PHOT 301: Quantum Photonics

LECTURE 03

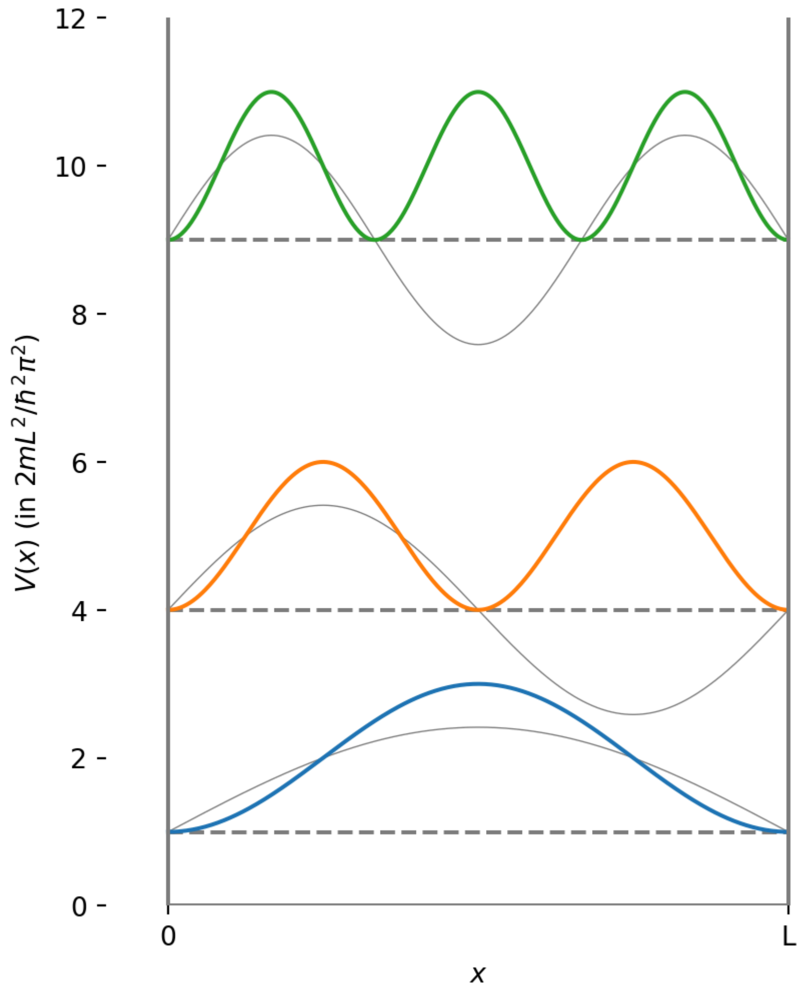
Michaël Barbier, Fall semester (2024-2025)

