EIGEN FUNCTIONS AND EIGEN VALUE OPERATORS:

$$\begin{aligned} \hat{p}f(x) &= -i\hbar\frac{d}{dx}f(x) = (-i\hbar)(ik)e^{i(kx-\omega t)} \\ &= \hbar k f(x) \end{aligned}$$

and since by the de Broglie relation $\hbar k$ is the momentum p of the particle, we have

$$\hat{p}f(x) = pf(x)$$

Note that this explains the choice of sign in the definition of the momentum operator!

We have repeatedly said that an operator is defined to be a mathematical symbol that applied to a function gives a new function.

Thus if we have a function $f(x)$ and an operator $\hat{A}$, then

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

is a some new function, say $\phi(x)$.

Exceptionally the function $f(x)$ may be such that $\phi(x)$ is proportional to $f(x)$; then we have

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

where a is some constant of proportionality. In this case $f(x)$ is called an **eigenfunction** of $\hat{A}$ and a the corresponding **eigenvalue**.

Example: Consider the function $f(x,t) = e^{i(kx-\omega t)}$.
This represents a wave travelling in x direction.
Operate on $f(x)$ with the momentum operator:

$$\begin{aligned} \hat{p}f(x) &= -i\hbar\frac{d}{dx}f(x) = (-i\hbar)(ik)e^{i(kx-\omega t)} \\ &= \hbar k f(x) \end{aligned}$$

and since by the de Broglie relation $\hbar k$ is the momentum p of the particle, we have

$$\hat{p}f(x) = pf(x)$$

Note that this explains the choice of sign in the definition of the momentum operator!

LINEAR OPERATORS:

An operator $\hat{A}$ is said to be linear if

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

and

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

where $f(x)$ and $g(x)$ are any two appropriate functions and c is a complex constant.

Examples: the operators $\hat{x}$, $\hat{p}$ and $\hat{H}$ are all linear operators. This can be checked by explicit calculation (Exercise!).

HERMITIAN OPERATORS:

The operator $\hat{A}^\dagger$ is called the **hermitian conjugate** of $\hat{A}$ if

$$\int \left(\hat{A}^\dagger\psi\right)^* \psi dx = \int \psi^* \hat{A}\psi dx$$

Note: another name for "hermitian conjugate" is "**adjoint**".

The operator $\hat{A}$ is called **hermitian** if

$$\int \left(\hat{A}\psi\right)^* \psi\, dx = \int \psi^* \hat{A}\psi\, dx$$

Examples:

(i) the operator $\hat{x}$ is hermitian. Indeed:

$$\int (\hat{x}\psi)^* \psi\, dx = \int (x\psi)^* \psi\, dx = \int \psi^*\, x\psi\, dx = \int \psi^*\, \hat{x}\psi\, dx$$

(ii) the operator $\hat{p} = -i\hbar d/dx$ is hermitian:

$$\begin{aligned}\int (\hat{p}\psi)^* \psi\, dx &= \int \left(-i\hbar\frac{d\psi}{dx}\right)^* \psi\, dx \\ &= i\hbar \int \left(\frac{d\psi}{dx}\right)^* \psi\, dx\end{aligned}$$

and after integration by parts, and recognizing that the wfn tends to zero as $x \to \infty$, we get on the right-hand side

$$-i\hbar \int \psi^* \frac{d\psi}{dx}\, dx = \int \psi^* \hat{p}\psi\, dx$$

(iii) the K.E. operator $\hat{T} = \hat{p}^2/2m$ is hermitian:

$$\begin{aligned}\int \left(\hat{T}\psi\right)^* \psi\, dx &= \frac{1}{2m}\int \left(\hat{p}^2\psi\right)^* \psi\, dx \\ &= \frac{1}{2m}\int (\hat{p}\psi)^*\, \hat{p}\psi\, dx \\ &= \frac{1}{2m}\int \psi^* \hat{p}^2\psi\, dx \\ &= \int \psi^* \hat{T}\psi\, dx\end{aligned}$$

(iv) the Hamiltonian is hermitian:

$$\hat{H} = \hat{T} + \hat{V}(\hat{x})$$

here $\hat{V}$ is a hermitian operator by virtue of being a function of the hermitian operator $\hat{x}$, and since $\hat{T}$ has been shown to be hermitian, so $\hat{H}$ is also hermitian.

