PHOT 301: Quantum Photonics

LECTURE 02

Michaël Barbier, Fall semester (2024-2025)

OVERVIEW

week	Topic	Reading
Week 1	Introduction & Required Mathematical Methods. Waves and Schrödinger's equation, Probability, Uncertainty and Time evolution. Infinite square well.	**Ch. 1 & Ch. 2 (up to the infinite well)**
Week 2	The harmonic oscillator, Creation and annihilation operators. Free particle, 1D Bound states & Scattering/Transmission, Finite well	
Week 3	Quantum mechanics formalism: Functions and operators, uncertainty. Approximation methods.	
Week 4	Angular momentum and the Hydrogen atom, Spin Magnetic fields, The Pauli equation, Minimal Coupling, Aharonov Bohm Perturbation: Fine Structure of Hydrogen, The Zeeman Effect	
Week 5	Identical particles, Periodic table, Molecular bonds, Periodic structures, Band structure, Bloch functions Time-dependent perturbation: Absorption, spontaneous emission, and stimulated emission	
Week 6	Final exam	

FOR NEXT WEEK

- Textbook Chapter 1: 1.1, 1.2, 1.3, 1.5, 1.8
- Textbook Chapter 2: 2.1(c), 2.3, 2.4, 2.5, 2.7
- Homework documents:
  - phot301_homework_integration.pdf
  - phot301_homework_solving_equations.pdf
  - phot301_homework_fourier.pdf
- Reading (by Thursday 24 July 2025): Chapter 2 of Griffiths

STATIONARY SOLUTIONS & ENERGY LEVELS

SOLVING THE 1D SCHRODINGER EQUATION

The Schrodinger equation was given by:

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

- The complex wave function $\Psi(x,t)$ is not observable
- Potential energy: $V \to V(x,y,z,t)$
- $\hbar = \frac{h}{2\pi} = 1.055 \times 10^{-34}$ J s
- Probability to find particle in x at time t given by $|\Psi(x,t)|^2$:

$$P(x \in [a,b]) = \int_a^b |\Psi(x,t)|^2 dx$$

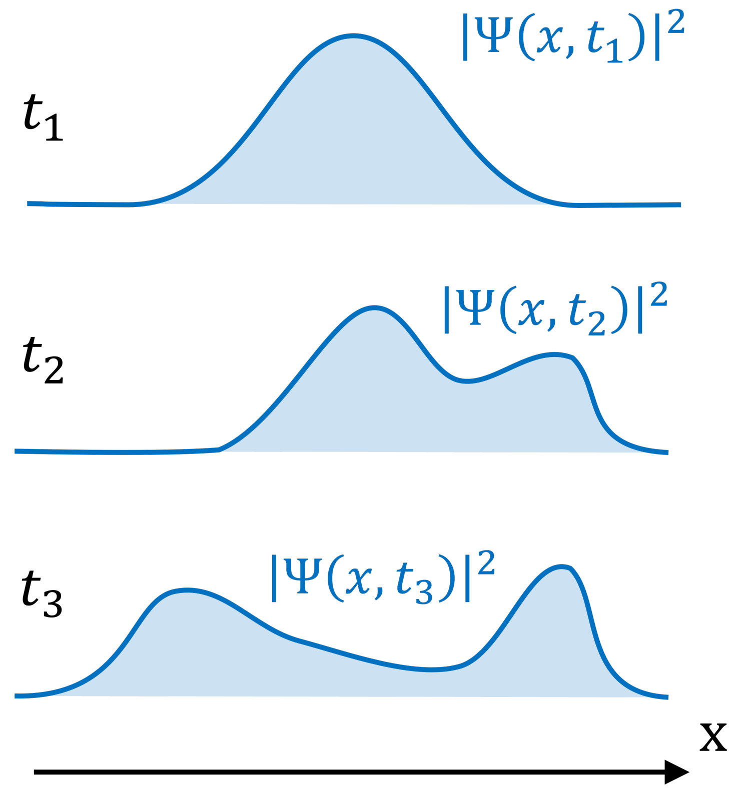
SOLVING THE 1D SCHRODINGER EQUATION

- Wave function $\Psi(x,t)$ defines $|\Psi(x,t)|^2$
- How to calculate $\Psi(x,t=0)$?
- Evolution in time of $\Psi(x,t)$?

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

$$+V(x,t)\Psi(x,t)$$

How do we solve for given $V(x,t)$?



SOLVING THE 1D SCHRODINGER EQUATION

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

How do we solve this equation for given $V(x,t)$?

