2026aug01 | 03_07003

Quantum Mechanics (QM)

A dive in and a Non-superficial Introduction

7.1) Schrödinger Equation

a) Discovered ~1925–1926 ~~over~~ Erwin Schrödinger's Christmas skiing holiday.

It CANNOT be derived, but there are physical intuitions leading to it.

In fact, the idea already existed that particles had wave properties, and that suggested there should be a wave equation determining their dynamics.

It is the fundamental dynamical equation of motion (wik) of non-relativistic (NR) QM. It is the analogue of Newton's 2nd law of motion (i.e., $\underset{\sim}{F}_{net} = m\underset{\sim}{a}_{cm}$).

In NR QM, fields (EM field etc.) are treated classically and are NOT quantized.

The relativistic generalization is quantum field theory (QFT) (wiki) which is the special relativistic generalization of QM. QFT is the current and probably forever theory of particle physics.

But NO established theory combines QM and gravity. This is elusive theory is called quantum gravity whose macroscopic limit will be general relativity or some replacement for that.

03_07004

b) The Sch. Equ
in 1-dimension for 1 particle
The particle has rest mass (i.e.,
a massive particle, NOT like
photon which has NO rest mass
and is a massless particle)

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

i) A 2nd order in space
1st order in time, linear differential equation.
It is what is true always
within its specified realm
of validity.

ii) Capital Greek Psi $\Psi = \Psi(x,t)$ is
the wave function and the solution
of the DE.

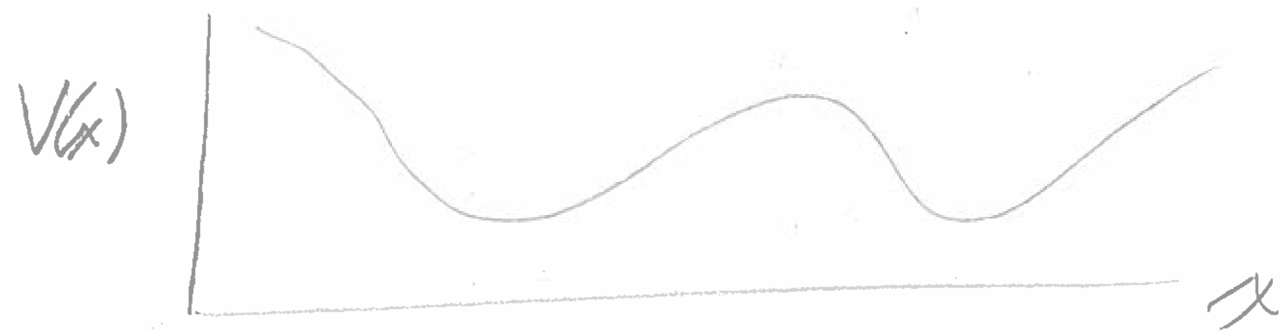
iii) Because the complex unit i appears
most physicists believe QM is intrinsically
a complex math theory, but like any
interpretations of QM there are dissenters (Google AI).

iv) $V(x)$ is potential energy

always given symbol V in QM and conventially called just Potential (which is confusingly different from Classical electromagnetism.

In QM jargon, it is called the Potential operator (or observable)

You have a potential (energy) landscape



v) m is the particle mass and since we are in NR limit, this is the same as rest mass.

vi) $\hbar = \frac{h}{2\pi}$ is Planck's constant divided by 2π

Sometimes called Dirac's constant or the reduced Planck's constant (Wiki), BUT usually just called h-bar

03_07006

$h = 6.626\ 070\ 15 \times 10^{-34}$ J/s

Exact in modern definition (Wik)

$= 4.135\ 667\ 696\ldots \times 10^{-15}$ eV/s

Note $1\,\mathrm{eV} \equiv 1.602\ 176\ 634 \times 10^{-19}$ J exactly

and the joule (J) is also specified exactly in term of fundamental constants

So the eV version is exact too, but with many unseen trailing digits

$\hbar$ is also exact, but irrational because of that 2π.

$\hbar = \frac{h}{2\pi} = 1.054\ 571\ 817\ldots \times 10^{-34}$ J/s

$= 6.582\ 119\ 569\ldots \times 10^{-16}$ eV/s

$\hbar$ is in units of <u>angular momentum</u> and is the natural and always used unit of angular momentum in QM, but also turns up the Sch. eqn where in 1-dimension it has <u>NO</u> obvious connection to <u>angular momentum</u>, but does to <u>momentum</u>.