INFINITE DEEP WELL

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



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

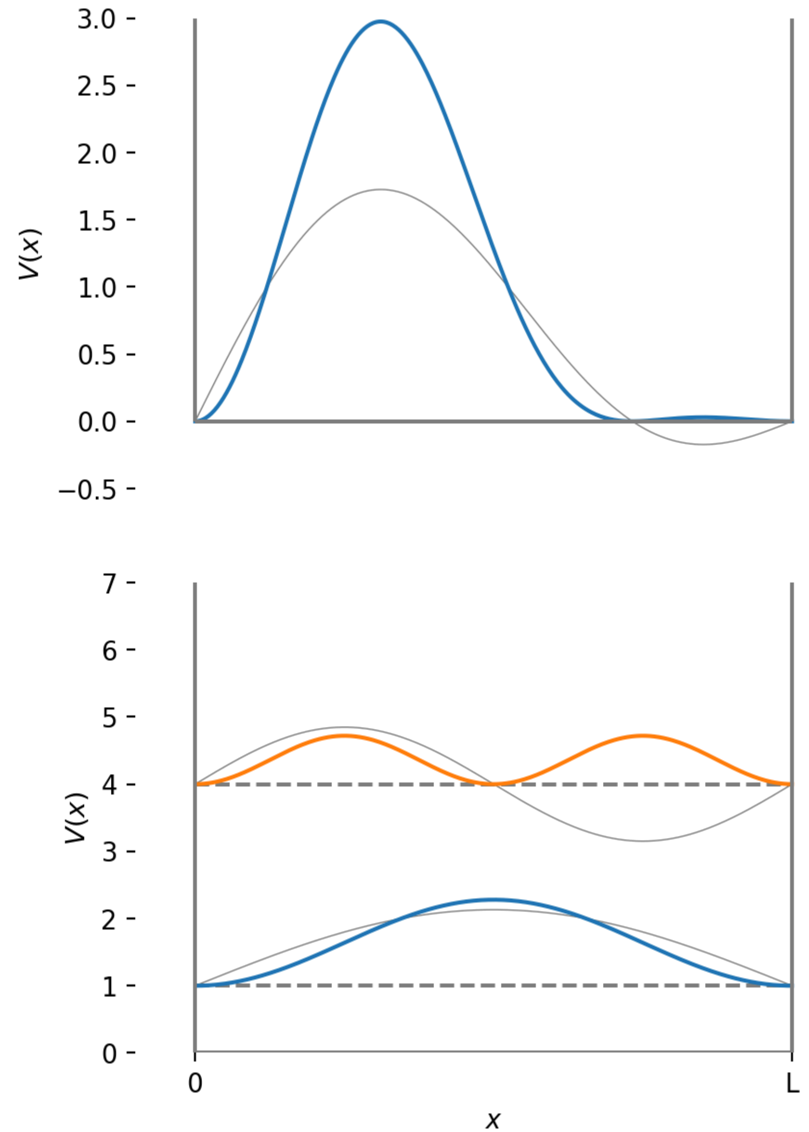
For the infinite well

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

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

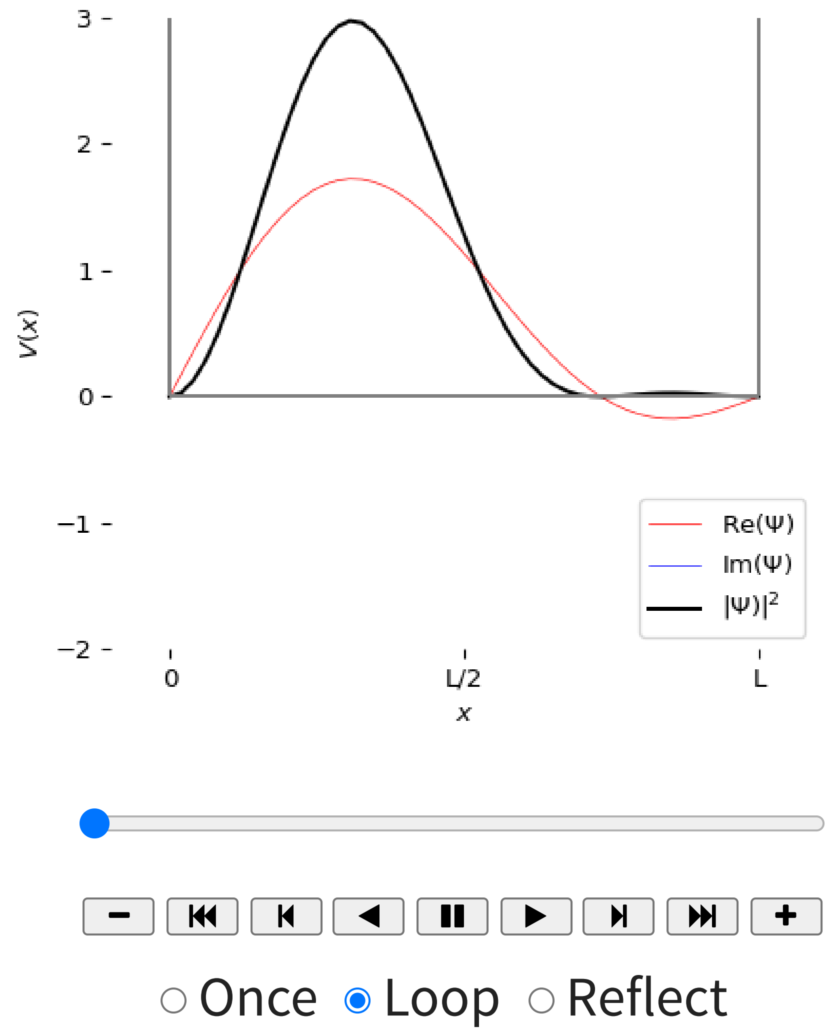
$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-iE_n t/\hbar}$$