- Assume $V(x,t)$ independent of time: $V(x) \leftarrow V(x,t)$
- Solve by separation of the variables $\Psi(x,t) = \psi(x)\phi(t)$

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

SOLVING THE 1D SCHRODINGER EQUATION

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

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

Divide the equation by $\Psi(x,t) = \psi(x)\phi(t)$

$$\Rightarrow i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)$$

$\longrightarrow$ the left hand side depends only on x and the right hand side only on t.

$$\Rightarrow i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = \text{constant } E$$

TIME-DEPENDENCE & STATIONARY EQUATION

$$i\hbar \frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = E$$

$\longrightarrow$ System of 2 ordinary differential equations:

$$\begin{cases} -\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2} + V(x) = E \\ i\hbar \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} = E \end{cases}$$

IF we can solve both equations $\Longrightarrow \Psi(x,t) = \psi(x)\phi(t)$ is a solution

TIME EVOLUTION

- Solving the equation for $\phi(t)$

$$i\hbar \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} = E \quad \Rightarrow \quad \frac{d\phi(t)}{dt} = -\frac{i}{\hbar} E\phi(t)$$

1st order differential equation with general solution:

$$\phi(t) = C\exp(-iEt/\hbar)$$

Full solution of the form (C is absorbed):

$$\Psi(x,t) = \psi(x)\phi(t) = \psi(x)\exp(-iEt/\hbar)$$

Notice that the probability $|\Psi(x,t)|^2 = |\psi(x)|^2$ is independent of t

TIME-INDEPENDENT EQUATION

Time-independent Schrodinger equation (TISE):

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

Or we can write

$$\hat{H}\psi = E\psi \quad \text{with Hamiltonian} \;\; \hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

The expectation value of $\hat{H}$ is:

$$\langle\hat{H}\rangle = \int \Psi^* \hat{H}\Psi dx = \int \Psi^* E\Psi dx = E\int |\Psi|^2 dx = E\int |\psi|^2 dx = E$$

GENERAL SOLUTION OF THE TDSE

- From the theory of differential equations:
  - The general solution is a **linear superposition** of solutions $\{\psi_n(x)\} = \psi_1(x), \psi_2(x), \psi_3(x), \ldots$
  - Independent solutions
  - Separate energies $\{E_n\}$ for corresponding $\{\psi_n(x)\}$
  - Solutions form an **infinite** and **complete basis**

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

Notice: General probability $\left|\Psi(x,t)\right|^2$ does depend on time

GENERAL SOLUTION OF THE TDSE

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

One can proof that $|c_n|^2$ is the probability to measure energy as E_n (Griffith's Chapter 3):

$$\langle \hat{H} \rangle = \int \Psi^* \hat{H} \Psi dx = \sum_{n=1}^{\infty} |c_n|^2 E_n \quad \text{and} \quad \sum_{n=1}^{\infty} |c_n|^2 = 1$$

POTENTIAL ENERGY FUNCTION V(X)

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

- Potential energy $V(x)$ is linked to force $F = -\frac{\partial V}{\partial x}$

$\Longrightarrow$ if $V(x)$ is a constant corresponds to zero force

$\Longrightarrow$ A linear $V(x)$ corresponds to a constant force

$\Longrightarrow$ A parabolic $V(x)$ corresponds to a linear force (like a spring)

SQUARE POTENTIAL ENERGY WELL

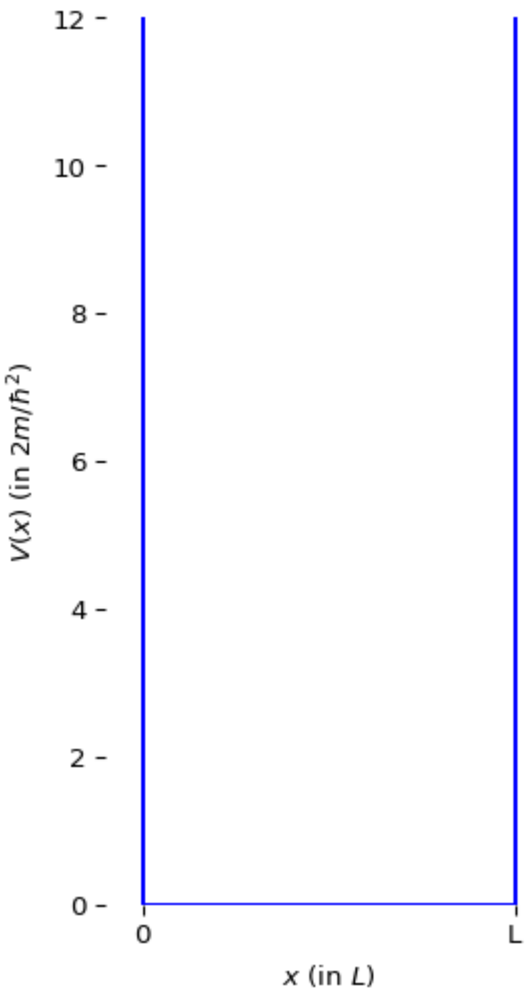
INFINITE WELL

- Inside the well a particle can exist
- Outside the well the potential is infinite

