Lecture 3

Operators and Observables

Study Goal of This Lecture

- Linear operators.
- Eigenvalues and eigenfunctions of Hermitian operators.
- Commutator.

The mathematical structure of quantum mechanics is highly related to linear algebra, especially topics concerning function space, linear operators and eigenvalue problem. (Three key things in this lecture.) This is apperant given the form of the T.I.S.E. :

So we will spend some time to cover the basics of linear algebra.

$$\hat{H}\psi = E\psi. \tag{3.1}$$

Although the T.I.S.E. is a differential equation.

3.1 Function Space (Hibert Space)

3.1.1 Basis of functions

- Key point: How do we write down a "function" mathematically?

The wave function mathematically represents the state of a system and must be "calculated". Generally speaking, we write down a function in term of "superposition of other pre-defined functions".

$$f(x) = \sin(x),\ \ f(x) = \sin(x) + \cos(x). \tag{3.2}$$

$$f(x) = \sum_{i=0}^{\infty} a_i x^i \leftarrow \text{polynomail!} \tag{3.3}$$

$$f(x) = \sum_{i=1}^{\infty} A_i e^{2\pi i k_i x} \leftarrow \text{Fourier series.} \tag{3.4}$$

These predefined functions are called ”basis functions”. The same $f(x)$ can be written in different basis $\rightarrow \psi(x)\ vs.\ \tilde{\psi}(k)$.

3.1.2 Inner product

We define “inner product” of the functions as:

$$\int_{-\infty}^{\infty} \psi^*(x)\phi(x)dx. \tag{3.5}$$

This is also called the “overlap” of two functions. If the two functions have zero overlap:

$$\int_{-\infty}^{\infty} \psi_1^*(x)\psi_2(x)dx = 0, \tag{3.6}$$

then we say $\psi_1(x)$ and $\psi_2(x)$ are “orthogonal” to each other.
For 3-D:

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz\ \psi_1^*(x,y,z)\psi_2(x,y,z) \tag{3.7}$$

$$\equiv \int \psi_1^*(\vec{r})\psi_2(\vec{r})d\tau. \tag{3.8}$$

3.2 Linear Operator

3.2.1 Linearity

Not just Hamiltonian are linear Hermitian operators, all quantum mechanical “observables” are linear and Hermitian operators. The math of quantum mechanical operators is linear algebra.

Basics of linear algebra.

We say an operator is linear if it satisfies the following properties:

$$1.\ \hat{A}(f_1 + f_2) = \hat{A}f_1 + \hat{A}f_2 \tag{3.9}$$

$$2.\ \hat{A}(cf) = c\hat{A}f,\ \text{while c is a number} \tag{3.10}$$

for example, differential operator, $\frac{d}{dx}$, is linear:

$$\frac{d}{dx}[f_1(x) + f_2(x)] = \frac{d}{dx}f_1(x) + \frac{d}{dx}f_2(x) = f_1'(x) + f_2'(x). \tag{3.11}$$

3.2.2 Hermitianity

An operator is Hermitian if it satisfies:

$$\int \psi^*(\hat{A}\phi)d\tau = \int \phi(\hat{A}\psi)^*d\tau \tag{3.12}$$

for any well-behaved functions ϕ and ψ. $(A\psi)^*$ is the complex conjugate of $A\psi$.

It is posulated that given the a wavefuntion ψ, the averaged value of an observable, $\langle a\rangle$, corresponding with an operator $\hat{A}$ is:

$$\langle a\rangle = \int \psi^*\hat{A}\psi d\tau \Leftarrow \text{expectation value.} \tag{3.13}$$

We will come back to this point later.

3.2.3 Other Properties

In linear algebra, quantum mechanical operators has the following important properties:

Very importants! experimental observables are real numbers!! e.g. $\hat{H}\psi = E\psi$, E must be real.

Theorem 3.2.1. *The eigenvalue of a Hermitian operator must be real.*

Proof. Suppose ϕ is an eigenfunction of $\hat{A}$, then

$$\hat{A}\phi = a\phi, \ (\hat{A}\phi)^* = a^*\phi^*. \tag{3.14}$$

Next,we write

$$\int \phi^* A\phi d\tau = \int \phi^* a\phi d\tau = a\int \phi^*\phi d\tau, \tag{3.15}$$

and

$$\int \phi(\hat{A}\phi)^* d\tau = \int \phi a^*\phi^* d\tau = a^*\int \phi^*\phi d\tau. \tag{3.16}$$

By definition of Hermitian operator, $\int \phi^*(\hat{A}\phi)d\tau = \int \phi(\hat{A}\phi)^*d\tau$,

$$\therefore a = a^*, \ a \text{ is real.}$$

□

Theorem 3.2.2. *The eigenfunctions of a Hermitian operator corresponding to different eigenvalues are orthogonal:*