2026aug01 | 03_07007

vii) $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

is in QM jargon

the kinetic energy operator

or kinetic energy observable

The operators determine which states (i.e., wave functions) have exact values for classical and QM variables like energy, momentum, angular momentum, spin.

and it shows how kinetic energy (KE) enters QM.

The more curvy Ψ,

the bigger $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

and the more KE there is.

$p_{op} = i\hbar\frac{\partial}{\partial x}$ is the momentum operator (CT-223)

KE "is" the curviness of the wave function Ψ.

Just accept it.

$k_{op} = i\frac{\partial}{\partial x}$ is the wavenumber operator

vii') $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$ is an operator

called the Hamiltonian

It's the mechanical energy operator

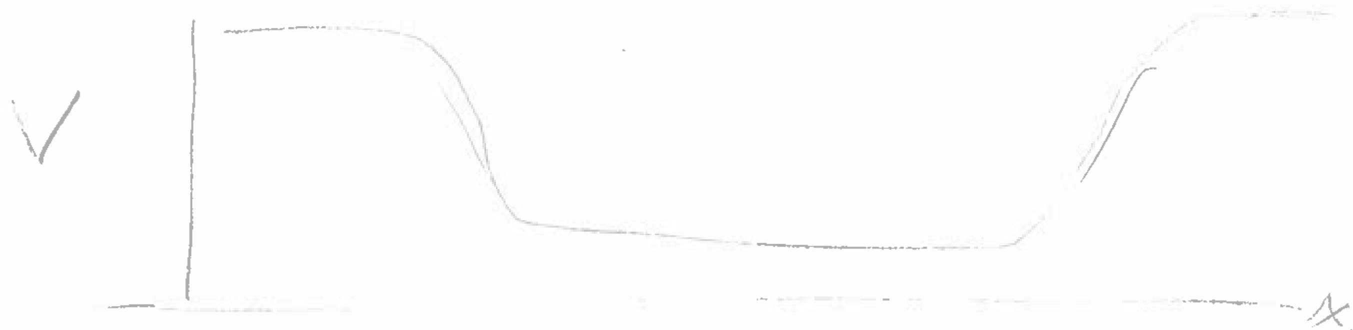
(or observable)

U3_07008

7.2 Solving the Sch. Equ. for the Infinite Square Well

the most elementary toy system in QM.

a) A NOT infinite, NOT square potential well is



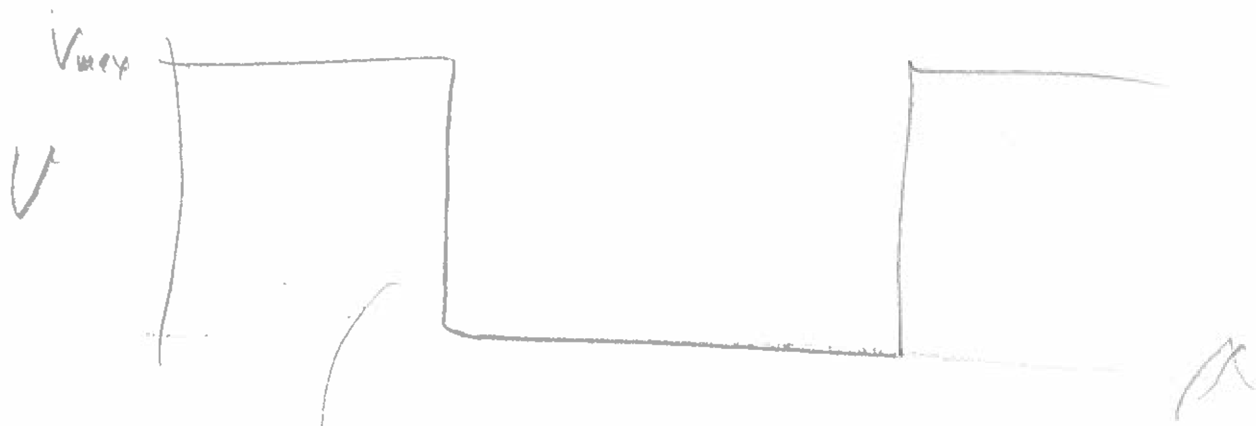
Recall, in classical mechanics

$$F_x = -\frac{\partial V}{\partial x}$$

$\therefore$ A classical particle can get trapped in potential well and oscillate forever *if* there is NO dissipation to waste heat

