**Lecture 14**

**Formalism of quantum mechanics**

In quantum mechanics, the state of the system is described by its wave function and the observables are represented by operators. Wave functions satisfy requirements for vectors and operators act on the wave functions as linear transformations. Therefore, it is natural to use language of linear algebra.

Only normalizable wave functions represent physical states. The set of all square-integrable functions, on a specified interval,

$$f(x) \text{ such that } \int_a^b |f(x)|^2 dx < \infty$$

constitutes a Hilbert space. Wave functions live in Hilbert space.

The inner product of two functions f and g is defined as

$$\langle f | g \rangle \equiv \int_a^b f^*(x)\, g(x)\, dx.$$

Dirac notations

[bra ~~x~~ ket]

$\langle f | g \rangle$

$|g\rangle$: ket

$\langle f |$: bra

$$\langle f | = \int f^* [\ldots]\, dx$$

In a finite-dimensional vector space, where the vectors expressed as columns,

$$|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

the corresponding bra is a row vector

$$\langle \alpha | = (a_1^* \; a_2^* \ldots a_n^*).$$

A function is said to be **normalized** if its inner product with itself is one.

$$\langle f | f \rangle = \int_a^b |f(x)|^2 \, dx$$

Two wave functions are **orthogonal** if their inner product is zero.

$$\langle f | g \rangle = 0$$

A set of functions is **orthonormal** if they are normalized and mutually orthogonal.

$$\langle f_m | f_n \rangle = \delta_{mn}$$

**Observables** in quantum mechanics are represented by **hermitian operators**, i.e. such as

$$\langle f | \hat{Q} f \rangle = \langle \hat{Q} f | f \rangle \quad \text{for all } f(x)$$

The **expectation value** of an observable Q (x, p) can be written as

$$\langle Q \rangle = \int \psi^* \hat{Q} \psi \, dx = \langle \psi | \hat{Q} \psi \rangle$$

**Determinate states :** such states that every measurement of Q is certain to return the same value q. **Determinate states are eigenfunctions of Q and q is the corresponding eigenvalue.**

$$\boxed{\hat{Q}\psi = q\psi}$$

Example: determinate states of the total energy are eigenfunctions of the Hamiltonian:

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

**Example:** Consider the operator $\hat{Q} \equiv i\frac{d}{d\phi}$

where $\phi$ is usual polar coordinate in two dimensions. Is $\hat{Q}$ operator hermitian? Find its eigenfunctions and eigenvalues.

**Solution**

$$f(\phi + 2\pi) = f(\phi)$$

[Functions on the finite interval $0 \le \phi \le 2\pi$ ]

Condition for the operator to be hermitian:

$$\langle f | \hat{Q} f \rangle = \langle \hat{Q} f | f \rangle \text{ or } \langle f | \hat{Q} g \rangle = \langle \hat{Q} f | g \rangle$$

We need to check if it is true for this operator.

$$\langle f | \hat{Q} g \rangle = \int_0^{2\pi} f^* \left( i \frac{dg}{d\phi} \right) d\phi = \text{(integrating by parts)}$$

$$= \cancel{i f^* g \Big|_0^{2\pi}}_{\,0} - \int_0^{2\pi} i \frac{df^*}{d\phi} g \, d\phi =$$

$$= \int_0^{2\pi} \left[ \left( -i \frac{d}{d\phi} \right) f^* \right] g \, d\phi = \langle \hat{Q} f | g \rangle$$

The solution of the eigenvalue equation

$$i \frac{d}{d\phi} f(\phi) = q f(\phi)$$

is $f(\phi) = A e^{-iq\phi}$.

The condition $f(\phi) = f(\phi + 2\pi)$ gives $e^{-iq2\pi} = 1$

Therefore, $q = 0, \pm 1, \pm 2, \ldots$

We say that the **spectrum** of this operator is the set of all integers, and it is **non-degenerate.**

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The collection of all the eigenvalues of an operator is called its **spectrum**. If all eigenvalues are different, spectrum is said to be **non-degenerate**. If two or more eigenvalues are the same, spectrum is said to be **degenerate**.

**Exercise 7**

Consider the operator $\hat{Q} = \frac{d^2}{d\phi^2}$, where $\phi$ is azimuthal angle in polar coordinates, and the functions are subject to

$$f(\phi + 2\pi) = f(\phi).$$

(1)Is $\hat{Q}$ hermitian?
(2) Find its eigenvalues and eigenfunctions.
(3) What is the spectrum of Q? Is the spectrum degenerate?

**Solution**

$$(1) \quad \langle f | \hat{Q} g \rangle = \int_0^{2\pi} f^* \frac{d^2 g}{d\phi^2} \, d\phi = f^* \frac{dg}{d\phi} \Big|_0^{2\pi}$$

$$- \int_0^{2\pi} \frac{df^*}{d\phi} \frac{dg}{d\phi} d\phi = f^* \frac{dg}{d\phi} \Big|_0^{2\pi} - \frac{df^*}{d\phi} g \Big|_0^{2\pi}$$

$$+ \int_0^{2\pi} \frac{d^2 f^*}{d\phi^2} g \, d\phi = \langle \hat{Q} f | g \rangle \qquad \text{Yes.}$$

$$(2) \quad \hat{Q} f = q f$$

$$\frac{d^2 f}{d\phi^2} = q f \Rightarrow f_{\pm}(\phi) = A^{\pm\sqrt{q}\phi}$$

$$e^{2\pi n i} = 1 \Rightarrow \sqrt{q}\, 2\pi = 2\pi n i \quad \text{so } f(\phi) = f(\phi + 2\pi) \Rightarrow$$

$$\boxed{\sqrt{q} = in}$$

The eigenvalues are $\boxed{q = -n^2}$ $(n = 0, \pm 1, \pm 2 \ldots)$

(3) The spectrum is doubly degenerate, for a given n there are two eigenfunctions

$$f_\pm(\phi) = A e^{\pm\sqrt{q}\phi} \qquad q=-n^2,$$

except special case n=0, which is not degenerate.