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

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!



EXPAND A FUNCTION IN EIGENSTATES

- Suppose we have a certain function

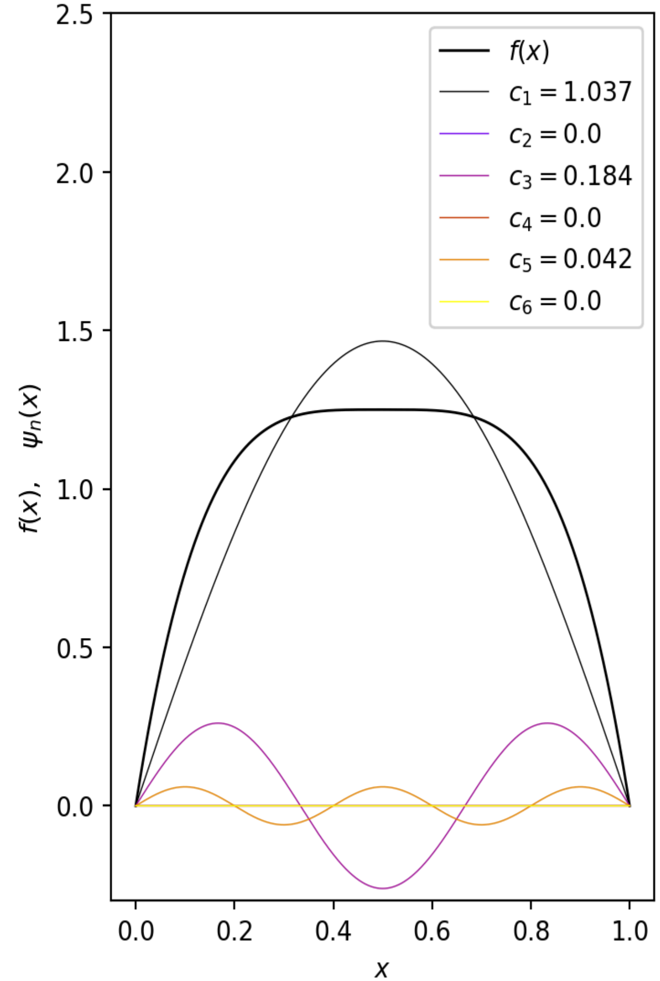
$$f(x) = (L/2)^4 - (x - L/2)^4, \quad \text{with } x \in [0, L]$$

- Since $f(0) = f(L) = 0$ we can expand $f(x)$ in eigenstates of the infinite well

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

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

- See the exercise sessions for the actual calculation



HARMONIC OSCILLATOR

INTRODUCTION

- Ball-spring problem
- Typical analog RCL electric circuit
- Many systems are approximately harmonic oscillators
  - Classical optics
  - 2nd order Taylor approximation of Potential wells
  - Phonons, vibrations in molecules/matter
  - Quantization of light: Photons

CLASSICAL HARMONIC OSCILLATOR

- mass attached to a spring
- The spring force counters any deviation: $F = -kx$
- Motion described by Newton's equation $F = ma$:

$$ma = m\frac{d^2x}{dt^2} = -kx$$

This is a linear equation with constant coefficients

$$\frac{d^2x}{dt^2} = -\frac{k}{m}x = -\omega^2 x$$

with $\omega = \sqrt{k/m}$.