$E_{mech} = KE + V$ is conserved and energy oscillates between KE and V forms.

b) Finite square well

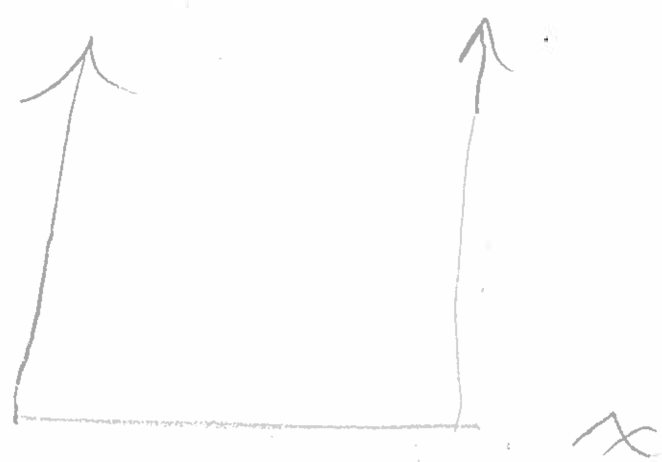


$F = -\frac{\partial V}{\partial x} = \infty$ at the boundaries.

A classical particle with some $KE < V_{max}$
just bangs back and forth
between the boundaries perpetually
if mechanical energy is conserved

c) Infinite square well

A classical particle is trapped forever unless it acquires infinite KE and QM particle too.



03_07010

d) First step in solving the Sch. eqn for any problem is separation of the space and time variables (Wiki: Separation of the Variables)

Posit a solution of the form

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

ψ is the small Greek psi

Now NOT all solutions will conform to this form, but you can get the other solutions by eigenfunction expansion (see p03_07021).

Substitute into the Sch. eqn. and divide by $\Psi(x,t)$ and you get:

$$\frac{-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi}{\psi} = \frac{i\hbar\frac{\partial T}{\partial t}}{T}$$

LHS (x only) = RHS (t only)

Must be equal for all x and t. ∴ Both sides cannot depend on x or t, and must equal a constant of separation.

03_07012

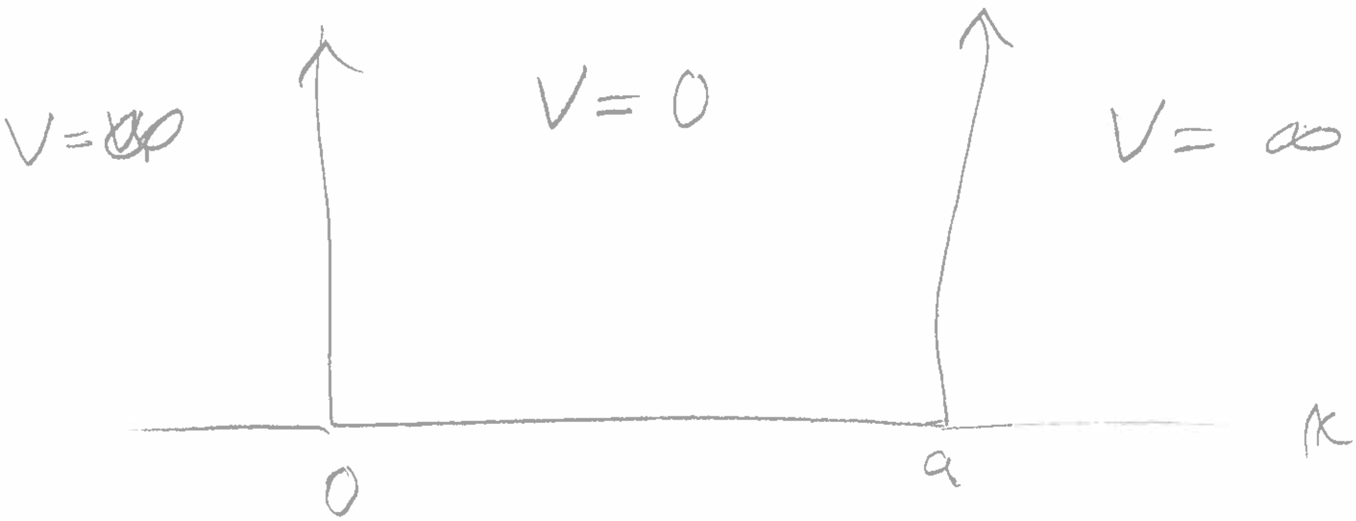
e) The space DE called the time-independent Sch. Eqn.

