Differential Equations

Two important rules of D.E.s.

- The best way to solve a D.E. is to guess a solution and try it.

- A D.E. which has a maximum of (n) order derivatives has
  ① (n) free parameters AND
  ② requires (n) initial conditions for a unique solution.

A few D.E. are so simple and common that you are required to know their solutions:

① $$\underset{\substack{\uparrow \\ 1^{st}\text{ order}}}{\frac{dy(t)}{dt}} = A \Longrightarrow \text{Soln: } y(t) = At + \underset{\substack{\uparrow \\ \text{one free} \\ \text{parameter}}}{C}$$

Need one initial condition to specify C.

② $$\underset{\substack{\uparrow \\ 1^{st}\text{ order.}}}{\frac{dy(t)}{dt}} = A\,y(t) \Longrightarrow \text{Soln: } y(t) = \underset{\substack{\uparrow \\ \text{one free} \\ \text{parameter}}}{C}\,e^{At}$$

③ $\frac{d^2y(t)}{dt^2} + Ay(t) = 0 \Rightarrow$ Many equivalent ways to write the solution:

↑ 2nd order

Solution : $y(t) = C_1\left(\sin(\sqrt{A}\,t) + C_2\right)$

OR $y(t) = C_1\left(\cos(\sqrt{A}\,t) + C_2\right)$

OR $y(t) = C_1\left(\sin(\sqrt{A}t)\right) + C_2\cos\left(\sin(\sqrt{A}t)\right)$

OR $y(t) = C_1 e^{i\sqrt{A}t} + C_2 e^{-i\sqrt{A}t}$

OR $\vdots$

~~Example: $\frac{d^2y(t)}{dt^2} + 4y(t) = 0$~~

~~Solution:~~

Wave Formula Sheet

λ = wavelength (meters)

K = "wave number" (meters^{-1}) $= \frac{2\pi}{\lambda}$

T = period (seconds)

ν = frequency $= \frac{1}{T}$ = (seconds^{-1} or Hz)

ω = angular frequency $= \frac{2\pi}{T} = 2\pi\nu$ (Hz)

Phase difference between two points in space:

$\Delta\phi = kx$, x = distance between the points

Phase difference after waiting for time (t):

$\Delta\phi = 2\pi\left(\frac{t}{T}\right) = \omega t$

Planck Formula: Light is composed of photons.

Energy of each photon is $E = \underset{\text{Planck's constant}}{h}\nu = \underbrace{\left(\frac{h}{2\pi}\right)}_{\hbar = \frac{h}{2\pi}} \underbrace{(2\pi\nu)}_{\omega} = \hbar\omega$

$\therefore \boxed{E = \hbar\omega}$ Energy of a photon

DeBroglie: Both matter particles and light particles have a wavelength:

$$\text{DeBroglie Wavelength} = \lambda = \frac{h}{\underset{\text{particle momentum}}{p}}$$

For photons, momentum $= p = \dfrac{E}{\underset{\boxed{\text{speed of light}}}{c}}$ from special relativity

$$\text{So} \quad \frac{h}{p} = \frac{h}{(E/c)} = \left(\frac{h}{E}\right)c = \left(\frac{1}{\nu}\right)c = \lambda$$

So DeBroglie's wavelength makes sense for photons

If $\lambda = \frac{h}{p}$ then $p = \frac{h}{\lambda} = \left(\frac{h}{2\pi}\right)\left(\frac{2\pi}{\lambda}\right) = \hbar k$

Summary: $$\boxed{\begin{aligned} E &= h\nu = \hbar\omega \\ p &= \hbar k \end{aligned}}$$

Postulate I of QM: Eigenvalues and Eigenfunctions

For any observable A, there exists

① an "operator" ⇒ $\hat{A}$ ← hat means operator.

② "eigenvalues" ⇒ a ← a numerical value

③ "eigenfunctions" ⇒ ϕ ← a function

These are related by:

$$\boxed{\hat{A}\phi = a\phi}$$

"An eigenvalue equation"

> If we measure A, the result will always be an eigenvalue of A.

