momenta p_i to operators (which we denote with a hat):

$$(q_i, p_j) \longrightarrow (\hat{q}_i, \hat{p}_j).$$

Together with the promotion of the Poisson bracket to the commutator by:

$$\{\ ,\ \}_{\text{Classical}} \longrightarrow \frac{1}{i\hbar}[\ ,\ ]_{\text{Quantum}}.$$

i.e. $[\hat{q}_i, \hat{p}_j] = i\hbar\, \delta_{ij}$.

Where $\hbar \equiv h/2\pi$ and h is Planck's constant.

In particular $\mathcal{H} \rightarrow \hat{H} = \sum_i \frac{\hat{p}_i^2}{2m_i} + V(\hat{q})$.

In quantum mechanics physical observables are represented by operators which act on a Hilbert space of quantum states. The states include eigenstates for the operators and the corresponding eigenvalue represents the value of a measurement. E.g. we may denote a position eigenstate with eigenvalue x (of $\hat{X}$ the position operator) by $|x\rangle$ then:

$$\hat{X}|x\rangle = x|x\rangle.$$

General states are formed from superpositions of eigenstates:

e.g. $|\psi\rangle = \int dx\, \psi(x)|x\rangle$.

or $|\psi\rangle = \sum_i \psi_i |q_i\rangle$

N.B. For a one particle system let $\varphi(q) \equiv c(q)|q\rangle$

then $\hat{q}\varphi = q\varphi$ and $[\hat{q},\hat{p}]\varphi = i\hbar\varphi$

is satisfied when $\therefore \hat{p} = (-i\hbar)\frac{\partial}{\partial q}$ as

$$
\begin{aligned}
[\hat{q},\hat{p}]\varphi &= (\hat{q}\hat{p}-\hat{p}\hat{q})\,c|q\rangle \\
&= \hat{q}(-i\hbar)\frac{\partial c}{\partial q}|q\rangle - \hat{p}\,cq|q\rangle. \\
&= (-i\hbar)\frac{\partial c}{\partial q}\,q|q\rangle - (-i\hbar)\frac{\partial}{\partial q}(cq)|q\rangle \\
&= +i\hbar\, c|q\rangle \\
&= +i\hbar\,\varphi.
\end{aligned}
$$

For a many particle system we may take the position eigenstates as a basis in Hilbert space and:

$$\varphi(q) \equiv \sum_i c_i(q)|q_i\rangle \qquad \text{and} \qquad \hat{p}_i \equiv (-i\hbar)\frac{\partial}{\partial q_i}.$$

Note that the Hamiltonian:

$$H = \sum \frac{1}{2m_i}p_i^2 + \sum_i V(q_i).$$

becomes:

$$\hat{H} = \sum_i -\frac{\hbar^2}{2m_i}\frac{\partial^2}{\partial q_i^2} + \sum_i V(q_i)$$

Def$^{\underline{n}}$ A Hilbert Space $\mathcal{H}$ is a complex vector space equipped with an inner product $\langle\ ,\ \rangle$ satisfying:

(i.) $\langle \phi, \psi\rangle = \overline{\langle \psi, \phi\rangle}$

(ii.) $\langle \phi, a_1\psi_1 + a_2\psi_2\rangle = a_1\langle\phi,\psi_1\rangle + a_2\langle\phi,\psi_2\rangle$

(iii.) $\langle\phi,\phi\rangle \geq 0 \quad \forall\ \phi\in\mathcal{H}$ if $\langle\phi,\phi\rangle = 0 \Rightarrow \phi = 0.$

The physical states in a system are described by normalised vectors in the Hilbert space i.e. those $\psi \in \mathcal{H}$ s.t. $\langle \psi, \psi \rangle = 1$.

Observables.

Observables are represented by Hermitean operators on $\mathcal{H}$.

Hermitean operators are self-adjoint.

An operator A^* is the adjoint operator of A if:

$$\langle A^* \phi, \psi \rangle = \langle \phi, A\psi \rangle.$$

A self-adjoint operator satisfies $A^* = A$.

Example

(1.) Let $\mathcal{H} = L^2(\mathbb{R})$ i.e. $\psi \in \mathcal{H} \Rightarrow \langle \psi, \psi \rangle < \infty$, and

$$\langle \psi, \phi \rangle \equiv \int_{\mathbb{R}} dq \, \psi^*(q) \phi(q).$$

The momentum operator is self-adjoint as:

$$\begin{aligned}
\langle \psi, \hat{p}\phi \rangle &= \int_{\mathbb{R}} dq \, \psi^*(q) \left(-i\hbar \frac{\partial}{\partial q} \phi(q)\right) \\
&= \int_{\mathbb{R}} dq \, i\hbar \frac{\partial}{\partial q}(\psi^*(q)) \, \phi(q) \\
&= \int_{\mathbb{R}} dq \left(-i\hbar \frac{\partial}{\partial q} \cdot \psi(q)\right)^* \phi(q) \\
&= \langle \hat{p}\psi, \phi \rangle.
\end{aligned}$$

N.B. $\psi(\pm\infty) \to 0$ and $\phi(\pm\infty) \to 0$.