$$H\psi = E\psi \quad \text{in short form}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi$$

E is the eigenenergy and ψ is the eigenstate

For the infinite square well outside of the well $V = \infty$.



Therefore, $\psi(\text{outside}) = 0$ to satisfy the DE.

Inside

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi$$

However, to fully specify the problem, we need to specify the boundary conditions (BCs).

2026aug01 | 03_07011

We give the constant the symbol E, and to no surprise it is the energy of a quantum mechanical state.

In this context, the state (i.e., the $\psi(x)$ function) is called an eigenstate and the energy an eigenenergy or just energy.

But it is NOT called mechanical energy usually though that is the classical analogue.

The time part is easily solved

$$E = \frac{i\hbar \frac{\partial T}{\partial t}}{T}$$

$$\frac{\partial T}{\partial t} = \frac{1}{i\hbar} E T$$

$$\frac{dT}{T} = (-iE/\hbar)\,dt$$

Recall

$$\frac{1}{i} = \frac{i}{i^2} = -i$$

$$\underbrace{T}_{|T|=1} = \underbrace{e^{-iEt/\hbar}}_{\text{But I think this the what people mostly write}} = \underbrace{e^{-i\omega t}}_{\omega = \text{angular frequency}} \quad \text{(CT-32)}$$

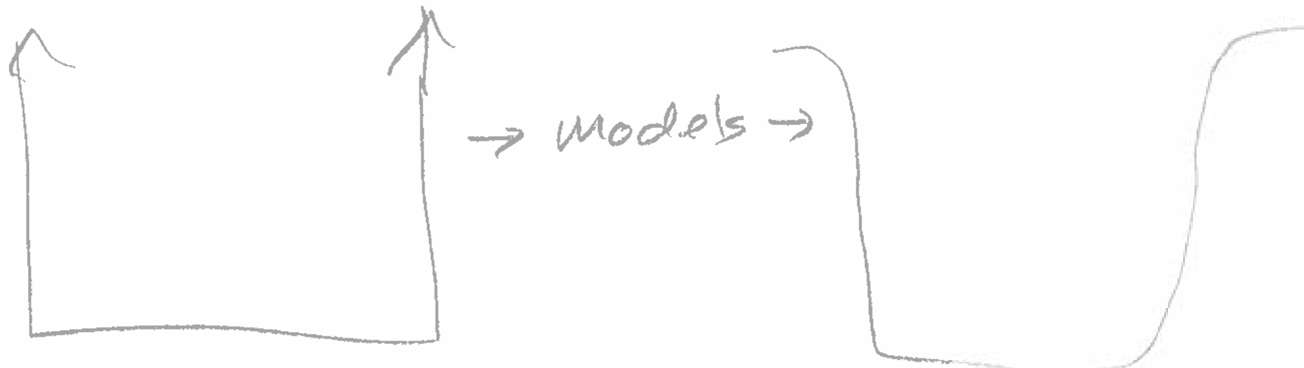
T is NOT a standard. Mostly people just write the function itself rather than a symbol. Just write $e^{-iEt/\hbar}$

2026aug01 | 03_07013

These are $\psi(x=0)=\psi(x=a)=0$.

The rationale for these BCs is this:

The infinite square well is a model for a deep steep well



And for smooth potentials which are believed to be most realistic, ψ should be smooth: i.e., differentiable to all orders everywhere.

The best we can do in making or ψ smooth at the boundaries is to make $\psi(x=0)=\psi(x=a)=0$ and so ψ is continuous at the boundaries

03_07014 |

What about making $\psi'(x=0) = \psi'(x=a) = 0$?