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

Operator	Instruction
$\hat{D} \equiv \frac{d}{dx}$	take the derivative : $\hat{D}\phi = \frac{d\phi}{dx}$.
Identity $= \hat{I} \equiv 1$	multiply by one : $\hat{I}\phi = \phi$.
$\hat{B}\phi$	Annihilate ϕ : $\hat{B}\phi = 0$.

The two most important operators in QM are

① Momentum : $\hat{p} = -i\hbar \frac{d}{dx}$ in 1D

② position : $\hat{x}$ = multiply by x in 1D.

Postulate II : The state function $\psi(x)$.

All properties of a QM system are described by the "state function" or "wave function" : $\psi(x)$.

Corallary ① : The expectation value for an observable C can be calculated by

$$\langle C \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, \hat{C}\, \psi(x)\, dx$$

where $\hat{C}$ is the operator for C.

Ex : $$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x)\, \hat{p}\, \psi(x)\, dx$$

$$\boxed{\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^*(x) \frac{d}{dx} \psi(x)\, dx}$$

Corallary ② : $|\psi(x)|^2 dx = \psi^*(x)\,\psi(x)\,dx$ = Probability to find the particle between x and $x+dx$.

"Born Interpretation of the wavefunction."

With the Born Interpretation,

$$\langle x\rangle = \int_{-\infty}^{\infty} \psi^*(x)\,\underset{\substack{\uparrow\\ \text{multiply}\\ \text{by } x}}{\hat{x}}\,\psi(x)\,dx = \int_{-\infty}^{\infty} \psi^* x\,\psi\,dx$$

$$= \int_{-\infty}^{\infty} x\,|\psi|^2\,dx$$

$\downarrow$ Born Interpretati

This is what →

$$\boxed{\langle x\rangle = \int_{-\infty}^{\infty} x\,P(x)\,dx}$$

we expect from the statistical definition of the expectation value of x.

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Postulate I: For every observable A, we have

$$\boxed{\underset{\substack{\uparrow\\ \text{an operator}}}{\hat{A}}\,\alpha = \underset{\substack{\uparrow\\ \text{an eigenvalue}}}{a}\,\underset{\substack{\uparrow\\ \text{an eigenfunction}}}{\alpha}} \leftarrow \text{eigenvalue equation}$$

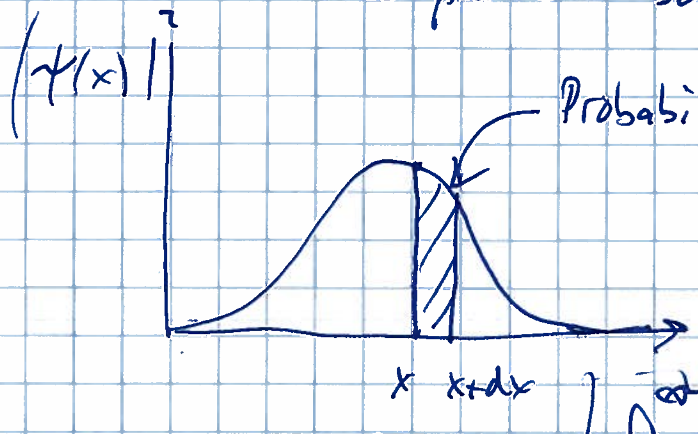
If we measure A, we always get eigenvalues of A.

Postulate II: Statistics & Wavefunctions

$$\langle C\rangle = \int_{-\infty}^{\infty} \psi^*(x)\, \underset{\curvearrowright}{\hat{C}\,\psi(x)}\, dx$$

$$\psi^*(x)\psi(x)dx = |\psi(x)|^2 dx = \underset{\uparrow}{P(x)dx}$$

Probability to find the particle between x and x + dx.



Probability to find particle between x & x + dx.

Also, note that

$$\boxed{\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \underset{\substack{\uparrow\\ \text{total probability to be anywhere}}}{1}}$$

"Normalization condition"

Postulate III: - Collapse of the Wavefunction

If we measure A, and eigenvalue (a) is the result, then after the measurement the state function for the system will be ϕ_a, the eigenfunction corresponding to (a).

Postulate IV: Time Evolution of the state function

If we make no measurements, then ~~ψ~~ the state function evolves in time according to the Time-Dependent Schroedinger Eq. (TDSE)

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

where $\hat{H}$ is the energy operator for the system (the Hamiltonian.)

