

These are related by

$$\boxed{\hat{A} \psi = a \psi} \quad \text{"An eigenvalue equation"}$$

Measurement of A ~~with ψ~~ always gives an eigenvalue (a) as a result

What is an operator? It is an instruction to do something.

CAMPAD

	<u>Operator</u>	<u>Instruction</u>	
	$\hat{D} \equiv \frac{d}{dx}$	take the derivative	$\hat{D}\psi = \frac{d\psi}{dx}$
Identity	$\equiv \hat{I}$	multiply by one	$\hat{I}\psi = \psi$
	\hat{P}	convert ψ to a polynomial	$\hat{P}\psi = a\psi^2 + b\psi$
	\hat{B}	annihilate ψ	$\hat{B}\psi = 0$

The most important operators in QM are

- Momentum : $\hat{p} = -i\hbar \frac{d}{dx}$ in 1-D.
- and
- position : $\hat{x} =$ multiplication by x in 1-D.

Eigenvalue equation for \hat{p}

$$-i\hbar \frac{d}{dx} \psi = p_x \psi \leftarrow \text{A D.E. for eigenfunction } \psi.$$

Solution : $\psi(x) = A e^{ikx}$, $k = p_x/\hbar.$

This is a plane wave. The eigenfunctions of momentum are plane waves. The wavelength λ is the value of x such that $k\lambda = 2\pi \leftarrow$ phase advances

so $\lambda = \frac{2\pi}{k} = \frac{2\pi}{p_x/\hbar} = \frac{h}{p_x}$ by 2π in one cycle

DeBroglie ..

The Energy Operator: "Hamiltonian"

In CM, the energy of a particle moving in a potential $V(x)$ is

$$\begin{aligned}
 \text{Energy} &= \text{KE} + \text{PE} = \frac{1}{2}mv^2 + V(x) \\
 &= \frac{1}{2m}(mv)^2 + V(x) \\
 &= \frac{p^2}{2m} + V(x).
 \end{aligned}$$

~~When~~ In QM, we assume that the energy operator - Hamiltonian - is given by

$$\begin{aligned}
 \hat{H} &= \frac{1}{2m}(\hat{p})^2 + V(x) = \frac{1}{2m} \hat{p} \hat{p} + V(x) \\
 &= \frac{1}{2m} \left(-i\hbar \frac{d}{dx}\right) \left(-i\hbar \frac{d}{dx}\right) + V(x).
 \end{aligned}$$

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

↑ Hamiltonian for one QM particle in potential $V(x)$.

The eigenvalue equation for \hat{H} is

$$\hat{H} \psi(x) = E \psi(x) \leftarrow \text{Also known as time-independent Schrödinger Eq.}$$

↑ eigenvalues of \hat{H} are the energies which the particle may have

Free Particle Case: $V(x) = 0$.

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) = E \psi(x)$$

$$\psi''(x) + \frac{2mE}{\hbar^2} \psi(x) = 0 \leftarrow \text{A.D.E. for } \psi(x)$$

Soln: $\psi(x) = Ae^{ikx} + Be^{-ikx}$.

Eigenfunctions of Energy for a free particle

$$k^2 = \frac{2mE}{\hbar^2}$$

$$E = \frac{(\hbar k)^2}{2m}$$

Also, $\hbar k = \text{momentum} = p$

so $E = \frac{p^2}{2m}$ as expected for a classical particle.



Let $f(x)$ be periodic with period $2L$, so that

$$-L < x < L$$

Then $f(x)$ can be represented by a Fourier Series:

$$f(x) = \sum_{n=0}^{\infty} \left[a_n \cos\left(\frac{n\pi x}{L}\right) + b_n \sin\left(\frac{n\pi x}{L}\right) \right]$$

If $f(x)$ = even, only cos terms appear ($b_n = 0$)

If $f(x)$ = odd, only sin terms appear ($a_n = 0$)

We can re-write this more compactly:

$$\cos \theta = \frac{1}{2} (e^{i\theta} + e^{-i\theta}) \Rightarrow \text{every cos has (+) and (-) exponents}$$

$$\sin \theta = \frac{1}{2i} (e^{i\theta} - e^{-i\theta}) \Rightarrow \text{every sin has (+) and (-) exponents}$$

\therefore Sum n from $(-\infty)$ to $(+\infty)$:

$$f(x) = \sum_{n=-\infty}^{+\infty} a_n e^{in\pi x/L}$$

$$\text{Then } A_n = \frac{1}{2} (a_{(n)} + a_{(-n)})$$

$$B_n = \frac{1}{2i} (a_{(n)} - a_{(-n)})$$

$$\text{and } A_0 = B_0 = 0. \quad a_0 = 1 = A_0$$

The set of functions $\{e^{in\pi x/L}\}$ form a complete set \Rightarrow Any periodic function can be expressed in terms of them by correctly choosing $\{a_n\}$.