(2.) Hermitian matrices on $\mathbb{C}^n$: $(a_{ij}^*)^T = a_{ij}$

i.e. Let $\langle \underline{x}, \underline{y} \rangle \equiv \underline{x}^\dagger \underline{y}$ then,

$$\langle \underline{x}, \underline{\underline{A}} \cdot \underline{y} \rangle = \underline{x}^{+} \cdot \underline{\underline{A}} \cdot \underline{y}$$

$$= \underline{x}^{+} \cdot \underline{\underline{A}}^{+} \cdot \underline{y} \qquad \text{As } \underline{\underline{A}}^{+} = \underline{\underline{A}}.$$

$$= (\underline{\underline{A}}\, \underline{x})^{+} \cdot \underline{y}$$

$$= \langle \underline{\underline{A}} \cdot \underline{x}, \underline{y} \rangle .$$

Eigenvalues and Eigenvectors.

Let $\underline{\underline{A}}$ be an operator and $\underline{u} \in \mathcal{H}$ be an eigenvector such that:

$$\underline{\underline{A}}\, \underline{u} = \alpha \underline{u} . \qquad \alpha \in \mathbb{C} .$$

The eigenvalues of self-adjoint operators are real.

$$\langle \underline{u}, \underline{\underline{A}}\, \underline{u} \rangle = \langle \underline{u}, \alpha \underline{u} \rangle = \alpha \langle \underline{u}, \underline{u} \rangle$$
$$\parallel$$
$$\langle \underline{\underline{A}}\, \underline{u}, \underline{u} \rangle = \langle \alpha \underline{u}, \underline{u} \rangle = \alpha^{*} \langle \underline{u}, \underline{u} \rangle .$$

$$\Rightarrow \alpha = \alpha^{*} \in \mathbb{R} .$$

The eigenvectors of two different eigenvalues are orthogonal:
($\underline{\underline{A}}$ is self-adjoint).
i.e. let $\underline{\underline{A}}\, \underline{u} = \alpha \underline{u}$ and $\underline{\underline{A}}\, \underline{u}' = \alpha' \underline{u}'$.

then,

$$\langle \underline{u}, \underline{\underline{A}}\, \underline{u}' \rangle = \langle \underline{u}, \alpha' \underline{u}' \rangle = \alpha' \langle \underline{u}, \underline{u}' \rangle$$
$$\parallel$$
$$\langle \underline{\underline{A}}\, \underline{u}, \underline{u}' \rangle = \alpha \langle \underline{u}, \underline{u}' \rangle$$

$$\therefore (\alpha' - \alpha) \langle \underline{u}, \underline{u}' \rangle = 0 \quad \Rightarrow \langle \underline{u}, \underline{u}' \rangle = 0 \quad \text{if} \quad \alpha \neq \alpha' .$$

Theorem. For every self-adjoint operator we can find a complete set of eigenvalues (a basis in $\mathcal{H}$).

The basis may be countable or continuous.
$\Rightarrow \underline{\underline{A}}\,\underline{u}_n = \alpha_n \underline{u}_n$ and every $\varphi \in \mathcal{H}$ may be written $\varphi = \sum \varphi_n \underline{u}_n$.

A Countable Basis.

Suppose $\{\underline{u}_n\}$ is a countable basis (can be put in a 1-to-1 correspondence with the natural numbers). Let $\{\underline{u}_n\}$ be an orthonormal set:

$$\langle \underline{u}_n, \underline{u}_m \rangle = \delta_{nm}$$

Then,

$$\langle \underline{u}_m, \varphi \rangle = \sum_n \langle \underline{u}_m, \varphi_n \underline{u}_n \rangle = \varphi_m .$$

Hence,

$$\varphi = \sum_n \langle \underline{u}_n, \varphi \rangle \underline{u}_n .$$

Let us now adopt the bra-ket notation of Dirac:

$$\varphi \rightarrow |\varphi\rangle$$

$$\underline{u}_n \rightarrow |u_n\rangle$$

$$\langle \underline{u}_n, \varphi \rangle \longleftrightarrow \langle u_n | \varphi \rangle$$

So we now write:

$$\varphi = \sum_n |u_n\rangle \langle u_n | \varphi \rangle$$

$$\Rightarrow \quad \sum_n |u_n\rangle\langle u_n| = \mathbb{1}_{\mathcal{H}} . \quad \text{(The Id. operator).}$$

This is known as the completeness operator.

In the $\{\underline{u}_n\}$ basis the inner product is:

$$\langle \varphi, \psi \rangle = \langle \varphi | \psi \rangle = \sum_n \langle \varphi | u_n \rangle \langle u_n | \psi \rangle = \sum_n \varphi_n^* \psi_n$$

We may insert an operator B between two states:

$$\langle \psi, B\psi \rangle = \langle \psi | B | \psi \rangle$$

$$= \sum_{n,m} \langle \psi | u_n \rangle \langle u_n | B | u_m \rangle \langle u_m | \psi \rangle .$$

$$\equiv \sum_{n,m} \psi_n^* B_{nm} \psi_m .$$

Where B_{mn} are the matrix elements of B, in the $\{\underline{u}_n\}$ basis.