$$\begin{cases} V(x<0)=\infty \\ V(0<x<L)=0 \\ V(x>L)=\infty \end{cases}$$

- Task: solve the stationary Schrodinger equation for $V(x)$

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



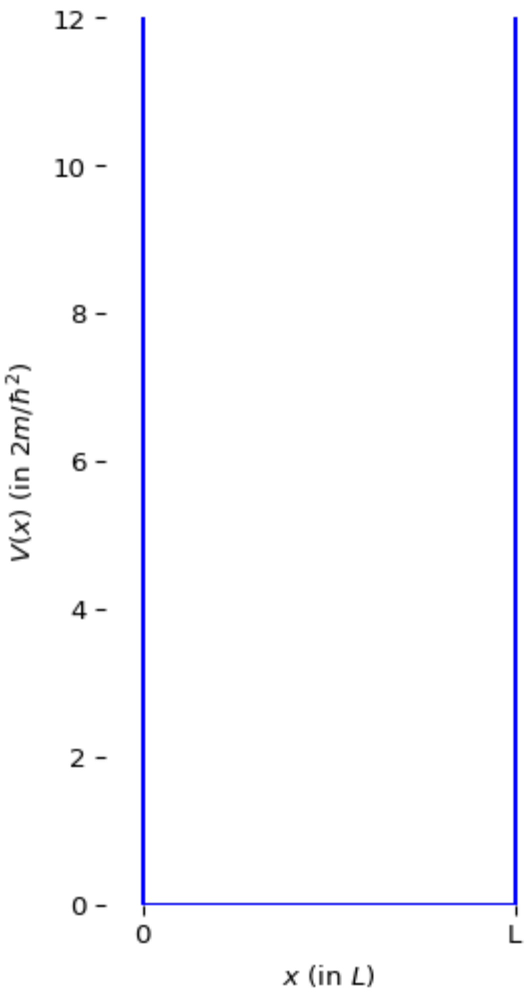
INFINITE WELL: SOLUTION IN THE WELL

- Particles outside would have infinite energy
- Wave function $\psi(x)$ should be zero outside
- Assume $\psi(0) = \psi(L) = 0 \longleftarrow \psi(x)$ ctu
- Inside the well $V(x) = 0$:

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

General solution:

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



INFINITE WELL: SOLUTION IN THE WELL

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

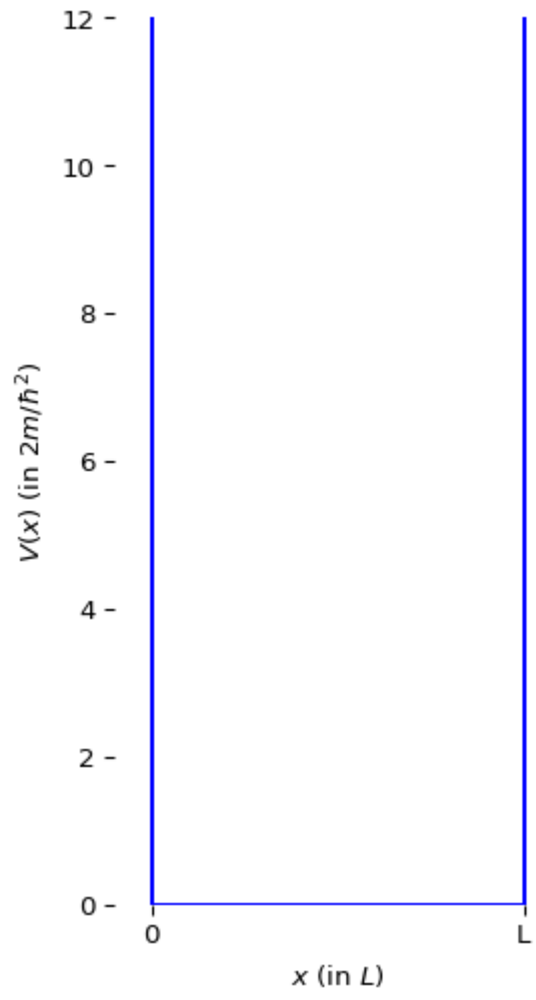
$$\psi(x) = A\cos(kx) + B\sin(kx)$$

- with A and B complex numbers
- $k = \sqrt{2mE/\hbar^2}$ a complex number

Apply BC's $\psi(0) = \psi(L) = 0$:

$$\psi(0) = 0 \quad \Rightarrow \quad A = 0$$

$$\psi(x) = B\sin(k\,x)$$



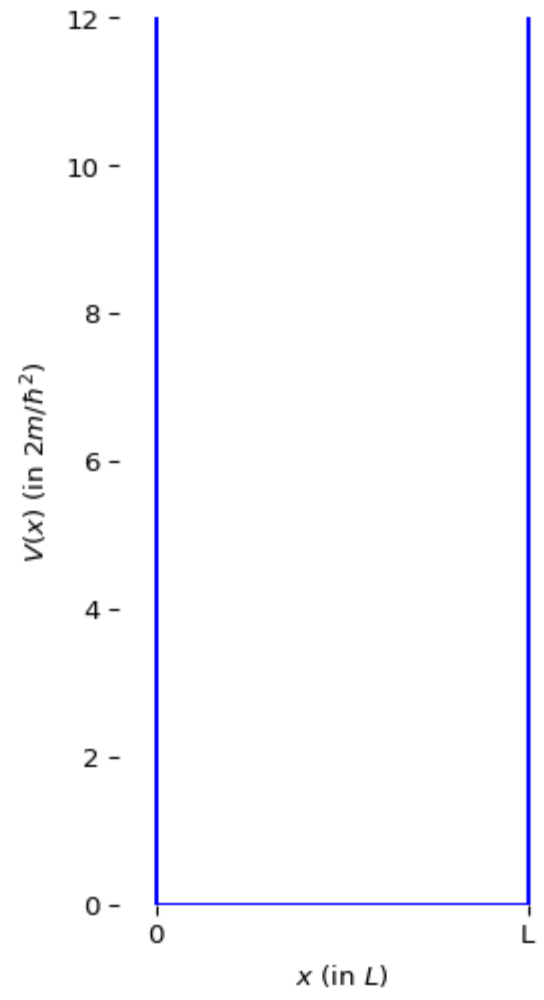
INFINITE WELL: ENERGIES

$$\psi(x) = B\sin(k\,x)$$

Apply the other BC: $\psi(L) = 0$:

$$k_n = \sqrt{2mE_n/\hbar^2} = n\pi/L$$

$$\implies \begin{cases} \psi_n(x) = A_n \sin\left(\dfrac{n\pi x}{L}\right) \\ E_n = \dfrac{\hbar^2 k_n^2}{2m} = \dfrac{\hbar^2}{2m}\left(\dfrac{n\pi}{L}\right)^2 \end{cases}$$



INFINITE WELL

$$\psi(x) = B\sin(k\,x)$$

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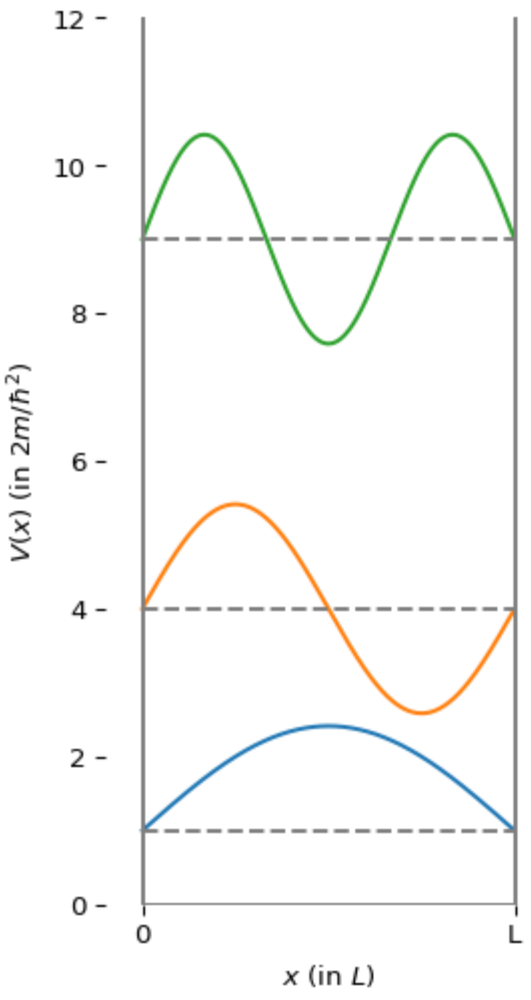