If we multiply two of these functions together and integrate them over $-L < x < L$, we get

$$\int_{-L}^L \left(e^{im\pi x/L} \right) \left(e^{-in\pi x/L} \right) dx = \begin{cases} 0 & \text{if } m \neq n \\ 2L & \text{if } m = n. \end{cases}$$

We write this more compactly as

$$\frac{1}{2L} \int_{-L}^L \left(e^{im\pi x/L} \right) \left(e^{-in\pi x/L} \right) dx = \delta_{mn}$$

Kronecker Delta

$$\delta_{mn} = \begin{cases} 1, & \text{if } m = n \\ 0, & \text{if } m \neq n \end{cases}$$

"Ortho-normality conditions for the functions $\{ e^{im\pi x/L} \}$ "

~~This Fourier series is perfect for representing functions which are periodic, or which are zero outside of $-L < x < L$ (then we just say~~

$$f(x) = \begin{cases} \text{Fourier series}, & -L < x < L \\ 0, & x < -L \text{ or } x > L. \end{cases}$$

To find the coefficients $\{a_n\}$ for any particular $F(x)$, we use the orthonormality condition: "Fourier Trick method"

Evaluate

$$\begin{aligned} \frac{1}{2L} \int_{-L}^L F(x) e^{-in\pi x/L} dx &= \frac{1}{2L} \int_{-L}^L \left(\sum_{n=-\infty}^{\infty} a_n e^{im\pi x/L} \right) e^{-in\pi x/L} dx \\ &= \sum_{n=-\infty}^{\infty} a_n \left[\frac{1}{2L} \int_{-L}^L \left(e^{im\pi x/L} \right) \left(e^{-in\pi x/L} \right) dx \right] \end{aligned}$$

$$= \sum_{n=-\infty}^{\infty} a_n \delta_{nm} = a_m$$

↑ Kronecker delta kills all terms except when $n \equiv m$.

∴ To calculate a coefficient a_m , we should evaluate $\frac{1}{2L} \int_{-L}^L F(x) e^{im\pi x/L} dx$:

$$a_m = \frac{1}{2L} \int_{-L}^L F(x) e^{im\pi x/L} dx$$

This discrete Fourier Series is useful for periodic Functions. For ~~continuous~~ non-periodic Functions, we can use a continuous limit:

Write it this way:

$$F(x) = \sum_{n=-\infty}^{\infty} a_n e^{im\pi x/L} \frac{1}{\Delta n} = \frac{L}{2\pi} \sum_{n=-\infty}^{\infty} a_n e^{im\pi x/L} \left(\frac{\pi \Delta n}{L}\right)$$

Define $k \equiv \frac{\pi n}{L}$, $\Delta k = \frac{\pi \Delta n}{L}$ and $A(k) \equiv \frac{L}{\pi} a_n$

Then $F(x) = \frac{1}{\sqrt{2\pi}} \sum_{k=-\infty}^{\infty} A(k) e^{ikx} \Delta k$

Let $L \rightarrow \infty$, $\Delta k \rightarrow dk$:

$$F(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk A(k) e^{ikx}$$

Fourier Series for a non-periodic Func.

$A(k)$ is the "Fourier Transform" of $F(x)$:

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx f(x) e^{-ikx}$$

"Prove via Fourier's Trick"

Postulate II - Existence and meaning of the state function

A QM system is described by a "state function" or "wave function" $\psi(x)$. All properties of the system are encoded in $\psi(x)$. For example, the expectation value of observable C can be calculated by

$$\langle C \rangle = \int \psi^* \hat{C} \psi dx$$

where \hat{C} is the operator corresponding to C .

Corollary: $|\psi|^2 dx =$ Probability to find particle between x and $x+dx$ (Born interpretation of the wavefunction.)

Example Expectation value of position:

$$\langle x \rangle = \int \psi^* \hat{x} \psi dx \quad \neq \int x |\psi|^2 dx = \int \psi^* x \psi dx$$

by postulate II

position operator = multiply by x

$$= \int x |\psi|^2 dx$$

↓ Born interpretation

$$= \int x P(x) dx$$

So Postulate II gives a reasonable result for $\langle x \rangle$, given the Born interpretation of $\psi(x)$.

this is what we expect from the statistical definition of ~~expectation~~ mean or average value.

