equation:

If we plug the stationary state solution into the Schrödinger equation we get:

$$E\,\phi_m(x,t) = \hat{H}\,\phi_m(x,t)$$

Because of the central role played by the energy eigenvalue problem we call the following equation, time-independent Schrödinger equation:

$$\boxed{\hat{H}\psi = E\psi}$$

It's solutions gives us the stationary states under time translation.

Momentum Space Representation & Fourier Transform

Analogous to position space representations of operators and state vectors we have momentum space representations of the same operators. In analogy to the position space analysis we can derive

$$\hat{p} \longrightarrow p$$

$$\& \qquad \hat{x} \longrightarrow i\hbar \frac{\partial}{\partial p}$$

On the other hand the momentum space wave function for the state $|\psi\rangle$ is given by:

$$\tilde{\psi}(p) = \langle p|\psi\rangle$$

We can easily relate it to the position space wave function $\psi(x) = \langle x|\psi\rangle$ by

$$\tilde{\psi}(p) = \langle p|\psi\rangle = \int dx\, \langle p|x\rangle\langle x|\psi\rangle$$

Note that $\langle x|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$

Then

$$\boxed{\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(x)\, e^{-ipx/\hbar}\, dx}$$

Using $\int_{-\infty}^{+\infty} e^{ix(p-p')/\hbar}\, dx = 2\pi\hbar\, \delta(p-p')$ we get

The Fourier Integral Theorem

$$\boxed{\int \tilde{\psi}(p)\, e^{+ipx'/\hbar}\, dp = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \psi(x)\, e^{ip(x-x')/\hbar}\, dp\, dx}$$

$$= \sqrt{2\pi\hbar} \int_{-\infty}^{+\infty} \psi(x)\, \delta(x-x')\, dx$$

$$\Rightarrow \boxed{\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{ipx/\hbar}\, \tilde{\psi}(p)\, dp}$$

$\psi(x)$ & $\tilde{\psi}(p)$ are Fourier transforms of each other.

The Fourier Integral Representation of Free Wave-Packets:

Let us consider a free particle in 1D. That means $V(x) = 0$ in $\hat{H}$:

$$\hat{H} = \frac{\hat{p}^2}{2m}$$

The solutions to the eigenvalue equation:

$$\hat{H}\psi = E\psi$$

are also solutions to the momentum eigenvalue eqn:

$$\hat{p}\psi = p\psi$$

Thus $\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}(Et + px)}$

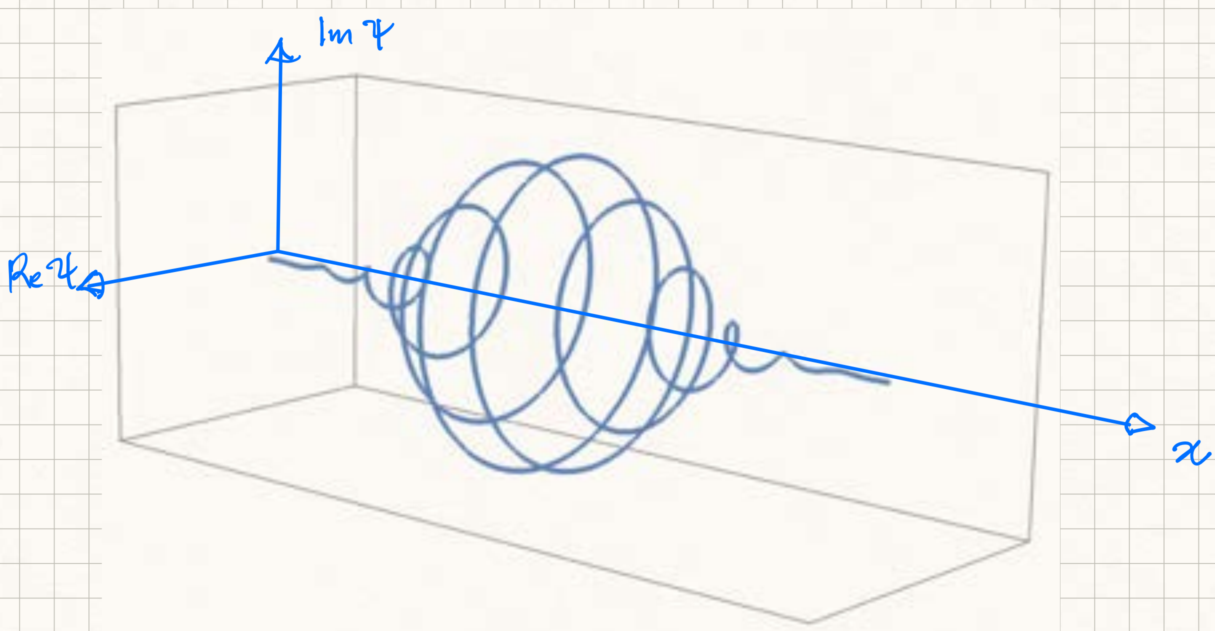
This is a plane wave solution with $E = \frac{p^2}{2m}$. It is not normalizable.

