OPERATORS

An operator is a recipe showing how to get a function g from a given function f:

$$g = \hat{O}f.$$

This is similar to a function, which tells us how to get a number y given a number x:

$$y = f(x).$$

Examples:

$$\begin{aligned}
\hat{A}f &\equiv f + 8 \\
\hat{x}f &\equiv xf \\
\hat{s}f &\equiv \sqrt{f} \\
\hat{\delta}f(x) &\equiv \frac{d}{dx}f(x)
\end{aligned}$$

Definitions:

Sum of operators: $(\hat{O} + \hat{P})f \equiv \hat{O}f + \hat{P}f$

Product: $(\hat{O}\hat{P})f \equiv \hat{O}(\hat{P}f)$.

Note that operators are always characterized by operations on functions.

Commutation:

Sum of operators is always commutative, product – not necessarily. Example:

$$(\frac{\hat{d}}{dx}\hat{x})f(x) = \frac{d}{dx}(xf) = f + xf'$$

$$(\hat{x}\frac{\hat{d}}{dx})f(x) = xf'.$$

Commutator:

$$[\hat{O}, \hat{P}] \equiv \hat{O}\hat{P} - \hat{P}\hat{O}.$$

The commutator is an operator, shows properties by operating on function:
$[\hat{x}, \frac{\hat{d}}{dx}]f = -f$ for arbitrary f, therefore $[\hat{x}, \frac{\hat{d}}{dx}] = -1$.

An operator $\hat{O}$ is linear if

$$\hat{O}(af(x) + bg(x)) = a\hat{O}f(x) + b\hat{O}g(x)$$

for arbitrary complex numbers a, b and functions f, g.
The operators $\hat{x}, \hat{\delta}$ defined above are linear, $\hat{A}, \hat{s}$ are not.
We will use only linear operators.

Eigenvalues and eigenfunctions of operators

Applying d/dx to the function e^{2x} gives the function multiplied by a constant, $(d/dx)e^{2x} = 2e^{2x}$. This shows a special relationship between the function and operator, which occurs only for certain functions. Thus, $(d/dx)x^3 \neq kx^3$.

Definition: if $\hat{O}f(x) = \alpha f(x)$, $f(x)$ is an eigenfunction of $\hat{O}$ with the eigenvalue α.

The eigenvalue equation for d/dx is $(d/dx)f(x) = \alpha f(x)$. Obviously, any $f(x) = e^{kx}$ with arbitrary k is an eigenfunction of the operator, with k the corresponding eigenvalue.

Going to the operator d^2/dx^2, again any e^{kx} is an eigenfunction, with the eigenvalue now k^2. Note: the same eigenvalue corresponds to the two eigenfunctions e^{kx} and e^{-kx}. The eigenvalue k^2 is degenerate, belonging to more than one eigenfunction. The degeneracy level is the number of linearly independent eigenfunctions belonging to the same eigenvalue (two in this example).

Theorem: If two (or more) eigenfunctions belong to the same eigenvalue, any linear combination of them $(af_1 + bf_2)$ will also be an eigenfunction with the same eigenvalue.

Proof (for 2 functions, similar for any number):

$$\left.\begin{array}{l} \hat{O}f_1(x) = \alpha f_1(x) \\ \hat{O}f_2(x) = \alpha f_2(x) \end{array}\right\} \Longrightarrow$$

$$\hat{O}(af_1 + bf_2) = a\hat{O}f_1 + b\hat{O}f_2 = a\alpha f_1 + b\alpha f_2 = \alpha(af_1 + bf_2)$$

The first equality uses the linearity of the operator $\hat{O}$.

Well behaved functions

Required properties:

1. Function must be single-valued and finite in the whole range.

   This applies primarily to trigonometric functions, e.g. $\sin(k\theta)$. Increasing θ by 2π does not change the physics, so we want to have $f(\theta + 2\pi) = f(\theta)$. The function $\sin(k\theta)$ must therefore have integer k.

2. Function must be continuous and have a continuous first derivative. This requirement comes from the appearance of the 2nd derivative in the Schrödinger equation. Exceptions occur when there are infinite jumps in the potential (e.g. the walls of a particle in a box).

3. The function is quadratically integrable, $0 < \int f^* f d\tau < \infty$. This makes possible the normalization of the function. A necessary (but not sufficient) condition is that $f \to 0$ as any of the arguments of the function goes to infinity.

Hermitian operators

Definition: The Hermitian conjugate $\hat{O}^\dagger$ of $\hat{O}$ is the operator satisfying $\int f\hat{O}^\dagger g d\tau = \int g\hat{O}^* f d\tau$ for any well-behaved f, g.

An operator is Hermitian if $\hat{O}^\dagger = \hat{O}$, i.e. $\int f\hat{O}g d\tau = \int g\hat{O}^* f d\tau$ for any well-behaved f, g.

We shall discuss only Hermitian operators (a few exceptions).

Examples:

- Is d/dx Hermitian? $\quad \hat{O} = \frac{d}{dx} \quad \hat{O}^* = \frac{d}{dx}$

$$\int_{-\infty}^{\infty} f\frac{d}{dx}g dx \overset{\text{integ by parts}}{=} [fg]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} g\frac{d}{dx} f dx =$$

$$= - \int_{-\infty}^{\infty} g\frac{d}{dx} f dx \neq \int_{-\infty}^{\infty} g\frac{d}{dx} f dx.$$

  The 2nd step is possible because f, g go to 0 at $\pm\infty$.