Resulting solutions are:

$$x \propto \sin(\omega t)$$

SOLVING THE QM HARMONIC OSCILLATOR

The time-independent Schrodinger equation (TISE):

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

Potential energy: $V(x) = \frac{1}{2}m\omega^2 x^2$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \frac{1}{2}m\omega^2 x^2\psi(x) = E\psi$$

Rewrite in dimensionless units: $\xi = \sqrt{\frac{m\omega}{\hbar}}$

$$\frac{1}{2}\frac{\partial^2}{\partial \xi^2}\psi(\xi) - \frac{1}{2}\xi^2\psi(\xi) = -\frac{E}{\hbar\omega}\psi$$

$\longrightarrow$ 2nd order linear differential equation

SOLVING THE QM HARMONIC OSCILLATOR

$$\frac{1}{2}\frac{\partial^2}{\partial\xi^2}\psi(\xi) - \frac{1}{2}\xi^2\psi(\xi) = -\frac{E}{\hbar\omega}\psi$$

$\longrightarrow$ Trial solution $\psi \propto \exp(-\xi^2/2)$

Substitute $A_n \exp(-\xi^2/2)H_n(\xi)$ with $H_n(\xi)$ yet unknown

$$\frac{d^2H_n(\xi)}{d\xi^2} - 2\xi\frac{dH_n(\xi)}{d\xi} + \left(\frac{2E}{\hbar\omega} - 1\right)H_n(\xi) = 0$$

Solutions exist for $\frac{2E}{\hbar\omega} - 1 = 2n, \qquad n = 0, 1, 2, 3\ldots$

$$\longrightarrow \qquad \begin{aligned} \psi_n &= A_n \exp(-\xi^2/2)H_n(\xi), \\ E_n &= (n + 1/2)\hbar\omega \;\text{ with } n = 0, 1, 2, \ldots \end{aligned}$$

