Lecture 6

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3.1 Operators

$$(\hat{A}+\hat{B})f(x) \equiv \hat{A}f(x)+\hat{B}f(x)$$

$$(\hat{A}-\hat{B})f(x) \equiv \hat{A}f(x)-\hat{B}f(x)$$

An operator can involve more than one variable. For example:

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)g(x,y) = \frac{\partial^2 g}{\partial x^2}+\frac{\partial^2 g}{\partial y^2}$$

The product of two operators $\hat{A}$ and $\hat{B}$ is defined by

$$\hat{A}\hat{B}f(x) \equiv \hat{A}\left[\hat{B}f(x)\right]$$

For example:

$$\hat{D} = \frac{d}{dx}, \quad \hat{3} = 3.$$

$$\hat{3}\hat{D}f(x) = \hat{3}\left[\hat{D}f(x)\right] = \hat{3}f'(x) = 3f'(x)$$

The operators $\hat{A}\hat{B}$ and $\hat{B}\hat{A}$ may not have the same effect. Consider:

$$\hat{D} = \frac{d}{dx} \,, \qquad \hat{x} = x .$$

$$\boxed{\hat{D}\hat{x}f(x)} = \hat{D}\left[\hat{x}f(x)\right]$$

$$= \frac{d}{dx}\left[x f(x)\right]$$

apply product rule

$$= f(x) + x f'(x)$$

$$= \boxed{\left(\hat{1} + \hat{x}\hat{D}\right)} f(x)$$

$$\hat{x}\hat{D}f(x) = \hat{x}\left[\frac{d}{dx}f(x)\right] = x f'(x)$$

$\hat{A}\hat{B}$ does not necessarily equal $\hat{B}\hat{A}$ for operators.

Two operators $\hat{A}$ and $\hat{B}$ are said to be equal if $\hat{A}f = \hat{B}f$ for all functions f.

$$\boxed{\hat{D}\hat{x} = \hat{1} + \hat{x}\hat{D}}$$

$\hat{1}$: unit operator

$\hat{0}$: null operator

(can usually omit ^ over numbers)

$$\hat{D}\hat{x} - \hat{x}\hat{D} - 1 = 0$$

we can move operators to the other side of the equation

Operators obey the associative law of multiplication:

$$\hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C}$$

For example, let

$$\hat{A} = \frac{d}{dx}, \quad \hat{B} = \hat{x}, \quad \text{and} \quad \hat{C} = 3$$

$$(\hat{A}\hat{B}) = \hat{D}\hat{x} = \underline{1+\hat{x}\hat{D}}$$

$$(\hat{B}\hat{C}) = \underline{3\hat{x}}$$

$$\begin{aligned}
[(\hat{A}\hat{B})\hat{C}]f &= (\hat{A}\hat{B})3f \\
&= (1+\hat{x}\hat{D})3f \\
&= 3f + 3xf'
\end{aligned}$$

$$\begin{aligned}
[\hat{A}(\hat{B}\hat{C})]f &= \hat{A}(3xf) \\
&= \frac{d}{dx}(3xf) \\
&= 3xf' + 3f
\end{aligned}$$

same result

A major difference between operator algebra and ordinary algebra is that numbers obey the commutative law of multiplication, but operators do not necessarily do so.

Commutative law : $ab = ba$

if a, b are numbers

Define the commutator $[\hat{A}, \hat{B}]$

$$\boxed{[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}}$$

If $\hat{A}\hat{B} = \hat{B}\hat{A}$, then $[\hat{A}, \hat{B}] = 0$, and we say that $\hat{A}$ and $\hat{B}$ commute.

Otherwise, they do not commute.

$$\left[\hat{3}, \frac{d}{dx}\right] = \hat{3}\frac{d}{dx} - \frac{d}{dx}\hat{3} = 0$$

$$\left[\frac{d}{dx}, \hat{x}\right] = \hat{D}\hat{x} - \hat{x}\hat{D} = 1$$

$\therefore$ $\frac{d}{dx}$ and $\hat{x}$ do not commute.

For example, find $\left[\hat{z}^3, \frac{d}{dz}\right]$

To find $\left[\hat{z}^3, \frac{d}{dz}\right]$, apply this to an arbitrary function $g(z)$.

$$\left[\hat{z}^3, \frac{d}{dz}\right] g(z) = \hat{z}^3\left[\frac{d}{dz} g(z)\right] - \frac{d}{dz}\left[\hat{z}^3 g(z)\right]$$

$$= \hat{z}^3 g'(z) - \frac{d}{dz} \underbrace{z^3 g(z)}_{\text{product rule}}$$

$$= \cancel{z^3 g'(z)} - \left[\cancel{z^3 g'(z)} + 3z^2 g(z)\right]$$

$$\boxed{\left[\hat{z}^3, \frac{d}{dz}\right] = -3z^2} \xleftarrow{\text{remove arbitrary function } g(z)}$$