  Conclusion: d/dx is not Hermitian. Its Hermitian conjugate is $-d/dx$.

- How about id/dx? $\quad \hat{O} = i\frac{d}{dx} \quad \hat{O}^* = -i\frac{d}{dx}$
  Steps similar to those above show that

$$\int_{-\infty}^{\infty} f\left(i\frac{d}{dx}\right) g dx = \int_{-\infty}^{\infty} g\left(-i\frac{d}{dx}\right) f dx.$$

  id/dx is therefore Hermitian.

- x is Hermitian.

Properties of Hermitian operators

1. All eigenvalues are real
2. Eigenfunctions belonging to different eigenvalues are orthogonal.
3. The set of all eigenfunctions f_i of a Hermitian operator forms a basis for the space of functions with the same boundary conditions, i.e. any function Ψ of this space may be spanned in the set of eigenfunctions, $\Psi = \sum_i c_i f_i$.

Proof of 1
$\hat{O}f = \alpha f$. Taking the complex conjugate gives $\hat{O}^* f^* = \alpha^* f^*$.
From the first equation, $\int f^* \hat{O} f d\tau = \alpha \int f^* f d\tau$,
and from the 2nd $\int f \hat{O}^* f^* d\tau = \alpha^* \int f f^* d\tau$.
The lhs of the last equation is equal (by the definition of Hermitian conjugate) to $\int f^* \hat{O}^\dagger f d\tau$. Since $\hat{O}$ is Hermitian, $\hat{O}^\dagger$ may be replaced by $\hat{O}$, and the lhs of the last two equations are equal. Therefore, the rhs are also equal; since $\int f^* f d\tau \neq 0$, $\alpha = \alpha^*$, and α is real.
Proof of 2. Given:
$\hat{O}f = \alpha f; \quad \hat{O}g = \beta g; \quad \alpha \neq \beta.$
From the 1st equation, $\int g^* \hat{O} f d\tau = \alpha \int g^* f d\tau$.
From the complex conjugate of the 2nd, $\int f \hat{O}^* g^* d\tau = \beta \int f g^* d\tau$.
Since $\hat{O}$ is Hermitian, the lhs of the last two equations are equal, therefore the rhs are equal. Since $\alpha \neq \beta$, $\int g^* f d\tau = 0$.
If $\alpha = \beta$, the functions f, g are degenerate, and any linear combination of them is an eigenfunction of $\hat{O}$ with the same eigenvalue. It is possible to choose orthogonal combinations.
3 will not be proved.

Theorem: Given two commuting Hermitian operators, there exists a complete set of eigenfunctions common to both operators.

Notes:

• a complete set – the set of all eigenfunctions, in which any function with the same boundary conditions may be spanned.

• there exists ... – an eigenfunction of one operator is not necessarily an eigenfunction of the other (remember the freedom of selecting eigenfunctions in case of degeneracy), but one can always find a complete set of eigenfunctions common to both operators.

Example: the hydrogen atom functions Ψ_{nlm} are eigenfunctions of the commuting Hermitian operators $\hat{H},\ \hat{L}^2,\ \hat{L}_z$:

$$\begin{aligned} \hat{H}\Psi_{nlm} &= E_n\Psi_{nlm} \\ \hat{L}^2\Psi_{nlm} &= l(l+1)\hbar^2\Psi_{nlm} \\ \hat{L}_z\Psi_{nlm} &= m\hbar\Psi_{nlm}. \end{aligned}$$

A linear combination such as $\sum_l c_l\Psi_{nlm}$ (constant n, m) will be an ef of $\hat{H}$ and $\hat{L}_z$, but not of $\hat{L}^2$.

The proof will be given only for the nondegenerate case:
Given $\hat{A}\hat{B} = \hat{B}\hat{A}$, $\quad \hat{A}f = af$, $\quad a$ nondegen ev.
$\hat{A}(\hat{B}f) \overset{commute}{=} \hat{B}\hat{A}f = \hat{B}af = a(\hat{B}f)$

$\hat{B}f$ is therefore an ef of $\hat{A}$ with the ev a. Since a is a nondegenerate ev, f and $\hat{B}f$ must be linearly dependent, which means they are proportional, or $\hat{B}f = bf$. The last equation shows that f is an ef of $\hat{B}$, QED.

It can be shown (exercise) that if two Hermitian operators have a complete set of common eigenfunctions, the operators commute.

Classical wave equation (one dimension):

$$\Psi = Ae^{2\pi i(kx-\nu t)}.$$

$k = 1/\lambda$ is the wave number.

From Planck's equation $E = h\nu \Rightarrow \nu = \frac{E}{h}$,
from de Broglie $\lambda = \frac{h}{p} \Rightarrow k = \frac{p}{h}$, giving
$\Psi = Ae^{2\pi i/h(px-Et)} = Ae^{i/\hbar(px-Et)}$.
Taking derivatives wrt x and t, we get

$$\frac{\partial\Psi}{\partial x} = \frac{i}{\hbar}p\Psi \Rightarrow p\Psi = \frac{\hbar}{i}\frac{\partial\Psi}{\partial x}$$
$$\frac{\partial\Psi}{\partial t} = -\frac{i}{\hbar}E\Psi \Rightarrow E\Psi = -\frac{\hbar}{i}\frac{\partial\Psi}{\partial t}.$$

This shows some relationship of p_x to the operator $\frac{\hbar}{i}\frac{\partial}{\partial x}$ and of E to $-\frac{\hbar}{i}\frac{\partial}{\partial t}$. This does not prove anything!!!.