- Convention: we'll use capital psi Ψ for state functions which depend on time: $\Psi(x,t)$ and lower case psi ψ for state functions which do not: $\psi(x)$.

Summary

$$\hat{A}\,\alpha = a\,\alpha$$

$$\langle A\rangle = \int_{-\infty}^{\infty} \psi^*(x)\,\hat{A}\,\psi(x)\,dx$$

$$|\psi(x)|^2\,dx = P(x)\,dx$$

$$\int_{-\infty}^{\infty} |\psi(x)|^2 = 1$$

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

Some important eigenvalue equations

Momentum: $\hat{p} = -i\hbar\dfrac{d}{dx}$

Eigenvalue Eq: $\hat{p}\,\alpha = p_x\,\alpha$

$-i\hbar\dfrac{d}{dx}\alpha = p_x\,\alpha$ ← A differential eq. for $\alpha(x)$.

Solution: $\alpha(x) = Ae^{i(p_x/\hbar)x}$

$$\frac{p_x}{\hbar} = k$$

$$\boxed{\alpha(x) = Ae^{ikx}}$$ ← The eigenfunctions ~~for~~ of momentum are exponential functions.

We call Ae^{ikx} a plane wave. The wavelength is $\lambda = \dfrac{2\pi}{k} = \dfrac{2\pi}{(p_x/\hbar)} = \dfrac{h}{p_x}$ ← DeBroglie

Ex: We measure the momentum of a particle, and the result is value $p = \hbar k'$.

After the measurement, the state function is

$$\psi(x) = u(x) = Ae^{ik'x}.$$

Energy : The Hamiltonian Operator $\hat{H}$.

In classical mechanics, Energy $= \frac{1}{2}mv^2 + V(x)$ for a single particle in a potential $V(x)$.

We can write this as

$$E = \frac{1}{2m}(mv)^2 + V(x)$$

$$= \frac{p^2}{2m} + V(x)$$

In QM, we assume that

$$\hat{H} = \text{energy operator} = \frac{1}{2m}(\hat{p})^2 + V(x)$$

$$= \frac{1}{2m}\hat{p}\,\hat{p} + V(x)$$

$$= \frac{1}{2m}\left(-i\hbar\frac{d}{dv}\right)\left(-i\hbar\frac{d}{dx}\right) + V(x)$$

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

Eigenvalue Equation for $\hat{H}$:

$$\boxed{\hat{H}u = Eu}$$ ← "Time-Independent Schroedinger Equation"

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

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

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

$$\boxed{\psi''(x) + \frac{2mE}{\hbar^2}\psi(x) = 0} \leftarrow$$ A D.E. for the eigenfunctions of energy.

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

where $k = \frac{\sqrt{2mE}}{\hbar}$

or $E = \frac{(\hbar k)^2}{2m} = \frac{(p_x)^2}{2m}$ as expected for the kinetic energy of a free particle.

Ex: Is $\psi(x) = A\cos(kx)$ an eigenfunction of

① momentum?

Answer: Try it: $\hat{p}\,A\cos(kx) = -i\hbar A\frac{d}{dx}\cos(kx)$

$$= +i\hbar kA\sin(kx)$$

$$\overset{?}{=} p_x A\cos(kx) \text{ ??}$$

No - $\sin(kx) \neq \cos(kx)$

So $\cos(kx)$ is not an e.f. of $\hat{p}$.

Is $\psi(x) = A\cos(kx)$ an eigenfunction of the free particle Hamiltonian: $\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$?

Try it: $\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} A\cos(kx)$

$$= \frac{\hbar^2 k^2}{2m} A\cos(kx) \overset{?}{=} E\, A\cos(kx)$$

Yes! and the eigenvalue is

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

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According to Postulate IV, the "equation of motion" of QM is the time-dependent Schroedinger Eq:

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

Given a wavefunction at $t = 0$, the TDSE tells us how it evolves in time.

<u>Good news</u>: We can solve this equation once and be done with it.

We guess a "seperable" solution:

$$\Psi(x,t) = \varphi(x)\, T(t)$$

$\varphi(x)$ only depends on position. $T(t)$ only depends on time

Plug in our guess:

$$i\hbar\, \varphi(x)\, T'(t) = \hat{H} \left[\varphi(x)\, T(t) \right]$$

To simplify, assume that $\hat{H}$ does not depend on time.

