Survival Facts from Quantum Mechanics

Operators, Eigenvalues and Eigenfunctions

An operator **O** may be thought as "something" that operates on a function to produce another function:

$$\mathbf{O}\,\mathrm{f}(x) = \mathrm{g}(x)$$

In most cases, the operators of quantum mechanics are *linear*. Operators are linear if they have properties:

$$\mathbf{O}[\mathrm{f}(x) + \mathrm{g}(x)] = \mathbf{O}\,\mathrm{f}(x) + \mathbf{O}\,\mathrm{g}(x)$$

$$\mathbf{O}c\,\mathrm{f}(x) = c\mathbf{O}\,\mathrm{f}(x)$$

where c is a constant (c can be a *complex number:* $c = a + ib,\ i = \sqrt{-1}$)

Examples:

linear operators:

x (multiplication by x):

$$x[\mathrm{f}(x) + \mathrm{g}(x)] = x\,\mathrm{f}(x) + x\,\mathrm{g}(x)$$

$\dfrac{d}{dx}$ (differentiation with respect to x):

$$\frac{d}{dx}[\mathrm{f}(x) + \mathrm{g}(x)] = \frac{d}{dx}\mathrm{f}(x) + \frac{d}{dx}\mathrm{g}(x)$$

A *non*linear operator: $\sqrt{}$ (square root operator):

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

The **eigenvalues** and **eigenfunctions** of an operator **A** are those numbers a_j and functions φ_j which satisfy

$$\mathbf{A}\varphi_j = a_j\varphi_j$$

where j is just a label for the various eigenfunctions and corresponding eigenvalues which satisfy this equation. In other words, when **A** operates on one of its eigenfunctions, say φ_3, the result is $a_3\varphi_3$ - just φ_3 back again, multiplied by the eigenvalue a_3.

Note that if we multiply an eigenfunction of a linear operator by a constant c we still have an eigenfunction:

$$\text{if } \mathbf{A}\varphi_j = a_j\varphi_j$$

$$\text{then } \mathbf{A}(c\varphi_j) = c\mathbf{A}\varphi_j = c(a_j\varphi_j) = a_j(c\varphi_j)$$

so that an eigenfunction φ_j and the function $\chi_j = c\varphi_j$ are not considered as independent eigenfunctions. (i.e., Since any eigenfunction is still an eigenfunction when multiplied by a constant, eigenfunctions which differ only by a multiplicative constant are not considered to be "distinct".)

Examples:

(1) The operator $\frac{d}{dx}$ has an eigenfunctions e^{kx} with eigenvalues k:

$$\frac{d}{dx}e^{kx} = ke^{x}$$

where k may take on any value.

(2) The operator $\left\{x\frac{d}{dx}\right\}$ also has an infinite set of eigenfunctions $\left\{x^n;\, n = 1,2,\ldots\infty,\, n \text{ may be nonintegral}\right\}$:

$$\left\{x\frac{d}{dx}\right\}x^n = x(nx^{n-1}) = nx^n$$

This example allows us to demonstrate that a linear combination of eigenfunctions is *not* an eigenfunction (unless the two eigenfunctions have the same eigenvalue). For example, there is no number c which satisfies the equation:

$$\left\{x\frac{d}{dx}\right\}\left[x^2 + x^3\right] = c\left[x^2 + x^3\right]$$

(3) The operator $\left\{\frac{d^2}{dx^2}\right\}$ has a set eigenfunctions of the form $\left\{\cos kx;\, k = \text{ real number}\right\}$ and $-k^2$ is the eigenvalue:

$$\frac{d^2}{dx^2}[\cos kx] = \frac{d}{dx}[-k\sin kx] = -k^2[\cos kx]$$

Note that the set of functions $\left\{\sin kx;\, k = \text{ any real number}\right\}$ are also eigenfunctions with the same eigenvalue:

$$\left\{\frac{d^2}{dx^2}\right\}[\sin kx] = \frac{d}{dx}[k\cos kx] = -k^2[\sin kx]$$

Therefore, for any given value of k, $\cos kx$, and $\sin kx$ are eigenfunctions of $\left\{\frac{d^2}{dx^2}\right\}$ with the same eigenvalue $-k^2$. This means that any combination of $\cos kx$ and $\sin kx$ is also an eigenfunction

$$\left\{\frac{d^2}{dx^2}\right\}[a\cos kx + b\sin kx] = -k^2[a\cos kx + b\sin kx]$$

In particular, if $a = 1$ and $b = i = \sqrt{-1}$ we have

$$\left\{\frac{d^2}{dx^2}\right\}[\cos kx + i\sin kx] = \left\{\frac{d^2}{dx^2}\right\}[e^{ikx}] = -k^2[e^{ikx}]$$

so that $\left\{e^{ikx}; k = \text{any real number}\right\}$ is an alternative set of eigenfunctions of $\left\{\frac{d^2}{dx^2}\right\}$.