Postulate III - Collapse of the wavefunction

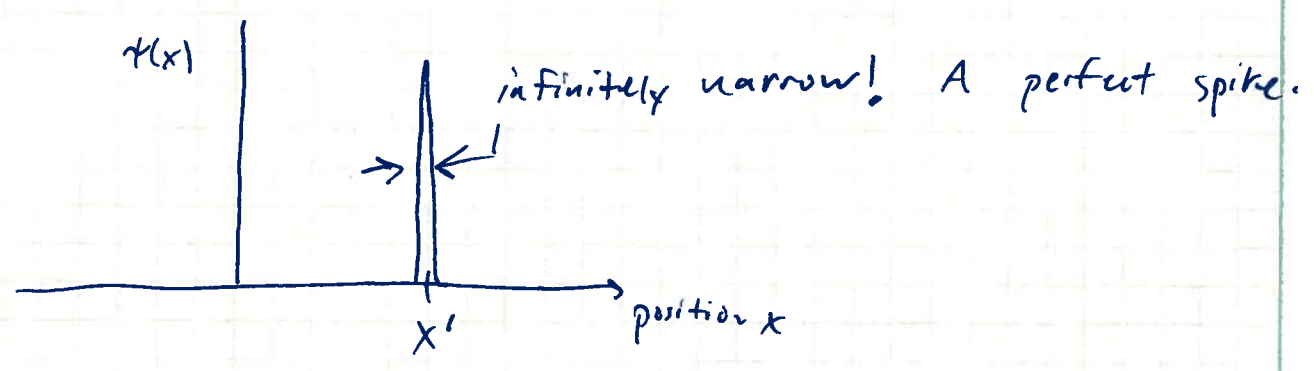
If observable A is measured, and eigenvalue a is the result (Postulate I), after the measurement the system will be left in the state ψ_a , where ψ_a is the eigenfunction of \hat{A} corresponding to eigenvalue a .

Ex: We measure the momentum of a free particle and find a particular value $p^* = \hbar k^*$. After the measurement, the wavefunction is

$$\psi(x) = A e^{ik^*x} \leftarrow \text{see the eigenfunction of } \hat{p} \text{ with eigenvalue } \hbar k^*$$

Ex: Measurement of position.

After a measurement of position (x), the particle's wavefunction will be 100% localized at x' ; the measured value:



We can think of this function as the Dirac Delta Function $\delta(x)$

Actually, $\delta(x)$ is not a well-defined function. It can really only exist inside an integral:

Definition of $\delta(x)$: $\int_{-\infty}^{\infty} f(x) \delta(x-x') dx = f(x')$

and $\int_{-\infty}^{\infty} \delta(x-x') dx = 1$, $\delta(x-x') = 0$ for $x \neq x'$

$\delta(0) = ??? (\rightarrow \infty)$ when $x = x'$.

~~The $\delta(x)$~~

In $\int_{-\infty}^{\infty} f(x) \delta(x-x') dx$, the $\delta(x-x')$ forces the integrand to be zero everywhere except the special value $x = x'$. At that point the integrand is $f(x') \delta(0)$, and the result of the ^{complete} integral is $f(x')$. The delta function "picks out" one value in the function $f(x)$.

Apparently, the eigenvalue equation for position measurement is

~~$\hat{x} \delta(x) = x \delta(x)$~~

$\hat{x} \delta(x-x') = x' \delta(x-x')$

But this truly only has meaning inside an integral:

$\int \hat{x} \delta(x-x') dx = \int x \delta(x-x') dx = x' \int \delta(x-x') dx$

\hat{x} means multiply by x

Postulate IV - Time evolution of the wavefunction.

When no measurements are being made, $\Psi(x)$ evolves in time governed by the Time-Dependent Schrodinger Eq:

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = \hat{H} \Psi(x,t)$$

- \hat{H} is the Hamiltonian for the system, or the Energy Operator.
- \hat{H} must be known if we want to know how $\Psi(x,t)$ evolves in time.
- We'll use Capital Ψ ; Ψ for wavefunctions which depend on time, and lower ψ ; ψ for wavefunctions which depend only on position (x).

~~The Time Dependent Schrodinger Eq. (TDSE) says that in a small time Δt the wavefunction changes by a small amount $\Delta \psi(x)$:~~

$$\frac{\Delta \psi(x)}{\Delta t} = \frac{-i}{\hbar} \hat{H} \psi(x, t \rightarrow t + \Delta t)$$

- According to Postulate III, if we make a measurement of an observable, the wavefunction "jump" discontinuously, instantaneously to ^{an} ~~and~~ eigenfunction of that observable. This "quantum jumping" or "wavefunction collapse" is not governed by the TDSE. It is entirely non-classical.