HARMONIC OSCILLATOR SOLUTIONS

$$\psi_n = A_n \exp(-\xi^2/2) H_n(\xi),$$

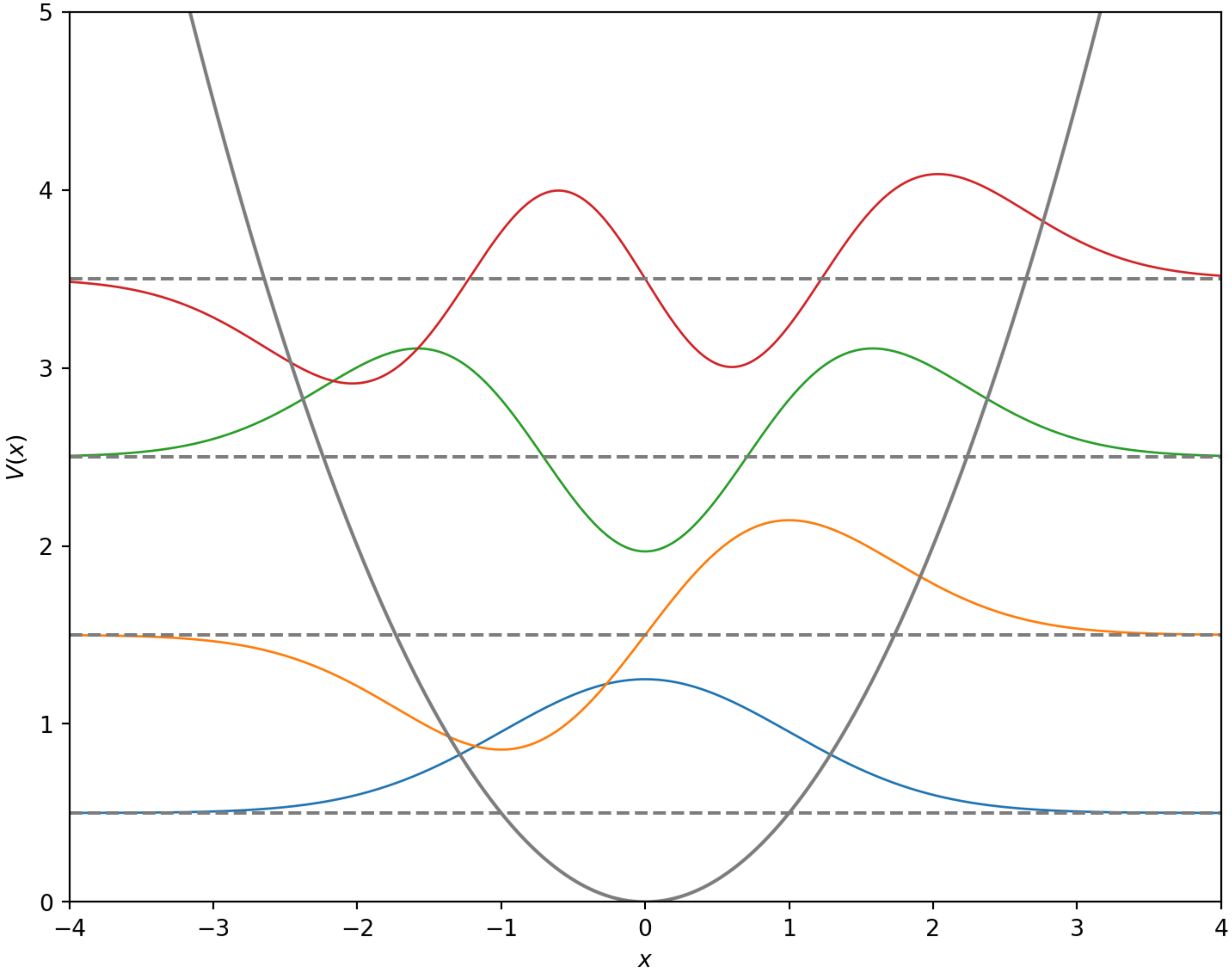
$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad \text{with } n = 0, 1, 2, \ldots$$

$$A_n = \sqrt{\frac{1}{\sqrt{\pi}\, 2^n n!}} \qquad \xi = \sqrt{\frac{m\omega}{\hbar}}$$