Commutators

The *commutator* of two operators **A** and **B** is defined as

$$[\mathbf{A},\mathbf{B}] = \mathbf{AB} - \mathbf{BA}$$

if $[\mathbf{A},\mathbf{B}] = 0$, then **A** and **B** are said to *commute*. In general, quantum mechanical operators can not be assumed to commute.

<u>Examples</u>:

When evaluating the commutator for two operators, it useful to keep track of things by operating the commutator on an arbitrary function, $\mathrm{f}(x)$.

(1) evaluate $\left[x, \frac{d}{dx}\right]$:

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

$$= x\frac{d\,\mathrm{f}(x)}{dx} - \frac{d}{dx}(x\,\mathrm{f}(x)) = x\frac{d\,\mathrm{f}(x)}{dx} - x\frac{d\,\mathrm{f}(x)}{dx} - \mathrm{f}(x)\frac{d}{dx}x = -\mathrm{f}(x)$$

$$\left[x, \frac{d}{dx}\right]\mathrm{f}(x) = -\mathrm{f}(x) \quad \Rightarrow \quad \left[x, \frac{d}{dx}\right] = -1$$

We see that the effect of operating on any *arbitrary* $\mathrm{f}(x)$ with $\left[x, \frac{d}{dx}\right]$ is to produce $-\mathrm{f}(x)$, so that the last equation is generally true.

(2) In quantum mechanics, the operator for linear momentum in the x direction is $\hat{p}_x = \frac{\hbar}{i}\frac{d}{dx}$ (where $\hbar = h/2\pi$). Let's evaluate $[x, \hat{p}_x]$:

$$[x, \hat{p}_x] = x\hat{p}_x - \hat{p}_x x = \frac{\hbar}{i}\left(x\frac{d}{dx} - \frac{d}{dx}x\right)$$
$$= \frac{\hbar}{i}\left[x, \frac{d}{dx}\right] = -\frac{\hbar}{i} = i\hbar$$

(3) In <u>classical</u> mechanics, the angular momentum of a particle around the origin is a vector quantity, **L**, which is defined as $\mathbf{L} = \mathbf{r} \times \mathbf{p}$,

$$\mathbf{L} = \begin{vmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = (yp_z - zp_y)\hat{\mathbf{x}} + (zp_x - xp_z)\hat{\mathbf{y}} + (xp_y - yp_x)\hat{\mathbf{z}}$$

so, identifying the components of **L**,

$$L_x = yp_z - zp_y \quad ; \quad L_y = zp_x - xp_z \quad ; \quad L_z = xp_y - yp_x$$

which are the components of a single particle's angular momentum. To get the <u>quantum mechanical</u> *operators* for **L**, we insert the quantum mechanical *operators* for the linear momenta to obtain:

$$\hat{L}_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \quad ; \quad \hat{L}_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \quad ; \quad \hat{L}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

The reader should use these expressions to operate on an *arbitrary* function $f(x, y, z)$ to evaluate the commutators

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \quad ; \quad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x \quad ; \quad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$$

Quantum Mechanical Operators and Wavefunctions

If φ is to be considered a "well behaved" function, then we demand that it have the following properties:

(a) φ must be continuous (no "breaks")

(b) φ must have continuous derivatives (no "kinks")

(c) φ must be normalizable. To be normalizable, φ must obey the condition (the symbol $d\tau$ symbolizes integration over all space):

$$\int \varphi^* \varphi \, d\tau = C, \text{ where } C \text{ is a finite constant.}$$

Then we can normalize φ if we multiply by $1/\sqrt{C}$:

$$\int\left(\varphi^*/\sqrt{C}\right)\left(\varphi/\sqrt{C}\right)\mathrm{d}\tau = 1.$$

Of central importance is the *time-independent Schrödinger equation*

$$\mathcal{H}\Psi = E\Psi.$$

where $\mathcal{H}$ is the *Hamiltonian* (or energy) *operator* for the system. Ψ is called the *wavefunction* or *state function* for the system and must be "well behaved" in the sense indicated above. In quantum mechanics, physically observable quantities are associated with *Hermitian* operators (eg., the energy of the system, the momentum of the system or of particles within the system, the position of particles in the system, etc.) If an operator $\mathbf{A}$ is Hermitian it has the property

$$\int\varphi^*\mathbf{A}\chi\mathrm{d}\tau = \int\chi(\mathbf{A}\varphi)^*\,\mathrm{d}\tau,$$

for all well behaved functions φ and χ.

If a system is in a state described by Ψ, then the *expectation value* we would observe for the property associated with the Hermitian operator $\mathbf{A}$ is given by

$$\langle\mathbf{A}\rangle = \int\Psi^*\mathbf{A}\Psi\,\mathrm{d}\tau,$$

if it is a physically observable quantity, it must real:

$$\langle\mathbf{A}\rangle^* = \langle\mathbf{A}\rangle \text{ so } \int\Psi^*\mathbf{A}\Psi\,\mathrm{d}\tau = \int\Psi(\mathbf{A}\Psi)^*\,\mathrm{d}\tau.$$

Thus, the Hermitian property of operators associated with observables guarantees that calculated quantities for these observables will be real.