That would be even smoother at the boundaries,

But $\psi'(x=0) = \psi'(x=a) = 0$

leads to $\psi(x) = 0$

everywhere solutions which are NOT physical solutions.

In fact, solutions that are physically real require

$$\int_{-\infty}^{\infty} |\psi|^2 dx \text{ be \underline{normalizable}} \begin{cases} \neq 0 \\ \neq \infty \end{cases}$$

and, in fact, the final solution is normalized: i.e.,

$$1 = \int_{-\infty}^{\infty} |\psi|^2 dx = \int_0^a |\psi|^2 dx$$

for the infinite square well.

$|\psi|^2$ = modulus of the in-general complex function squared.

$|\psi|^2$ is called the probability density

[2026aug01] [03-07015

$|\psi|^2$ according the longstanding

Born rule

(really Born axiom of quantum mechanics).

f) The Born Rule

Due to Max Born in 1920s who was a Nobel Prize winner and remarkably the grandfather of Olivia Newton-John

The interpretation of the Born rule is that if you make a measurement of the position of a particle, you collapse the wave function (or do whatever "collapse" really is) and the probability of finding the particle in dx is $|\psi(x)|^2 dx$

03_07016

My personal view is to think of $|\Psi(x)|^2$ as the density of existence at x, but this is view and there are many views and QM is indifferent to our opinions. The formalism is always right as far as we know.

The particle exists in a superpositions in my view which is just following a herd

But what constitutes a measurement?

Empirical experience for any particular system tells you when to break off calculating wave function evolution (which is completely deterministic according the Sch. eqn.) and calculate probabilities. And when you calculate probabilities at the right moment, you always get the right answer!!!

Google AI confirms this, but I knew it from a Brian Greene for years, but no QM text book I know of states it plainly.

The lack of a theory
to tell you when to
calculate probabilities
remains one of the
great and frustrating
mysteries of QM.
The mystery is called
the measurement problem.

Some believe in wave function "collapse"
happens due some unknown
mechanism.
Some suggest Many Worlds.
There is NO collapse
or equivalent. Every possibility
in realized in parallel worlds.

But all is NOT ~~lost~~.
AI will solve the measurement problem
next week.

9) To return to theme: Solving for eigenstate K

$\psi(x=0) = \psi(x=a) = 0$ for most smoothness
at boundaries consistent with $\psi(x)$ being
normalizable and actually normalized
$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$ since the particle must be somewhere

03_07018

or in my view
have a total existence of 1.

At this point solving the DE

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x} = E\psi$$

ψ is usually called the eigenstate or eigenfunction

is easy.

It is the simple harmonic oscillator eq.n of classical physics. recall.

But this is NOT the quantum simple harmonic oscillator, That has $V(x) = \frac{1}{2}k x^2$ where

k is some constant ; for [illegible]
[illegible]
simple harmonic oscillator potential energy

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi$$

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

or

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

or

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

where we identify k with our old friend from waves on a string as the wave number k

2026aug01 | 03_07019

The general solution is

2nd order DE and so 2 independent solution

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

The cosine solution cannot match $\psi(x=0)=0$, and so $B=0$.

$\therefore$ $\psi(x) = A\sin(kx)$

where A is the normalization constant and match the BC $\psi(x=a)=0$, we require $ka = n\pi$ with n an integer ≥ 1

Negative integer solutions are NOT needed. In fact, overall solutions that differ by a phase factor $e^{i\phi}$ which can be ± 1 are mathematically and physically the same solution. See p. 03-07021

We require

$$1 = \int_0^a |A\sin(kx)|^2 dx$$

$$1 = A^2 \frac{1}{k}\int_0^{n\pi} \sin^2 y \, dy$$

$$= A^2 \frac{1}{k}\int_0^{n\pi} \frac{1}{2}\left[1 - \cos(2y)\right] dy$$

(Wiki: trig identities: double-angle formulae)

$$= A^2 \frac{1}{k}\,\frac{1}{2}\left[y - \frac{1}{2}\sin(2y)\right]_0^{n\pi}$$

$= A^2 \frac{1}{k}\left(\frac{1}{2}\right) n\pi = A^2\frac{a}{2}$, and so $A = \sqrt{\frac{2}{a}}$ where again the overall sign is physically irrelevant

Actually, ψ is a pure real here, NOT a complex function. But in general ψ's are complex.