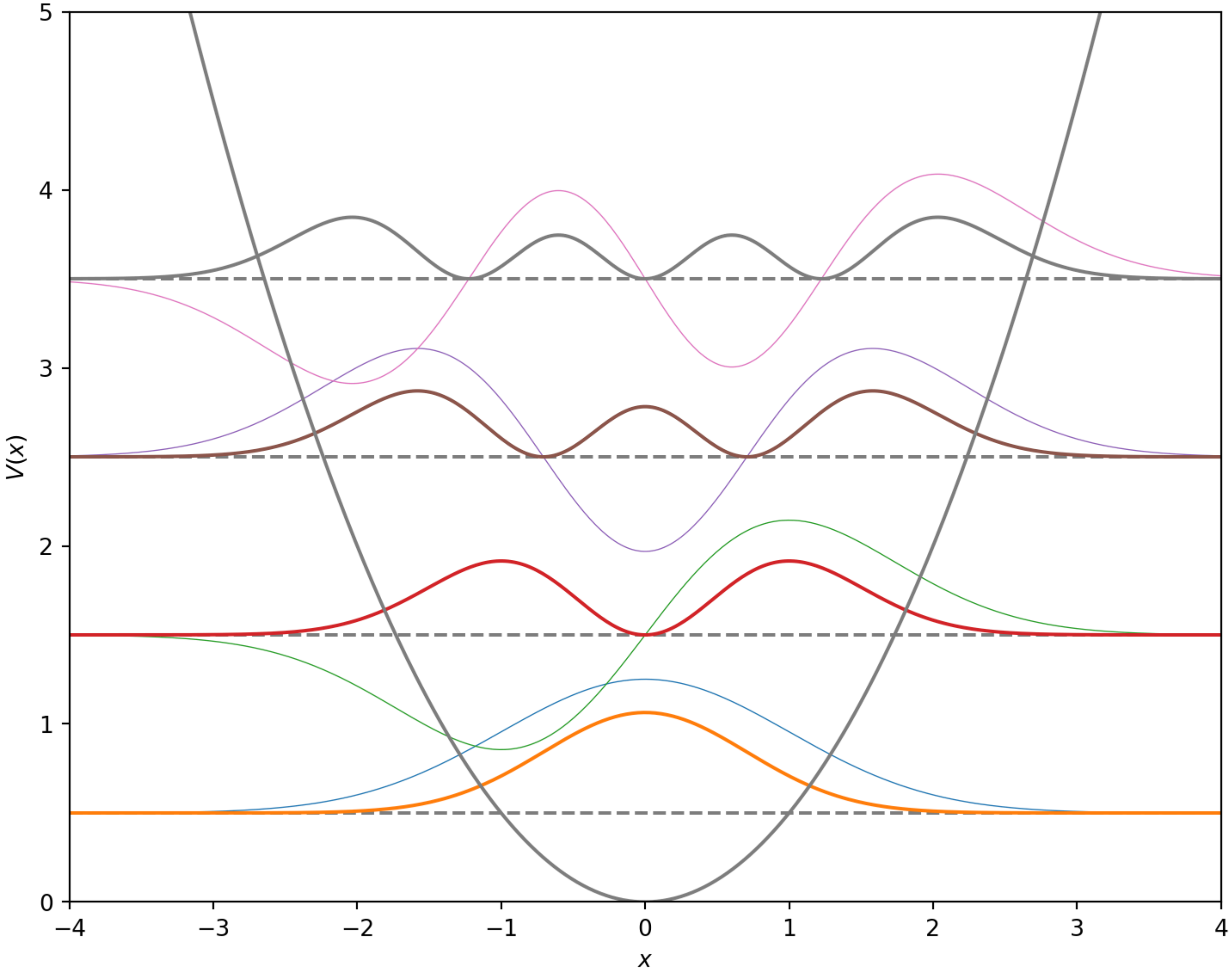
Hermite polynomials $H_n(\xi)$

$$H_0 = 1$$
$$H_1 = 2\xi$$
$$H_2 = 4\xi^2 - 2$$
$$H_3 = 8\xi^3 - 12\xi$$
$$\vdots$$
$$H_n(\xi) = 2\xi H_{n-1}(\xi) - 2(n-1)H_{n-2}(\xi)$$

HARMONIC OSCILLATOR SOLUTIONS



HARMONIC OSCILLATOR SOLUTIONS



ALTERNATIVE (ALGEBRAIC) DERIVATION

The time-independent Schrodinger equation (TISE):

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

with potential energy: $V(x) = \frac{1}{2}m\omega^2 x^2$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \frac{1}{2}m\omega^2 x^2\psi(x) = E\psi$$

Operator form:

$$\frac{1}{2m}\left(\hat{p}^2 + \frac{1}{2}m\omega^2 x^2\right)\psi(x) = E\psi, \qquad \hat{p} = -i\hbar\frac{\partial}{\partial x}$$

This is a sum of squares $\longrightarrow$ factorize $u^2 + v^2 = (iu+v)(-iu+v)$

LADDER OPERATORS

Ladder operators $\hat{a}_-\hat{a}_+ = (iu+v)(-iu+v) = u^2+v^2$

$$\hat{a}_\pm = \frac{1}{\sqrt{2\hbar m\omega}}(\mp i\hat{p} + m\omega x)\,, \qquad [\hat{x},\hat{p}] = x\hat{p} - \hat{p}x = i\hbar$$