Example: Is $\hat{p}_x$ Hermitian?

$$\int_{-\infty}^{\infty}\Psi^*\hat{p}_x\Psi\mathrm{d}x = \int_{-\infty}^{\infty}\Psi^*\left(\frac{\hbar}{i}\frac{d}{dx}\Psi\right)\mathrm{d}x = \frac{\hbar}{i}\int_{-\infty}^{\infty}\Psi^*\left(\frac{d}{dx}\Psi\right)\mathrm{d}x =$$

(Integrate by parts, $\int_{-\infty}^{\infty}u\mathrm{d}v = uv\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}v\mathrm{d}u$)

$$= \frac{\hbar}{i}\Psi\Psi^*\Big|_{-\infty}^{\infty} - \frac{\hbar}{i}\int_{-\infty}^{\infty}\Psi\left(\frac{d}{dx}\Psi^*\right)\mathrm{d}x = \int_{-\infty}^{\infty}\Psi\left(\frac{\hbar}{i}\frac{d}{dx}\Psi\right)^*\mathrm{d}x = \int_{-\infty}^{\infty}\Psi(\hat{p}_x\Psi)^*\mathrm{d}x$$

note that if $\hat{p}_x$ didn't have the factor of *i* in front, it wouldn't be Hermitian.

Orthogonality (Definition):

two functions φ and χ are said to be *orthogonal* if

$$\int \varphi^* \chi \, \mathrm{d}\tau = 0$$

<u>Important property of Hermitian Operators</u>: Eigenfunctions of a Hermitian operator *are orthogonal*. (In the case where two or more eigenfunctions have the same eigenvalue, then the eigenfunctions can be made to be orthogonal).

proof: suppose φ_i and φ_j are eigenfunctions of $\mathbf{A}$ with respective eigenvalues a_i and a_j such that $a_i \neq a_j$.

$$\mathbf{A}\varphi_i = a_i \varphi_i$$

$$\mathbf{A}\varphi_j = a_j \varphi_j$$

By use of the Hermitian property we get:

$$\int \varphi_i^* \mathbf{A} \varphi_j \, \mathrm{d}\tau = \int \varphi_j (\mathbf{A}\varphi_i)^* \, \mathrm{d}\tau,$$

now operate with $\mathbf{A}$ on both sides of the equation:

$$a_j \int \varphi_i^* \varphi_j \, \mathrm{d}\tau = a_i^* \int \varphi_j \varphi_i^* \, \mathrm{d}\tau.$$

a_i is real because $\mathbf{A}$ is Hermitian. Then we have

$$(a_i - a_j) \int \varphi_j \varphi_i^* \, \mathrm{d}\tau = 0.$$

$$\therefore \int \varphi_j \varphi_i^* \, \mathrm{d}\tau = 0.$$

Now, if $a_i = a_j$, then we are free to combine φ_i and φ_j and we will still have an eigenfunction (see the example concerning $\frac{d^2}{dx^2}$ above). For example, suppose φ_1 and φ_2 both have eigenvalue a with respect to operator $\mathbf{A}$. Then we can take

$$\chi_1 = \varphi_1 \text{ and } \chi_2 = \varphi_2 + c\varphi_1$$

and we can choose $c = -\int \varphi_1^* \varphi_2 \, \mathrm{d}\tau \Big/ \int \varphi_1^* \varphi_1 \, \mathrm{d}\tau$.

You can show that χ_1 and χ_2 are orthogonal and both still have eigenvalue a.

QED.

Very Important Fact:

Commuting operators have common eigenfunctions.

suppose $\mathbf{A}$ and $\mathbf{B}$ commute: $[\mathbf{A},\mathbf{B}] = \mathbf{AB} - \mathbf{BA} = 0$.

Let $\{\varphi_i\}$ be the set of eigenfunctions of $\mathbf{A}$:

$$\mathbf{A}\varphi_i = a_i\varphi_i$$

$$\text{then, } \mathbf{B}(\mathbf{A}\varphi_i) = \mathbf{B}(a_i\varphi_i) = a_i(\mathbf{B}\varphi_i)$$

$$\text{but } \mathbf{AB} = \mathbf{BA} \text{ so } \mathbf{A}(\mathbf{B}\varphi_i) = a_i(\mathbf{B}\varphi_i)$$

$\therefore$ the function $\mathbf{B}\varphi_i$ is an eigenfunction of $\mathbf{A}$ with eigenvalue a_i. If φ_i is the *only* eigenfunction of $\mathbf{A}$ with eigenvalue a_i, then $\mathbf{B}\varphi_i \propto \varphi_i$ (in other words, $\mathbf{B}\varphi_i$ can only be an eigenfunction of $\mathbf{A}$ with eigenvalue a_i if it differs from φ_i by a constant multiplicative factor – p. 2 of this handout). Thus,

$$\mathbf{B}\varphi_i = b_i\varphi_i \text{ for some constant } b_i.$$

If a_i is a degenerate eigenvalue, i.e. there are more than one eigenfunctions of $\mathbf{A}$ with eigenvalue a_i, then we can take linear combinations of these eigenfunctions to satisfy this condition.