03_07020

$\therefore \quad \chi(x) = \sqrt{\frac{2}{a}} \sin(kx)$ are the eigenstates or eigenfunctions

where $\quad k = \frac{n\pi}{a}$, n integer ≥ 1

$\boxed{\text{n is a quantum number}}$

Quantum number index allowed variable values

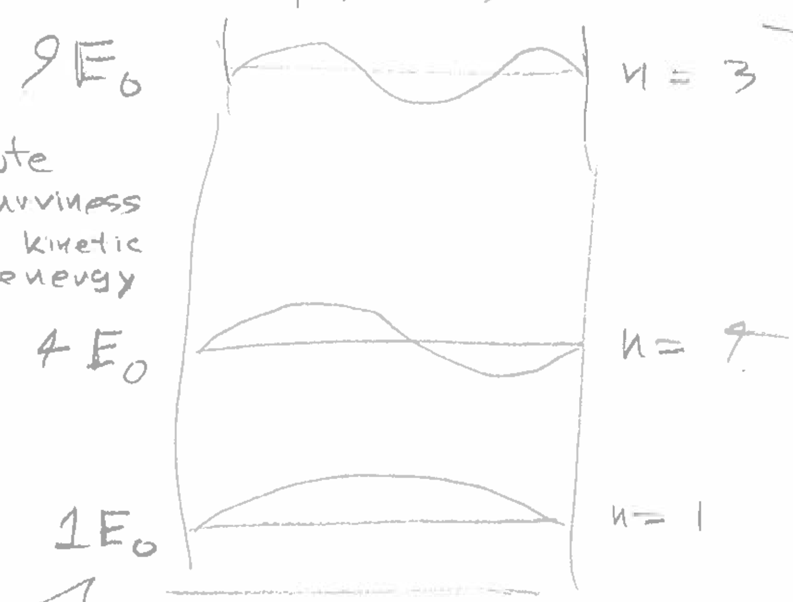
and from p. 03_07018

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

$$\therefore \quad E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2$$

$$E = E_0 n^2$$ → (Wiki: Infinite square well agrees)

$n = 1$ gives the ground state. The state of lowest energy.



Note curviness is kinetic energy

Ground state or Zero-point energy

The infinite square well problem illustrates a basic feature of QM. Bound systems only have quantized states, NOT a continuum of them. Also there is a zero point energy and so there is NO at-rest state in a classical sense

202Gaug01

03_07021

The total eigenstate wave function is

$$\Psi_n(x,t) = \left[\frac{1}{\sqrt{2}} \sin(k_n x)\right] e^{-iE_n t/\hbar}$$

Solving the infinite square problem is on every intro QM final!

h) Now what about $\Psi(x,t)$ that cannot be separated?

The formalism also guarantees the eigenfunctions are othogonal: $\int \chi_m^* \chi_n \, dx = \delta_{mn}$

There is a formalism of eigenfunctions (Arf-510) that tells us that any normalizable function $\chi(x)$ that matches the BCs can be expanded in eigen functions

Thus $a_n = \int \chi_n^* \chi \, dx$ is how the coefficients are determined

Say you are give $\chi(x)$ as an initial condition

$$\chi(x) = \sum_{n=1}^{\infty} a_n \chi_n(x)$$

So only mathematically and physically distinct eigenfunction occur in expansion

Note χ_n that just differ in sign or phase factor $e^{i\phi}$, all just get included in one term with coefficient a_n, and so are mathematically NOT distinct solutions in an expansion sense,

But this means that are also NOT distinct in a physical sense since the expansion is the general for the initial condition Ψ_0. They are also NOT distinct a Born rule sense, but we CANNOT explicate that here but they are NOT

03_07022

Since $\psi(x)$ is the initial condition

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

Recall, the Schrödinger equation is linear and so the sum of solutions is a solution.

So $\Psi(x,t)$ is a solution of the Sch. equ. and since it satisfies the initial conditions, it just is the general solution for our initial condition

7.3 Lots More to QM

- spin
- symmetrization principle
- other standard ideal solutions
- perturbation theory, etc.

We leave it all to be covered sine die

(without specifying a day).