But because of the linearity of the Schrödinger equation linear combinations of plane-waves is also a solution. Thus one can describe wave-packets in which particles are localized in terms of L^2-integrable functions using Fourier integral of plane waves:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int dp \; \tilde{\Psi}(p) \; e^{-\frac{i}{\hbar}(Et - px)}$$

Plane waves ~ non-normalizable

Wave-packet ~ normalizable



An Example of a Wavepacket at t=0

The figure above shows an example of a wavepacket with a Gaussian profile:

$$\Psi(x,0) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} \; e^{-\frac{(x-x_0)^2}{2\sigma^2}} \; e^{i p_0 x/\hbar}$$

$x_0 \longrightarrow$ The centre of the wave packet at time $t=0$.

$p_0 \longrightarrow$ The average momentum (see below).

The Time-Evolution Operator in the Position Representation:

The time evolution operator $\mathcal{U}(t-t_0)$ evolves a state $|\psi(t_0)\rangle$ at time t_0 to a state $|\psi(t)\rangle$ at time t:

$$|\psi(t)\rangle = \mathcal{U}(t-t_0)|\psi(t_0)\rangle$$

We want to understand what this equation looks like in the position representation. Before doing that we want to list some of the more important properties of $\mathcal{U}(t,t_0)$ {the evo. operator in the more general case}:

1. $\hat{\mathcal{U}}(t,t) = \hat{\mathbb{1}}$

2. $\hat{\mathcal{U}}(t,t_0)^{-1} = \hat{\mathcal{U}}(t_0,t)$.

$$|\psi(t)\rangle = \hat{\mathcal{U}}(t,t_0)|\psi(t_0)\rangle \Rightarrow |\psi(t_0)\rangle = \hat{\mathcal{U}}^{-1}(t,t_0)|\psi(t)\rangle$$

But $|\psi(t_0)\rangle = \hat{\mathcal{U}}(t_0,t)|\psi(t)\rangle \Rightarrow \hat{\mathcal{U}}^{-1}(t,t_0) = \hat{\mathcal{U}}(t_0,t)$

3. $\hat{\mathcal{U}}(t,t_0) = \hat{\mathcal{U}}(t,t')\hat{\mathcal{U}}(t',t_0)$ Markovian Property

Now we compute $K(x,t;x_0,t_0) \equiv \langle x|\mathcal{U}(t,t_0)|t_0\rangle$

$K(x,t;x_0,t_0)$ is known as Green's function or the propagator. $\mathcal{U}(t,t_0)$ is also called the propagator.