INFINITE WELL: NORMALIZATION

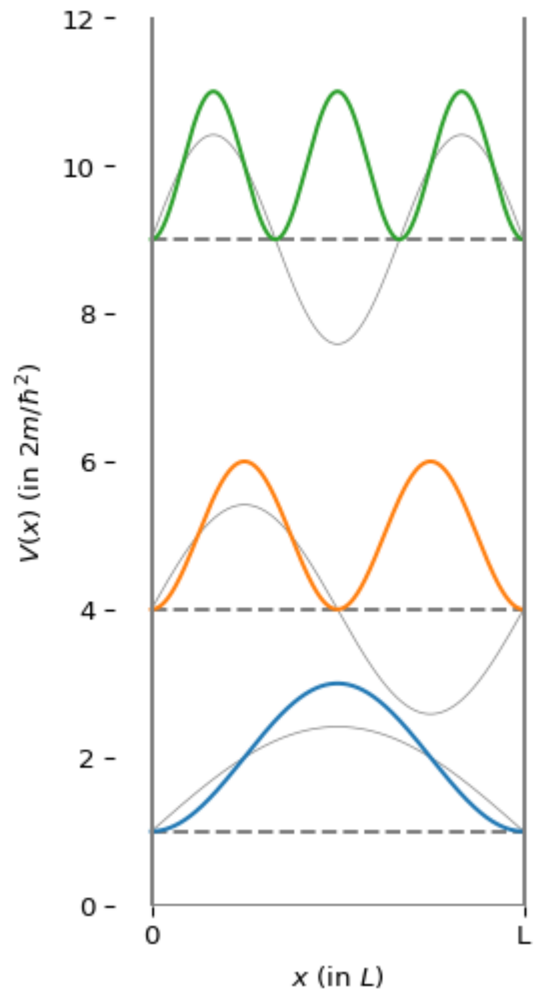
$$\psi_n(x) = A_n \sin\left(\frac{n\pi x}{L}\right)$$

- Obtain A_n from normalization $\int |\psi|^2 = 1$

$$1 = \int_0^L |A_n|^2 \left|\sin\left(\frac{n\pi x}{L}\right)\right|^2 dx = \frac{|A_n|^2 L}{2}$$

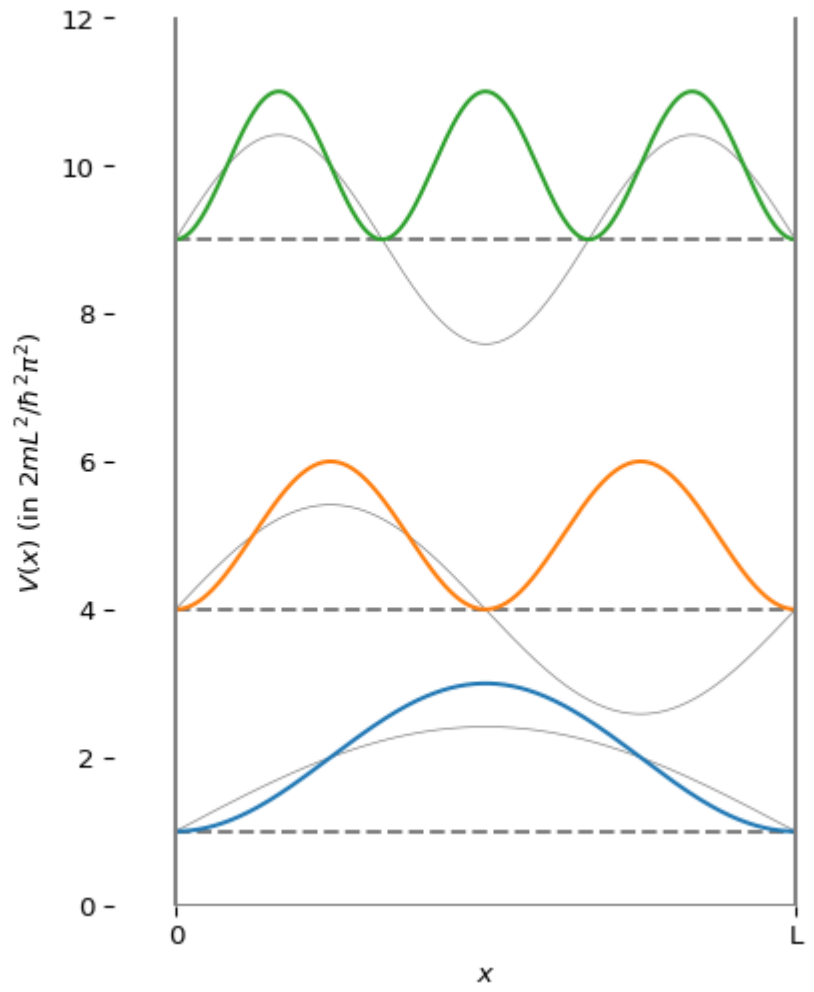
$$\implies \quad |A_n|^2 = \frac{2}{L} \Rightarrow |A_n| = \sqrt{\frac{2}{L}}$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$