For example, assume that $\hat{H} = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$.

Then $$\hat{H}\left[\varphi(x) T(t)\right] = T(t)\, \hat{H}\, \varphi(x)$$

$$\therefore \quad i\hbar\, \psi(x)\, T'(t) = T(t)\, \hat{H}\, \psi(x)$$

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

only depends on time

only depends on x

If these are equal to each other for all t & x, they must both be equal to a constant.

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

Separation constant, a number.

Two equations:

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

$$\boxed{\hat{H}\psi(x) = E\,\psi(x)} \Leftarrow \text{Time-Independent Schroedinger Eq}$$

$\therefore$ Our solution is

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

where E = energy of the system

$\psi(x)$ = an energy eigenfunction of the system.

In general, there will be many energy eigenfunctions for a system, each with its own eigenvalue:

$$\phi_1(x)\,,\ \phi_2(x),\ \phi_3(x),\ \ldots$$

$$E_1\,,\ E_2\,,\ E_3\,,\ \ldots$$

Each of these is a solution to the TDSE:

$$\Psi_1(x,t) = A_1\,\phi_1(x)\,e^{-i(E_1/\hbar)t}$$

$$\Psi_2(x,t) = A_2\,\phi_2(x)\,e^{-i(E_2/\hbar)t}$$

$$\Psi_3(x,t) = A_3\,\phi_3(x)\,e^{-i(E_3/\hbar)t}$$

$$\vdots$$

Question: What if we add together some of these solutions? Is the sum a solution to the TDSE?

Answer: Try it!

$$\text{Let } \Psi(x,t) = \sum_{n=1}^{\infty} a_n\,\phi_n(x)\,e^{-iE_nt/\hbar}$$

↑ any set of coefficients at all!

Plug it in:

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

$$i\hbar \frac{\partial}{\partial t}\left[\sum_{n=1}^{\infty} a_n \varphi_n(x) e^{-iE_nt/\hbar}\right] \overset{?}{=} \hat{H}\left[\sum_{n=1}^{\infty} a_n \varphi_n(x) e^{-iE_nt/\hbar}\right]$$

$$i\hbar \sum_{n=1}^{\infty} a_n \varphi_n(x) \underbrace{\frac{\partial}{\partial t}\left[e^{-iE_nt/\hbar}\right]}_{\frac{-iE_n}{\hbar} e^{-iE_nt/\hbar}} \overset{?}{=} \sum_{n=1}^{\infty} a_n e^{-iE_nt/\hbar} \underbrace{\hat{H}\left[\varphi_n(x)\right]}_{E_n \varphi_n(x)}$$

because φ_n is an e.f. of $\hat{H}$

$$\sum_{n=1}^{\infty} a_n e^{-iE_nt/\hbar} E_n \varphi_n(x) \overset{\checkmark}{=} \sum_{n=1}^{\infty} a_n e^{-iE_nt/\hbar} E_n \varphi_n(x)$$

↑

Yes!

Any linear combination of seperable solutions is a solution

This is the principle of superposition. In QM, we can add two ~~solutions~~ valid states together and the result is another valid state.

Our strategy with every system in QM will be:

① ~~Find~~ Guess the Hamiltonian for our system.
(Usually $\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$ in Phys 401)

② Find the energy eigenfunctions for our $\hat{H}$ by solving the TIDE:

$$\hat{H}\varphi(x) = E\varphi(x)$$

Solutions: $\varphi_1(x), \varphi_2(x), \varphi_3(x), \varphi_4(x) \ldots$

$E_1, E_2, E_3, E_4, \ldots$

③ ~~For~~ If we know that at $t=0$, the wavefunction is $\Psi(x,t=0) = \psi(x)$, then to get $\Psi(x,t)$ for all time do this:
Find the set of coefficients $\{a_n\}$ such that

$$\psi(x) = \sum_{n=1}^{\infty} a_n \varphi_n(x).$$

Then $$\Psi(x,t) = \sum_{n=1}^{\infty} a_n \varphi_n(x) e^{-iE_n t/\hbar}$$