Proof. For two eigenfunctions with different eigenvalues, we have:

$$\hat{A}\phi_1 = a_1\phi_1,\ \hat{A}\phi_2 = a_2\phi_2 \text{ for } a_1 \neq a_2. \tag{3.17}$$

Apply the hermitianity:$\int \phi_1^* \hat{A}\phi_2 d\tau = \int \phi_2(\hat{A}\phi_1)^* d\tau$, we have:

$$\text{LHS: } \int \phi_1^* \hat{A}\phi_2 d\tau = \int \phi_1^* a_2 \phi_2 d\tau = a_2 \int \phi_1^* \phi_2 d\tau, \tag{3.18}$$

$$\text{RHS: } \int \phi_2(\hat{A}\phi_1)^* d\tau = \int \phi_2 a_1 \phi_1^* d\tau = a_1 \int \phi_1^* \phi_2 d\tau, \tag{3.19}$$

then

$$\text{Equ (3.18)} - \text{Equ (3.19)} = 0 \Rightarrow (a_2 - a_1) \int \phi_1^* \phi_2 d\tau = 0. \tag{3.20}$$

$$\because a_1 \neq a_2,\ a_1 - a_2 \neq 0,$$

$$\therefore \int \phi_1^* \phi_2 d\tau = 0,\ \phi_1 \text{ and } \phi_2 \text{ are orthogonal.}$$

□

Therefore, eigenfunctions of a Hermitian operator are orthogonal to each other,we can further require that they are normalized, therefore, eigenfunctions of an Hermitian operator form an orthonormal set of functions:

$$\hat{A}\psi_n = a_n\psi_n, \text{ where } \int \psi_n^* \psi_m d\tau = \delta_{nm}. \tag{3.21}$$

3.2.4 Commutability

The multiplication of operators is associative. That is:

$$\hat{A}\hat{B}f = \hat{A}(\hat{B}f), \tag{3.22}$$

$$\hat{A}\hat{B}\hat{C} = (\hat{A}\hat{B})\hat{C} = \hat{A}(\hat{B}\hat{C}), \tag{3.23}$$

but they in general do not commute to each other. i.e. orders are important. $\Rightarrow \hat{A}\hat{B} \neq \hat{B}\hat{A}$.
For example, $\hat{A} = \hat{x} = x\cdot$ and $\hat{B} = \frac{\partial}{\partial x}$, then:

$$\hat{A}\hat{B}f(x) = x \cdot \frac{\partial}{\partial x} f(x) = x \cdot f'(x), \tag{3.24}$$

$$\hat{B}\hat{A}f(X) = \frac{\partial}{\partial x}[x \cdot f(x)] = x \cdot f'(x) + f(\dot{x}). \tag{3.25}$$

The outcome of the above two equation are different → operator $\hat{A}$ and $\hat{B}$ do not commute. We can define commutator of two operators:

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}. \tag{3.26}$$

For example, $\hat{A} = \hat{x}$, $\hat{B} = \frac{\partial}{\partial x}$,

$$[\hat{A}, \hat{B}]f(x) = \hat{A}\hat{B}f(x) - \hat{B}\hat{A}f(x), \tag{3.27}$$

$$x \cdot f'(x) - x \cdot f'(x) - f(x) = -f(x), \tag{3.28}$$

$$\therefore [\hat{A}, \hat{B}] = -1 \cdot \quad \text{[Multiply by -1]}.$$

Note that commutator itself is an operator and must be valid for all $f(x)$.

Here is an important theorem:

Theorem 3.2.3. *If and only if* $[\hat{A}, \hat{B}]$ *commute, then they can share the same set of eigenfunctions.*

Proof. consider $\hat{A}\psi = a\psi$, because $\hat{A}$ and $\hat{B}$ commute, we have $\hat{A}\hat{B} = \hat{B}\hat{A}$. then

$$\hat{B}\hat{A}\psi = \hat{B}a\psi = a\hat{B}\psi \Rightarrow \hat{A}\hat{B}\psi = a\hat{B}\psi. \tag{3.29}$$

$\therefore$ $\hat{B}\psi$ is also an eigenfunction of $\hat{A}$. Because each independent eigenfunction of $\hat{A}$ has an unique eigenvalue(consider non-degenerate case). □

Therefore, $\hat{B}\psi$ must be proportional to ψ. $\Rightarrow \hat{B}\psi = b\psi \rightarrow \psi$ is also an eigenfunction of $\hat{B}$!!

Later we will come back to this point and show that the theorem is deeply connected to the Heisenberg uncertainty principle. Final piece in this lecture we give a postulate that given a wave function and an observable(operator $\hat{A}$), then experimentally measured "averaged value" of $\hat{A}$ is:

$$\langle a \rangle = \int \psi^*(x)\hat{A}\psi(x)dx = \int |\psi(x)|^2 A(x)dx. \tag{3.30}$$

Expectation value: after averaging.

This is an "expectation value" for $\hat{A}$.