INFINITE WELL: SUMMARY

$$\begin{cases} \psi_n(x) = \sqrt{\dfrac{2}{L}} \sin\left(\dfrac{n\pi x}{L}\right) \\ E_n = \dfrac{\hbar^2 k_n^2}{2m} = \dfrac{\hbar^2}{2m}\left(\dfrac{n\pi}{L}\right)^2 \\ n = 1, 2, 3, 4, \ldots \end{cases}$$



Plot shows the wave function (ψ, grey), probability ($|\psi|^2$, color) for first 3 eigenstates

EIGENENERGIES AND EIGENSTATES

$$\text{Eigenstates} \quad \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

$$\text{Eigenenergies} \quad E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

$$n = 1, 2, 3, 4, \ldots$$

- Lowest state $n = 1$ we call ground state
- Higher states $n > 1$ are excited states
- Parity of wave functions is either:
    - Even $(n = 1, 3, 5, \ldots)$
    - Odd $(n = 2, 4, 6, \ldots)$

PROPERTIES

$$\text{Eigenstates} \quad \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

The eigenstates are orthonormal:

$$\int \psi_m(x)^* \, \psi_n(x) dx = \delta_{nm}$$

Eigenstates form a complete basis
Every $f(x)$ we can expand as a series:

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{L}\right)$$

PROPERTIES OF STATIONARY EIGENSTATES

$$\psi_n \text{ are orthonormal} \qquad \int \psi_m(x)^* \, \psi_n(x) \, dx = \delta_{mn}$$

$$\psi_n \text{ form a complete basis} \qquad f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) \qquad \forall f(x)$$

$$\text{Coefficients } c_n \text{ are given by} \qquad c_n = \int \psi_n(x)^* \, f(x) \, dx$$

Proof of last property:

$$\int \psi_m(x)^* \, f(x) \, dx = \int \psi_n(x)^* \, \sum_{n=1}^{\infty} c_n \psi_n(x) \, dx$$

$$= \sum_{n=1}^{\infty} c_n \int \psi_m(x)^* \, \psi_n(x) \, dx = \sum_{n=1}^{\infty} c_n \delta_{mn} = c_m$$