The square of an operator is defined as the product of the operator with itself.

$$\hat{B}^2 = \hat{B}\hat{B}$$

For example:

$$\hat{D}^2 f(x) = \hat{D}\left[\hat{D} f(x)\right] = \hat{D} f'(x) = f''(x)$$

$$\hat{D}^2 = \frac{d^2}{dx^2}$$

$\hat{B}^n$: apply $\hat{B}$ n times in succession $(n = 1, 2, 3, \ldots)$

It turns out that operators occurring in quantum mechanics are linear. $\hat{A}$ is a linear operator if and only if it has the following two properties:

$$\boxed{\hat{A}[f(x) + g(x)] = \hat{A}f(x) + \hat{A}g(x)}$$

$$\boxed{\hat{A}[cf(x)] = c\hat{A}f(x)}$$

where $f(x)$ and $g(x)$ are arbitrary functions, and c is an arbitrary constant.

$$\sqrt{f(x) + g(x)} \neq \sqrt{f(x)} + \sqrt{g(x)}$$

the square root function is a

nonlinear operator.

Identities in linear-operator manipulations:

$$\boxed{(\hat{A}+\hat{B})\hat{C} = \hat{A}\hat{C} + \hat{B}\hat{C}}$$

$$\boxed{\hat{A}(\hat{B}+\hat{C}) = \hat{A}\hat{B} + \hat{A}\hat{C}}$$

3.2 Eigenfunctions and Eigenvalues

$$\boxed{\hat{A} f(x) = k f(x)}$$

$\hat{A}$: linear operator

$f(x)$ is not identically zero

For example, e^{2x} is an eigenfunction of the operator $\frac{d}{dx}$ with eigenvalue 2.

$$\frac{d}{dx} \underbrace{e^{2x}}_{\text{eigenfunction of } \frac{d}{dx}} = \underset{\substack{\uparrow \\ \text{eigenvalue}}}{2}\, e^{2x}$$

$\sin 2x$ is not an eigenfunction of $\frac{d}{dx}$.

$$\frac{d}{dx}\sin(2x) = 2\cos(2x)$$

a) Find the eigenfunctions and eigenvalues of the operator $\frac{d}{dx}$.

$$\hat{A} f(x) = k f(x)$$

$$\frac{d}{\boxed{dx}} f(x) = k \boxed{f(x)}$$

$$\frac{1}{f(x)}\, df(x) = k\, dx$$

$$\int \frac{1}{f}\, df = k \int dx$$

$$\ln f + c_1 = kx + c_2$$

$$\ln f = kx + c$$

$$f = e^{c} e^{kx}$$

$$\boxed{f = A e^{kx}}$$

$$e^{(a+b)} = e^{a} e^{b}$$

b) If we impose the boundary condition that the eigenfunctions remain finite as $x \to \pm\infty$, find the eigenvalues.

k can be complex

$$k = a + ib$$

$$f(x) = A e^{kx}$$

$$f(x) = A e^{(a+ib)x}$$

$$\boxed{f(x) = A e^{ax} e^{ibx}}$$

if $a > 0$: $e^{ax} \to \infty$ as $x \to \infty$

if $a < 0$: $e^{ax} \to \infty$ as $x \to -\infty$

$\therefore\ a = 0$

$$f(x) = A e^{ibx}$$

$k = ib$, where b is real

3.3 Operators and Quantum Mechanics

$$\underbrace{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]}_{\text{Hamiltonian operator}}\psi(x) = E\psi(x)$$

eigenvalue problem

Newtonian mechanics: $\overset{\text{velocity}}{\vec{v}}, \vec{x}$

Hamiltonian mechanics: $\underset{\text{momenta}}{\vec{p}}, \underset{\text{generalized coordinates}}{\vec{q}}$

Conjugate momenta:

$$\boxed{p_x \equiv mv_x},\ p_y \equiv mv_y,\ p_z = mv_z$$

E = kinetic + potential

$$E = T + V$$

$$v_x = \frac{p_x}{m}$$

$$T = \frac{1}{2} m v_x^2$$

$$\boxed{v_x^2 = \frac{p_x^2}{m^2}}$$

$$T = \frac{p_x^2}{2m}$$

$$H = T + V$$

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

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$ QM

$$\boxed{\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}, \quad \hat{p}_y = \frac{\hbar}{i}\frac{\partial}{\partial y}, \quad \hat{p}_z = \frac{\hbar}{i}\frac{\partial}{\partial z}}$$

operators for the components of linear momentum

$$\hat{p}_x^2 = \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 = \frac{\hbar}{i}\frac{\partial}{\partial x}\frac{\hbar}{i}\frac{\partial}{\partial x} = -\hbar^2\frac{\partial^2}{\partial x^2}$$

$$\boxed{\hat{p}_x^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}}$$

$$\hat{H} = -\underbrace{\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{\frac{\hat{p}_x^2}{2m}} + V(x)$$

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