Theorem: The eigenvalues of hermitian operators are real.
Proof: Let ψ be an eigenfunction of $\hat{A}$ with eigenvalue a:

$$\hat{A}\psi = a\psi$$

then we have

$$\int \left(\hat{A}\psi\right)^* \psi \, dx = \int (a\psi)^* \psi \, dx = a^* \int \psi^* \psi \, dx$$

and by hermiticity of $\hat{A}$ we also have

$$\int \left(\hat{A}\psi\right)^* \psi \, dx = \int \psi^* \hat{A}\psi \, dx = a \int \psi^* \psi \, dx$$

hence

$$(a^* - a) \int \psi^* \psi \, dx = 0$$

and since $\int \psi^* \psi \, dx \neq 0$, we get

$$a^* - a = 0$$

The converse theorem also holds: an operator is hermitian if its eigenvalues are real.
The proof is left as an exercise.

Note: by virtue of the above theorems one can define a hermitian operator as an operator with all real eigenvalues.

Corollary: *The eigenvalues of the Hamiltonian are real.*
In fact, since by definition the Hamiltonian has the dimension of energy, therefore the eigenvalues of the Hamiltonian are the energies of the system described by the wave function.

1.5 Expectation values.

Consider a system of particles with wave function $\psi(x)$
(x can be understood to stand for all degrees of freedom of the system; so, if we have a system of two particles then x should represent
$\{x_1, y_1, z_1; x_2, y_2, z_2\}$).

The expectation value of an operator $\hat{A}$ that operates on ψ is defined by

$$\langle \hat{A} \rangle \equiv \int \psi^* \, \hat{A}\psi \, dx$$

If ψ is an eigenfunction of $\hat{A}$ with eigenvalue a, then, assuming the wave function to be normalized, we have

$$\langle \hat{A} \rangle = a$$

Now the rate of change of the expectation valueof A is:

$$\begin{aligned}
\frac{d\langle\hat{A}\rangle}{dt} &= \int \frac{\partial}{\partial t}\left(\psi^* \hat{A}\,\psi\right) dx \\
&= \int \left\{ \frac{\partial \psi^*}{\partial t}\hat{A}\psi + \psi^* \frac{\partial \hat{A}}{\partial t}\psi + \psi^* \hat{A}\frac{\partial \psi}{\partial t} \right\} dx \\
&= \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{i}{\hbar}\int \left\{ \left(\hat{H}\psi\right)^* \hat{A}\psi - \psi^* \hat{A}\hat{H}\psi \right\} dx
\end{aligned}$$

where we have used the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$$

Now by hermiticity of $\hat{H}$ we get on the r.h.s.:

$$\begin{aligned}
&\frac{i}{\hbar}\int \left\{ \psi^* \hat{H}\hat{A}\psi - \psi^* \hat{A}\hat{H}\psi \right\} dx \\
=\; &\frac{i}{\hbar}\int \psi^* \left(\hat{H}\hat{A} - \hat{A}\hat{H}\right)\psi\, dx
\end{aligned}$$

hence

$$\frac{d\langle\hat{A}\rangle}{dt} = \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle$$

Of particular interest in applications are linear hermitian operators that do not explicitly depend on time, *i.e.* such that

$$\partial\hat{A}/\partial t = 0$$

For this class of operators we get the following equation of motion:

$$i\hbar\frac{d\langle\hat{A}\rangle}{dt} = \langle[\hat{A},\hat{H}]\rangle$$

Here the expectation values are taken with arbitrary square integrable functions. Therefore we can re-write this equation as an operator equation:

$$i\hbar\frac{d\hat{A}}{dt} = [\hat{A},\hat{H}]$$

If in particular $\hat{A}$ is an observable that commutes with $\hat{H}$, *i.e.* if $[\hat{A},\hat{H}] = 0$, then

$$\frac{d\hat{A}}{dt} = 0$$

i.e. $\hat{A}$ is a conserved observable.

We can also prove the following theorem:
if two operators $\hat{A}$ and $\hat{B}$ commute, then they have common eigenfunctions.
Proof: Let ψ be an eigenfunction of $\hat{A}$ with eigenvalue a:

$$\hat{A}\psi = a\psi$$

operating on both sides with $\hat{B}$ we get

$$\hat{B}(\hat{A}\psi) = a\hat{B}\psi$$

on the l.h.s. we can write $\hat{B}\hat{A}\psi$, and then since by assumption $\hat{A}$ and $\hat{B}$ commute, we get

$$\hat{A}\hat{B}\psi = a\hat{B}\psi$$

thus $\hat{B}\psi$ is an eigenfunction of $\hat{A}$ with the same eigenvalue as ψ; therefore $\hat{B}\psi$ can differ from ψ only by a constant factor, *i.e.* we must have

$$\hat{B}\psi = b\psi$$

i.e. ψ is also an eigenfunction of $\hat{B}$.