STATIONARY SOLUTION OF THE TISE

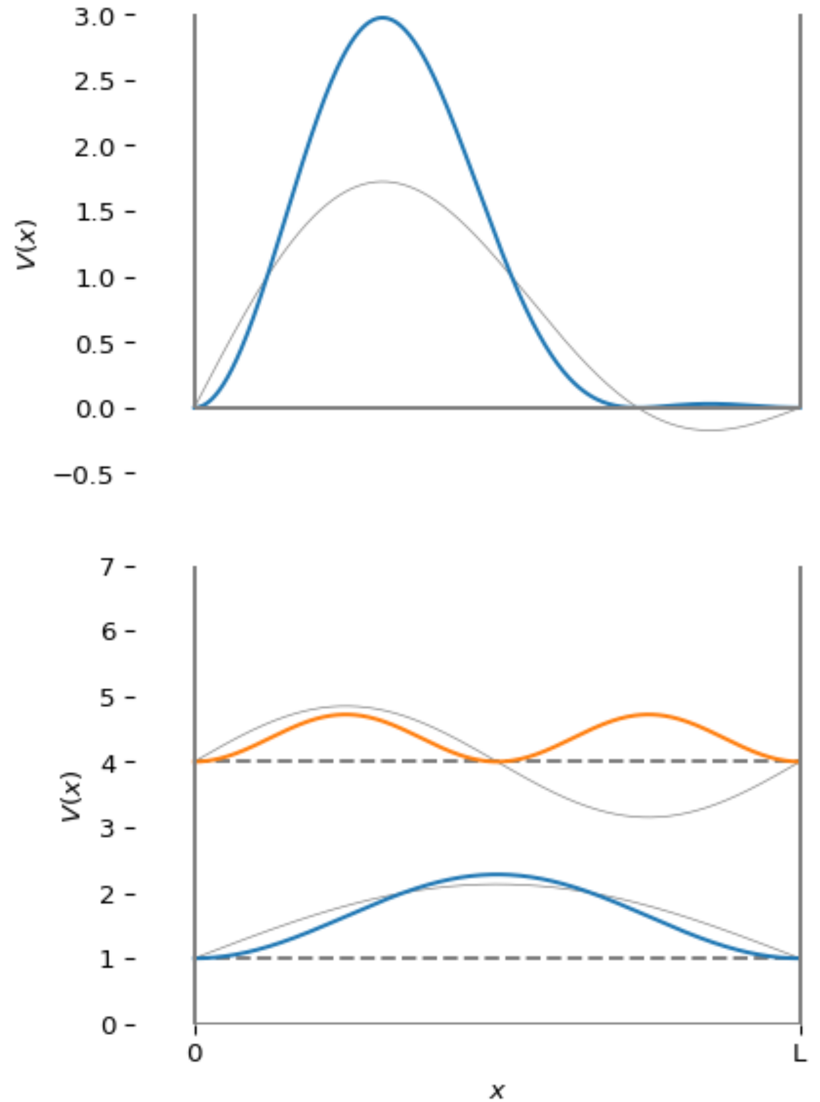
For the infinite well

$$\psi(x) = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{L}x\right)$$

Example state:

$$\begin{cases} c_1 = 4/5, \\ c_2 = \sqrt{1 - c_1^2} = 3/5, \\ n > 2 \longrightarrow c_n = 0 \end{cases}$$

- How does the wave function (ψ, color) and the probability ($|\psi|^2$, gray) look?
- What if we let time evolve?



INFINITE WELL: SOLUTION OF THE TDSE

Adding time evolution

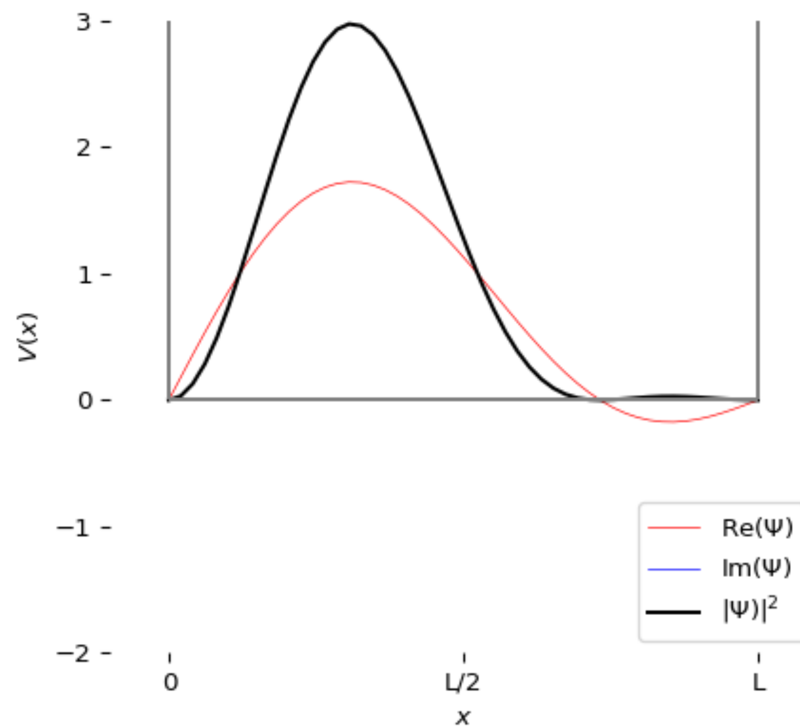
$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-iE_n t/\hbar}$$

$$\text{with } \sum_{n=1}^{\infty} |c_n|^2 = 1$$

Coefficients $|c_n|^2$ give the probability to measure energy as E_n:

$$\langle \hat{H} \rangle = \int \Psi^* \hat{H} \Psi dx = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

But $\langle \hat{x} \rangle = \int x \Psi^* \Psi \, dx$ is not constant!