Thus if $\{\underline{u}_n\}$ were eigenvectors of an operator A then:

$$A_{nm} = \begin{pmatrix} \alpha_1 & & \\ & \alpha_2 & 0 \\ 0 & \ddots & \alpha_D \end{pmatrix}_{nm} = \alpha_n \delta_{nm} .$$

Theorem. Given any two commuting self-adjoint operators A and B:

$[A, B] = 0$ one can find a basis $\{\underline{u}_n\}$ such that A

and B are simultaneously diagonalizable:

$$A \underline{u}_n = \alpha_n \underline{u}_n \quad \text{and} \quad B\underline{u}_n = \beta_n \underline{u}_n$$

i.e. A is self-adjoint hence $\exists$ a basis of eigenvectors $\{\underline{u}_n\}$

such that $A\underline{u}_n = \alpha_n \underline{u}_n$.

Now $\quad AB\underline{u}_n = BA\underline{u}_n = \alpha_n B\underline{u}_n$

$\therefore \quad B\underline{u}_n$ is in the eigenspace of A

$$B\underline{u}_n = \beta_n \underline{u}_n$$

$$\therefore \quad A(B\underline{u}_n) = \beta_n \alpha_n \underline{u}_n$$

And evidently $\underline{u}_n$ is a basis of eigenvectors for B too.

Example.

Let $(\hat{x}, \hat{y}, \hat{z})$ be the position operators of a particle in $\mathbb{R}^3$ then $[\hat{x}, \hat{y}] = 0$, $[\hat{x}, \hat{z}] = 0$, $[\hat{y}, \hat{z}] = 0$ (using the canonical quantum commutation rules) and hence are simultaneously diagonalizable. One can say the same for p_x, p_y and p_z.

Probabilistic Interpretation.

If a system is in a state ψ the probability to find it in the eigenstate ϕ_i is:

$$P(\psi, \phi_i) \equiv \frac{|\langle \psi, \phi_i \rangle|^2}{\langle \psi, \psi \rangle}.$$

Where ϕ_i are an orthonormal basis of eigenstates for some self-adjoint operator.

A Continuous Basis (or Continuous Spectrum).

If an operator A has eigenstates $\underline{u}_\alpha$ where the eigenvalue α is a continuous variable then an arbitrary state in the Hilbert space is:

$$|\varphi\rangle \equiv \int d\alpha \, \phi_\alpha |u_\alpha\rangle$$

Then,

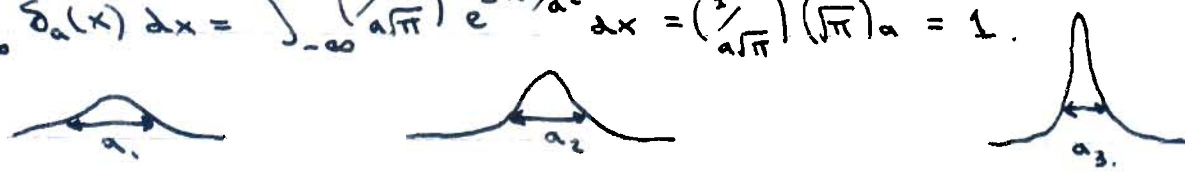
$$\langle u_\beta | \varphi \rangle = \int d\alpha \, \langle u_\beta | u_\alpha \rangle \phi_\alpha = \phi_\beta$$

The mathematical object that satisfies the above statement is the Dirac delta function:

$$\langle u_\beta | u_\alpha \rangle = \delta(\alpha - \beta).$$

Formally it is a distribution or measure that is equal to zero everywhere apart from 0 when $\delta(0) = +\infty$. One may regard it as the limit of a sequence of functions having a spike at the origin: $\delta_a(x) = \frac{1}{a\sqrt{\pi}} e^{-x^2/a^2}$ so that as $a \to 0$ the limit of the Gaussians is the Dirac delta function, as

$$\int_{-\infty}^{\infty} \delta_a(x)\, dx = \int_{-\infty}^{\infty} \left(\frac{1}{a\sqrt{\pi}}\right) e^{-x^2/a^2} dx = \left(\frac{1}{a\sqrt{\pi}}\right)\left(\sqrt{\pi}\right)a = 1.$$



Then $$\int_{-\infty}^{\infty} f(x)\, \delta(x)\, dx = f(0).$$ But the notation here is an abuse.

The eigenstate $|u_\alpha\rangle$ is no longer a vector in the Hilbert space because:

$$\langle u_\alpha | u_\beta \rangle = \delta(\alpha - \beta) \Rightarrow \langle u_\alpha | u_\alpha \rangle = \infty.$$

However with the integral notation in place we can use them as basis vectors:

$$\langle \varphi | \psi \rangle = \int d\alpha \, \langle \varphi | u_\alpha \rangle \langle u_\alpha | \psi \rangle$$

$$\Rightarrow \int d\alpha \, |u_\alpha\rangle\langle u_\alpha| = \mathbb{1}_{\mathcal{H}}.$$