Let's solve the time-dependent Schrödinger Eq once and for all, and be done with it.

$$i\hbar \frac{d}{dt} \Psi(x,t) = \hat{H} \Psi(x,t) \leftarrow \text{T D S E.}$$

Remember, \hat{H} is an operator which describes the system. It is the operator of an energy measurement.

We guess a solution where $\Psi(x,t)$ is a product of two functions \Rightarrow one that only depends on time, and one that only depends on position.

$$\Psi(x,t) = \cancel{\Psi(x,t)} \quad \alpha(x) T(t) \leftarrow \text{We guess this solution}$$

Plus it in to the TDSE:

$$i\hbar \alpha(x) T'(t) = \hat{H} \alpha(x) T(t)$$

To simplify, assume that \hat{H} does not depend on time. Physically, this means that the ^{total} energy of the system is not changing (a conservative system.) Then \hat{H} can contain ^{only} \hat{x} and \hat{p} , but these operators will not act on $T(t)$. So we can bring $T(t)$ out front:

$$i\hbar \alpha(x) T'(t) = T(t) \hat{H} \alpha(x)$$

$$\frac{i\hbar T'(t)}{T(t)} = \frac{\hat{H} \alpha(x)}{\alpha(x)}$$

The left hand side depends only on time.

The right hand side depends only on position.

For them to be equal, they must both be constant:

$$\frac{i\hbar T'(t)}{T(t)} = E = \frac{\hat{H} Q(x)}{Q(x)}$$

↑
separation constant, a number.

We can now write two equations:

$$i\hbar T'(t) = E T(t) \Rightarrow \text{Soln: } \boxed{T(t) = A e^{-iEt/\hbar}}$$

$$\hat{H} Q(x) = E Q(x) \Rightarrow \text{Time Independent Schrödinger Eq.}$$

AKA, the eigenvalue equation

for energy.

- ∴ E , the separation constant, is the ^{energy eigenvalue} ~~energy of the~~ system and therefore is the energy of the system for our solution.
- ∴ $Q(x)$ is the energy eigenfunction corresponding to E .
- ∴ The solution to the TDSE is

$$\boxed{\Psi(x,t) = A Q(x) e^{-iEt/\hbar}}$$

Where $Q(x)$ is an eigenfunction of \hat{H} , and E is its eigen value.

To specify a solution more specifically, we must know exactly what \hat{H} is for our system. If we know \hat{H} , we can solve for $Q(x)$ by solving

Remarks

• Is our solution, $\Psi(x,t) = A \psi(x) e^{-iEt/\hbar}$ the only solution?

Three

⇒ Answer: No! Two reasons:

• We assumed a separable solution. There could ^{also} be non-separable solutions.

• In general, there will be many eigenfunctions of \hat{H} : $\psi_1(x), \psi_2(x), \psi_3(x), \dots$ each with its own energy eigenvalue: E_1, E_2, E_3, \dots

~~• Any linear combination of $\psi_n(x)$'s will also be a solution. For example, if $\psi_1(x)$ and $\psi_2(x)$ both satisfy $\hat{H}\psi_n = E_n\psi_n$, then~~

~~$\tilde{\psi}(x) \equiv a\psi_1(x) + b\psi_2(x)$ is also a solution for any a & b :~~

$$\hat{H}\tilde{\psi}(x) = \hat{H}(a\psi_1(x) + b\psi_2(x))$$

Each eigenfunction has its own separable solution:

$$\Psi_1(x,t) = \psi_1(x) e^{-iE_1 t/\hbar}$$

$$\Psi_2(x,t) = \psi_2(x) e^{-iE_2 t/\hbar}$$

⋮

ect.

Even more importantly, ~~we~~ can any linear combination of the separable solutions is also a solution:

Is $\Gamma(x,t) \equiv \sum_{\text{all } n} a_n \psi_n(x) e^{-iE_n t/\hbar}$ a ~~the~~ solution to the TDSE?
any set of coefficients at all!

Let's see:

$$i\hbar \frac{\partial}{\partial t} \Gamma(x,t) \stackrel{?}{=} \hat{H} \Gamma(x,t)$$

$$i\hbar \sum_{\text{all } n} a_n \psi_n(x) \left(-i \frac{E_n}{\hbar}\right) e^{-iE_n t/\hbar} \stackrel{?}{=} \sum_{\text{all } n} a_n \left[\hat{H} \psi_n(x) \right] e^{-iE_n t/\hbar}$$

$$\cancel{\hat{H}} \left(\sum_{\text{all } n} a_n \overset{E_n}{\psi_n(x)} e^{-iE_n t/\hbar} \right) \stackrel{?}{=} \sum_{\text{all } n} a_n \left(E_n \psi_n(x) \right) e^{-iE_n t/\hbar}$$

yes! $\rightarrow \sum_{\text{all } n} a_n \psi_n(x) e^{-iE_n t/\hbar}$

Any linear combination of separable solutions is also a solution.