$$K(x,t;x_0,t_0) = \langle x|\mathcal{U}(t,t_0)|x_0\rangle$$

Let us now take a time t' such that $t_0 < t' < t$. Since we can write

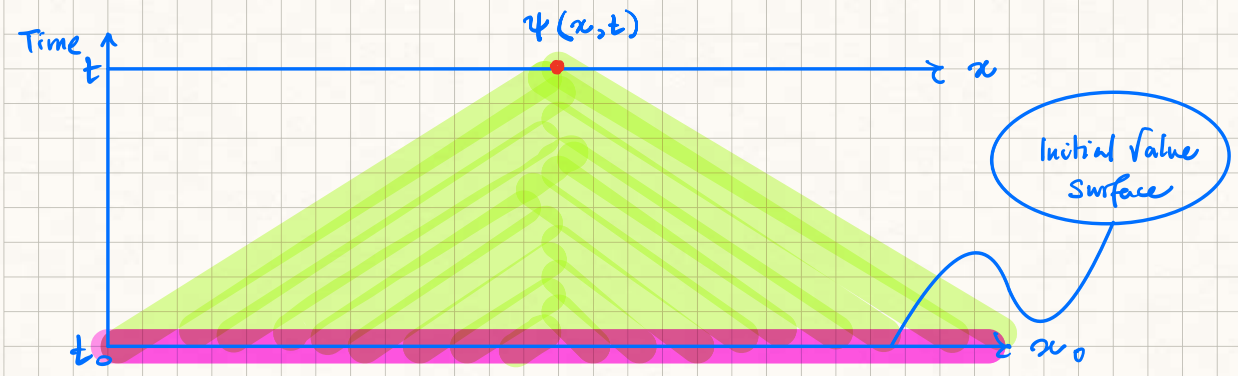
$$\mathcal{U}(t,t_0) = \mathcal{U}(t,t')\mathcal{U}(t',t_0)$$

We write
$$K(x,t;x_0,t_0) = \int dx' \langle x|\mathcal{U}(t,t')|x'\rangle\langle x'|\mathcal{U}(t',t_0)|x_0\rangle$$
$$= \int dx' \, K(x,t;x',t')\, K(x',t';x_0,t_0)$$

Interpretation of K:

K propagates the wavefunction forward in time. The wavefunction at time t at position x is the result of interference of the wavefunction on the whole spatial surface at t' propagated forward in time according to K:

$$\psi(x,t) = \int_{-\infty}^{+\infty} dx_0 \; K(x,t;x_0,t_0)\, \psi(x_0,t_0)$$



Comments:

1. $K(x,t;x_0,t_0)$ may be thought of as the time evolved wavefunction of a unit wave-funtion $\psi(x_0,t_0) = \delta(x-x_0)$. This justifies calling it a Green's function.

2. If we subdivide $t-t_0$ into an infinite number of subintervals we get the path-integral representation of $K(x,t;x_0,t_0)$.

3. The propagator for the free one-dimensional free particle is: [Assignment 1]

$$K(x,t;x_0,t_0) = \left[\frac{m}{2\pi i\hbar\,(t-t_0)}\right]^{\frac{1}{2}} \exp\left\{\frac{im\,(x-x_0)^2}{2\hbar\,(t-t_0)}\right\}$$

Averages & Expectation Values of Observables:

According to quantum mechanics if we measure an observable represented by a self-adjoint operator $\hat{A}$ we are only guaranteed a probility distribution $p_\psi(a_i)$ that we will obtain the result a_i. Since this distribution depends on the state $|\psi\rangle$ of the system we label $p_\psi(a_i)$ with ψ (This is not the standard practice).

Given $\hat{A}$ & $|\psi\rangle$, the problem is how do we calculate $p_\psi(a_i)$? Here we adopt a frequentist approach.

To experimentally determine $p_\psi(a_i)$ we first prepare a large collection of systems all in the state $|\psi\rangle$. Then as we measure $\hat{A}$ for those systems [the collection is called an ensemble] we build up a histogram of a_i. In the limit in which the sample size $\longrightarrow \infty$, we identify the histogram to $p_\psi(a_i)$.

Mathematically, if we are given $|\psi\rangle$ we can express it in the eigenbasis of $\hat{A}$:

$$|\psi\rangle = \sum_i c_i |a_i\rangle$$

Then according to the Born rule:

$$P_\psi(a_i) = |c_i|^2$$

which is given by $P_\psi(a_i) = |\langle a_i|\psi\rangle|^2$

Verify : $|\langle a_i|\psi\rangle|^2 = |\langle a_i| \sum_j c_j |a_j\rangle|^2 = |\sum_j c_j \delta_{ij}|^2 = |c_i|^2.$

<u>Note added</u>

If the eigenvalue is degenerate then to compute $p_\psi(a_i)$ one needs to first project down to the eigenspace by using the projection operator $\hat{P}_i = \sum_k |a_i^{(k)}\rangle\langle a_i^{(k)}|$ where the k index labels the different eigenvectors $|a_i^{(k)}\rangle$ corresponding to the eigenvalue a_i. Then we find $P_\psi(a_i) = \sum_k |c_i^{(k)}|^2$ where $|\psi\rangle = \sum_{i,k} c_i^{(k)} |a_i^{(k)}\rangle$ with the i-index labelling the different eigenvalues while k refers to the different eigenvectors belonging to a_i.

