General Structure of QM

In this final lecture, we present a simplified version of the general structure of quantum mechanics.

The objective is to illustrate, in a more direct way, the connection between linear algebra and quantum mechanics.

The general structure of wave mechanics placed equal weight on the operators that represent the observables, and on their eigenfunctions.

This allows one to go far toward finding the eigenvalue spectrum using the operators alone.
The Hamiltonian Operator

The state of a physical system is described by a wave function, which contains all the information about the system. The wave function depends on time, and its temporal development is given by

\[ i\hbar \frac{\partial \Psi(x, t)}{\partial t} = H \Psi(x, t) \]

The wave function \( \Psi(x, t) \) is acted on by an operator \( H \), the Hamiltonian, which plays a central role in quantum mechanics. The operator \( H \) for a simple system of a single particle in a potential \( V \) has the form

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

If \( V(x) \) does not have an explicit time dependence, the wave equation can be solved by

\[ \Psi(x, t) = \psi_E(x)e^{-iEt/\hbar} \]

where

\[ H\psi_E(x) = E\psi_E(x) \]

The solutions of this equation are called the eigenfunctions of the Hamiltonian, and \( E \) are the eigenvalues.
Eigenfunctions and Eigenvalues

There are two important properties of eigenfunctions of $H$:

- Eigenfunctions corresponding to different eigenvalues are orthogonal, that is

$$\int \psi_E(x)^* \psi_E(x) dx = 0 \quad E \neq E'$$

- The eigenfunctions form a complete set. An arbitrary function $\psi(x)$ that is square integrable so that

$$\int \psi(x)^* \psi(x) dx < \infty$$

may be expanded in terms of eigenfunctions of the Hamiltonian

$$\psi(x) = \sum_E c_E \psi_E(x)$$
Spectrum

The spectrum of $H$ may be discrete. If the potential $V(x)$ goes to zero as $x \to \infty$, the eigenvalues may be discrete as well as form a continuum. This occurs for an attractive potential, deep enough to form one or more bound states. If this is the case, then it is the total set of continuum and discrete eigenfunctions that are required for the complete set. In that case

$$\psi(x) = \sum_n c_n \psi_n(x) + \int c(p) \psi_p(x) dp$$

Here the integer $n$ labels the bound states and $p$ labels the continuum states.

The eigenfunctions can be normalized. The orthomomality conditions are

$$\int \psi_m(x)^* \psi_n(x) dx = \delta_{mn}$$

$$\int \psi_q(x)^* \psi_p(x) dx = \delta(p - q)$$

$$\int \psi_n(x)^* \psi_p(x) dx = 0$$
Wave Function $\Psi(x, t)$

The wave function $\Psi(x, t)$ can be determined by noting that each eigenfunction has a simple time dependence given by

$$\psi_E(x, t) = \psi_E(x) e^{-iEt/\hbar}$$

It follows from this that

$$\Psi(x, t) = \sum_E c_E \psi_E(x) e^{-iEt/\hbar}$$

More generally,

$$\Psi(x, t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar}$$

$$+ \int c(p) \psi_p(x) e^{-i p^2 t / 2m \hbar} dp$$
Other Variables

Just as the energy is an eigenvalue of the energy (Hamiltonian) operator $\hat{H}$, the momentum is an eigenvalue of the momentum operator $\hat{p}$. The momentum operator eigenvalue equation has the form

$$\hat{p}\psi_p(x) = \frac{\hbar}{i} \frac{d}{dx} \psi_p(x) = p\psi_p(x)$$

The eigenfunctions form a continuum $(-\infty < p < \infty)$, and the eigenfunctions take the form

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

The eigenfunctions form an orthonormal set

$$\int_{-\infty}^{\infty} \psi_{p_1}(x) \ast \psi_{p_2}(x) dx = \delta(p_1 - p_2)$$

and the expansion theorem is usually written in the form

$$\psi(x) = \int_{-\infty}^{\infty} \psi(p) \psi_p(x) dp$$
The Expansion Postulate

For an arbitrary observable, which we denote by $Q$, there will be eigenfunctions corresponding to the real eigenvalue $q$,

$$\hat{Q}\psi_q(x) = q\psi_q(x)$$

The eigenfunctions form an orthogonal set, and they can be normalized so that

$$\int \psi_{q_1}(x)^*\psi_{q_1}(x)dx = \delta_{q_1q_2}$$

Here $\delta_{q_1q_2}$ is a Kronecker delta for discrete eigenvalues and a Dirac delta function for continuous eigenvalues.