This is one manifestation of the Principle of Superposition. A QM particle can be in a linear combination of states. This is fundamentally the same physics as in the two-slit experiment, when the particle apparently sees or travels through both slits.

The "Equation of Motion" of QM is the Time-Dependent Schrodinger Eq: (TDSE)

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H} \Psi(x,t)$$

Given an arbitrary wavefunction at $t=0$, $\Psi(x,t=0) \equiv \psi(x)$, the TDSE tells us how it changes or evolves in time. Specifically, it says that the rate of change is proportional to the Hamiltonian operating on Ψ .

We found "separable" solutions to the TDSE that look like

$$\Psi(x,t) = \underbrace{Q(x)}_{\text{this } E \text{ goes with this } Q(x)} e^{-iEt/\hbar}$$

where $Q(x)$ is an energy eigenfunction of the system, and E is its energy eigenvalue.

In general, we have many eigenfunctions of partner eigenvalues:

$$\Psi_1(x,t) = Q_1(x) e^{-iE_1 t/\hbar} \quad \text{where } \hat{H} Q_1(x) = E_1 Q_1(x)$$

$$\Psi_2(x,t) = Q_2(x) e^{-iE_2 t/\hbar} \quad \hat{H} Q_2(x) = E_2 Q_2(x)$$

⋮

$$\Psi_n(x,t) = Q_n(x) e^{-iE_n t/\hbar} \quad \hat{H} Q_n(x) = E_n Q_n(x)$$

Question : Can I put together a solution with an energy eigenvalue & a different energy eigenfunction?

$\Psi(x,t) = Q_3(x) e^{-i E_3 t / \hbar}$?? For example

Is this a solution to the TDSE??

Answer : No! Each e.f. evolves in time with a frequency determined by its own e.v.

BTW, $\frac{E}{\hbar}$ has units of frequency ($\text{Hz} = \frac{1}{\text{second}}$),

so we usually define

$$\omega_n \equiv \frac{E_n}{\hbar}$$

then we write

$\Psi(x,t) = Q_n(x) e^{-i\omega_n t}$. where $\omega_n = E_n/\hbar$,
& $\hat{H} Q_n = E_n Q_n$.

Bottom line : We have a bunch of separable solutions to the TDSE, one for each pair of e.f. & e.v.

We also found that any linear combination of separable solutions is also a solution:

$$\Psi(x,t) = \sum_n a_n \psi_n(x) e^{-iE_n t / \hbar} \leftarrow \text{Also a valid solution}$$

↑
any arbitrary set of coefficients

This is the principle of superposition, which

we saw in the two slit experiment: a QM particle can be in two or more states at the same time.

The following is one of the most important results in QM:

~~Any for any physical system~~

Any physical state Ψ can be written as a linear combination of the energy eigenfunctions

$$\Psi(x,t) = \sum_n a_n \psi_n(x) e^{-iE_n t / \hbar}$$

for any arbitrary $\Psi(x,t)$.

It's only a matter of choosing the right set of coefficients $\{a_n\}$.

We say that "the energy e.f.s are complete"

\Rightarrow we mean that any state can be written in terms

Specifically, $\Psi(x, t=0)$, the initial wave function, can be written as

$$\Psi(x, t=0) \equiv \psi(x) = \sum_n a_n \phi_n(x)$$

\uparrow lower case \uparrow coefficients.

Therefore, the typical procedure for solving a QM problem is this:

1) Find the energy e.f.s & e.v. by solving

$$\hat{H} \phi_n(x) = E_n \phi_n(x) \leftarrow \text{"Time-Independent Schrodinger Eq?"}$$

Solution yields a set of eigenfunctions $\{\phi_n\}$ and the corresponding eigenvalues $\{E_n\}$.

2) ~~Find~~ Find the appropriate coefficients so that

$$\Psi(x, t=0) = \psi(x) = \sum_n a_n \phi_n(x)$$

\uparrow initial state, usually given to us \uparrow Find $\{a_n\}$ so that this is true.

4) ~~Write~~ Write down the complete solution:

$$\Psi(x, t) = \sum_n a_n \phi_n(x) e^{-iE_n t}$$

\uparrow $\{a_n\}$ found in step (2). \uparrow ϕ_n & E_n found in step (1).

We typically never even write down the TDSE.