A characterization of the distribution of a_i obtained from the above ensemble is the average value of a_i:

$$\bar{a}\Big|_\psi = \frac{\sum_i a_i\, p_\psi(a_i)}{\sum_i p_\psi(a_i)}$$

This is the standard expression for average. Quantum mechanically this equivalent to

$$\langle \hat{A} \rangle_\psi \equiv \frac{\langle \psi | \hat{A} | \psi \rangle}{\langle \psi | \psi \rangle}.$$

$$\langle \hat{A} \rangle_\psi = \frac{\sum_{i,j} (c_i^* \langle a_i |) \hat{A} (c_j | a_j \rangle)}{\sum_{i,j} c_i^* c_j \langle a_i | a_j \rangle}$$

$$= \frac{\sum_{i,j} c_i^* c_j a_j \delta_{ij}}{\sum_{i,j} c_i^* c_j \delta_{ij}}$$

$$= \frac{\sum_i |c_i|^2 a_i}{\sum_i |c_i|^2} = \frac{\sum_i P_\psi(a_i) a_i}{\sum_i P_\psi(a_i)}$$

The Standard Deviation or The Uncertainty

The average is the first moment but it doesn't tell us any thing about the spread of the eigenvalue distribution of $\hat{A}$ in the state $|\psi\rangle$. That is given by the standard deviation or the variance or the uncertainty of $\hat{A}$:

$$(\Delta \hat{A})_\psi = \langle (\hat{A} - \langle \hat{A} \rangle_\psi)^2 \rangle_\psi^{1/2} = \langle (\hat{A}^2 - 2\hat{A} \langle \hat{A} \rangle_\psi + \langle \hat{A} \rangle_\psi^2) \rangle^{1/2}$$

$$= \sqrt{\langle \hat{A}^2 \rangle_\psi - 2 \langle \hat{A} \rangle_\psi^2 + \langle \hat{A} \rangle_\psi^2}$$

$$= \sqrt{\langle \hat{A}^2 \rangle_\psi - \langle \hat{A} \rangle_\psi^2}$$

From now on we shall drop the subscript ψ if there is no room for confusion.

In quantum mechanics, if we have two observables $\hat{A}$ & $\hat{B}$ st $[\hat{A}, \hat{B}] \neq 0$ then we say they are incompatible observables. If we try to measure $\hat{A}$ & $\hat{B}$ simultaneously then ΔA & ΔB will depend on $|\psi\rangle$. But quantum mechanics puts a limit on how precisely $\hat{A}$ & $\hat{B}$ can be measured. It turns out that if one tries to minimize $\Delta \hat{A}$ by tuning $|\psi\rangle$, the uncertainty, ΔB, in $\hat{B}$ increases.

If $[\hat{A}, \hat{B}] = \hat{C}$, then one can show that the product of ΔA & ΔB has a minimum bound

$$\boxed{(\Delta A)^2 (\Delta B)^2 \geq \left(\frac{1}{2i} \langle \hat{C} \rangle\right)^2}$$

This is the generalized uncertainty principle. For $\hat{A} = \hat{X}$ & $\hat{B} = \hat{P}$ one gets:

$$\boxed{\Delta x \, \Delta p \geq \frac{\hbar}{2}}$$

with the inequality saturated for $\psi(x) \sim e^{-(x-x_0)^2/2\sigma}$ [Gaussian wave functions.]

Comment:

It should be noted that the uncertainty principle derived here is different from the one derived by Heisenberg. The one derived here is a mathematical expression whereas Heisenberg's original derivation was related to what he thought was experimentally possible.