The eigenfunctions $\psi_q(x)$ also form a complete set, which is equivalent to the statement that an arbitrary (square integrable) function $\psi(x)$ may be expanded in terms of the $\psi_q(x)$,

$$\psi(x) = \sum_q c_q \psi_q(x)$$

with

$$c_q = \int \psi_q(x)^*\psi(x)dx$$
The Expansion Coefficients

The interpretation of the expansion coefficients $c_q$ is the following: If the observable $Q$ is measured for a collection of systems each of which is described by the wave function $\psi(x)$, which is normalized to unity, so that

$$\int \psi(x)\psi(x) \, dx = 1$$

then

1. The result of any given measurement can only be one of the eigenvalues $q$.
2. The probability that the eigenvalue $q$ will be found, or, equivalently, the fraction of systems in the collection that will be found to have the eigenvalue $q$, is $|c_q|^2$.
3. After a measurement on a member of the collection yields a given eigenvalue $a_1$, for example, then that particular system in the collection must be projected by the measurement into the state $\psi_{q_1}(x)$. It is only in this way that we can be sure that a subsequent measurement of the observable $Q$ gives the same result.
The Vector Space Analogy

The expansion theorem may be viewed as a generalization of the expansion of a vector $\vec{A}$ in terms of orthonormal unit vectors in an $N$-dimensional vector space

$$\vec{A} = A_1\hat{i}_1 + A_2\hat{i}_2 + \cdots + A_N\hat{i}_N$$

The unit vectors satisfy

$$\hat{i}_k \cdot \hat{i}_l = \delta_{kl}$$

and they are the analogs of the eigenfunctions $\psi_q(x)$. The coefficients $A_n$ are given by

$$A_n = \hat{i}_n \cdot \vec{A}$$

and these are the analogs of the $c_q$. Thus, $c_q$ can be referred as the projections of $\psi(x)$ along the basis vectors $\psi_q(x)$. 

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The Hilbert Space

The analogy between wave functions $\psi(x)$ and $N$-dimensional vectors is actually quite profound. In both cases we deal with linear spaces: just as a sum of any two vectors in the vector space yields a vector $\vec{A} + \vec{B} = \vec{C}$ so is the sum of two wave functions an acceptable wave function, and in both cases we define an inner product.

The difference between the vector space of quantum mechanics and a simple $N$-dimensional vector space is that the vector space in quantum mechanics is continously infinite-dimensional. Thus the finite, discrete sum in an inner product $\vec{A} \cdot \vec{B} = \sum_i A_i B_i$ is replaced by an integral in $\int \phi(x) \psi(x) dx$.

This means that in quantum mechanics one has to worry about convergence of integrals. Proving the expansion theorem is very complicated. In mathematics parlance the vector space in quantum mechanics is a Hilbert Space.
Operators and Observables

In vector space an operator transforms one vector into another. Linear operators are such that

\[ A[\alpha_1 \psi_1(x) + \alpha_2 \psi_2(x)] = \alpha_1 A\psi_1(x) + \alpha_2 A\psi_2(x) \]

and if they are to represent observables, they need to be *Hermitian*. For Hermitian operators

\[ \int \Psi(x)^* A \Psi(x) dx = \int [A \Psi(x)]^* \Psi(x) dx \]
Dirac Notation

Dirac introduced a very economical and powerful notation that applies equally well to finite dimensional vector spaces and to Hilbert spaces. We associate with each wave function $\psi$, a state vector, $|\psi\rangle$, called a ket. We also associate with each complex conjugate wave function $\phi^*$ the quantity $\langle \phi |$, called a bra. The inner product of $\psi$ and $\phi^*$ is associated with the braket relation

$$\int \phi^* \psi \, dx = \langle \phi | \psi \rangle$$

It follows that

$$\langle \phi | \psi \rangle^* = \langle \psi | \phi \rangle$$

The expression for the integral involving an operator may be written in two equivalent ways

$$\int \phi^* A \psi \, dx = \langle \phi | A \psi \rangle = \langle \phi | A \psi \rangle$$

An Hermitian operator satisfies

$$\langle A\phi | \psi \rangle = \langle \phi | A^\dagger | \psi \rangle$$

for any pair of states.
Dirac Notation

If $A$ is a number, rather than an operator, then it can be taken out of the brackets. Thus

$$\langle \phi | a \psi \rangle = a \langle \phi | \psi \rangle$$

and

$$\langle a \phi | \psi \rangle = a^* \langle \phi | \psi \rangle$$

Eigenvalue equations take the form

$$Q | \psi_q \rangle = q | \psi_q \rangle$$

The orthonormality condition in Dirac notation reads

$$\langle \psi_{q_1} | \psi_{q_2} \rangle = \delta_{q_1 q_2}$$
**Dirac Notation**

The expansion theorem reads

\[
|\psi\rangle = \sum_q c_q |\psi_q\rangle
\]

On multiplication by a particular eigenstate from the left

\[
\langle \psi_q'|\psi \rangle = \sum_q c_q \langle \psi_q'|\psi_q \rangle = \sum_q c_q \delta_{qq'} = c_{q'}
\]

With this form we can write

\[
\langle \phi|\psi \rangle = \sum_q c_q \langle \phi|\psi_q \rangle = \sum_q \langle \phi|\psi_q \rangle \langle \psi_q|\psi \rangle
\]

Since this is true for all $\phi$ and $\psi$, we can “take apart” this relation

\[
\sum_q |\psi_q\rangle \langle \psi_q| = 1
\]