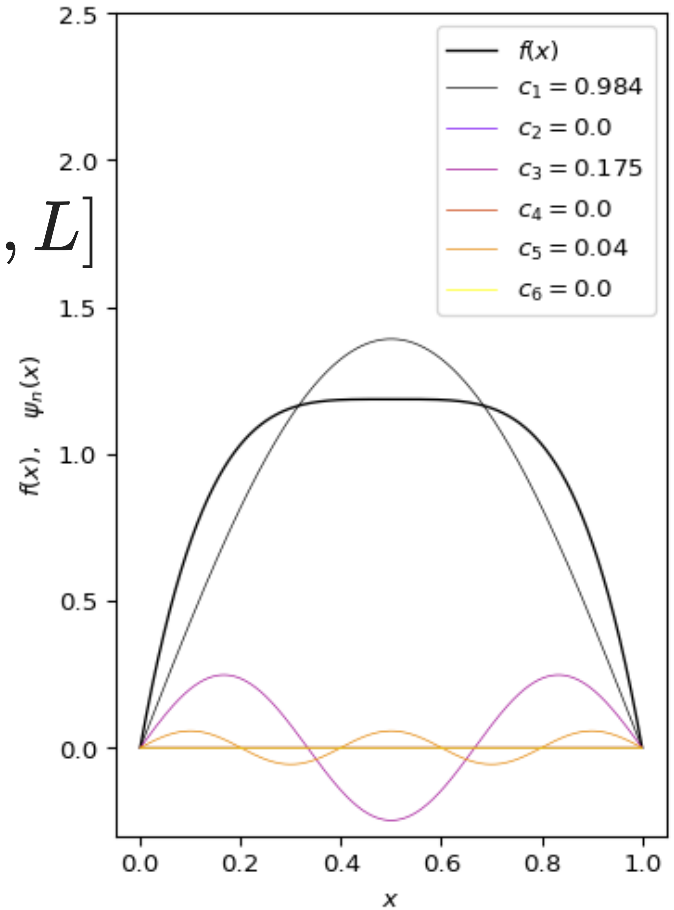
Once Loop Reflect

EXPAND A FUNCTION IN EIGENSTATES

- Suppose we have a certain wave function

$$f(x) = A\left((L/2)^4 - (x - L/2)^4\right),\ \text{with } x \in [0, L]$$

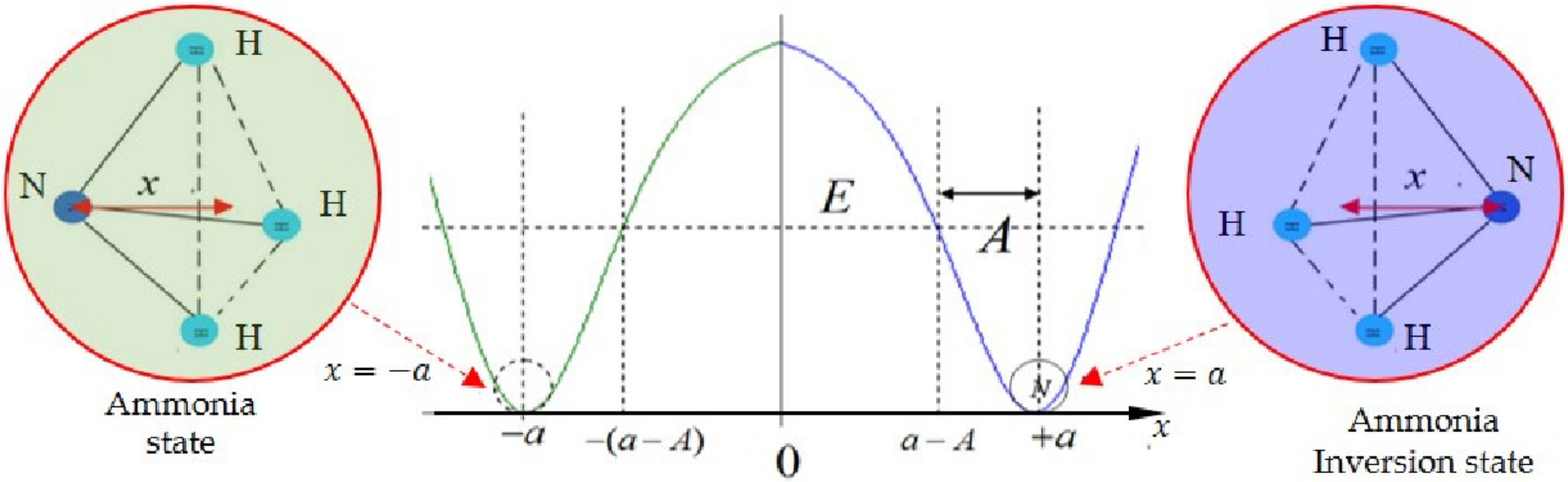
- Normalization constant $A = \sqrt{\frac{64}{45}\left(\frac{L}{2}\right)^9}$
- Since $f(0) = f(L) = 0$ we can expand $f(x)$ in eigenstates of the infinite well



$$f(x) = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{L} x\right)$$

$$\text{with} \quad c_n = \int_0^L \psi_n(x)^* \, f(x) \, dx$$

A MORE COMPLEX EXAMPLE



Ammonia molecule has two possible geometries

- The ammonia molecule NH_3 has two possible geometries
- Experiments tell that NH_3 flips between states
- Possible by quantum tunneling