The product is:

$$\begin{aligned}
\hat{a}_-\hat{a}_+ &= \frac{1}{2\hbar m\omega}(i\hat{p}+m\omega x)(-i\hat{p}+m\omega x) \\
&= \frac{1}{2\hbar m\omega}\left(\hat{p}^2 + (m\omega x)^2 - im\omega(x\hat{p}-\hat{p}x)\right) \\
&= \frac{1}{2\hbar m\omega}\left(\hat{p}^2 + (m\omega x)^2\right) - \frac{i}{2\hbar}(x\hat{p}-\hat{p}x) \\
&= \frac{1}{2\hbar m\omega}\left(\hat{p}^2 + (m\omega x)^2\right) + \frac{1}{2} \\
&= \frac{1}{\hbar\omega}\hat{H} + \frac{1}{2}
\end{aligned}$$

LADDER OPERATORS

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We can also flip the ladder operators:

$$\hat{H} = \left(\hat{a}_-\hat{a}_+ - \frac{1}{2}\right)\hbar\omega$$
$$\hat{H} = \left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)\hbar\omega$$

Stationary Schrodinger equation becomes:

$$\hat{H}\psi = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)\psi = E\,\psi$$

LADDER OPERATORS GENERATE SOLUTIONS

If $\psi(x)$ is a solution, the $\hat{a}_+\psi(x)$ is another solution:

$$\hat{H}\psi(x) = E\psi \Rightarrow \hat{H}(\hat{a}_+\psi(x)) = (E + \hbar\omega)(\hat{a}_+\psi(x))$$

If $\psi(x)$ is a solution, then $\hat{a}_-\psi(x)$ is another solution:

$$\hat{H}\psi(x) = E\psi \Rightarrow \hat{H}(\hat{a}_-\psi(x)) = (E - \hbar\omega)(\hat{a}_-\psi(x))$$

LADDER OPERATORS GENERATE SOLUTIONS

Since energy $E > 0$ operating with $\hat{a}_-$ leads at some point to:

$$\hat{a}_- \psi_0 = 0$$

The leads to the following differential equation

$$\frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0(x) = 0$$

$$\Rightarrow \frac{d\psi_0(x)}{dx} = -\frac{m\omega}{\hbar}\, x\, \psi_0(x)$$

$$\Rightarrow \int \frac{d\psi_0(x)}{\psi_0(x)}\, dx = -\frac{m\omega}{\hbar}\int x\, dx$$

$$\Rightarrow \ln(\psi_0(x)) = -\frac{m\omega}{2\hbar}x^2 + C$$

$$\Rightarrow \psi_0(x) = A\, e^{-\frac{m\omega}{2\hbar}x^2}$$

LADDER OPERATORS GENERATE SOLUTIONS

$$\Rightarrow \psi_0(x) = A\, e^{-\frac{m\omega}{2\hbar}\, x^2}$$

Normalization requires $\int |\psi_0(x)|^2 = 1$

$$\int_{-\infty}^{\infty} |\psi_0(x)|^2\, dx = |A|^2 \int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar}\, x^2} = |A|^2 \sqrt{\frac{\pi\hbar}{m\omega}}$$

where we used the identity

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

This results in the solution:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}\, x^2}$$

SOLUTIONS WITH THE LADDER OPERATORS

Other solutions $\psi_n(x)$ can now be generated:

$$\psi_n(x) = A_n \left(\hat{a}_+\right)^n \psi_0(x), \quad \text{with} \quad E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

The normalization factor A_n can be calculated

$$\psi_n(x) = \frac{1}{\sqrt{n!}} \left(\hat{a}_+\right)^n \psi_0(x), \quad \text{with} \quad E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

And operating with a single ladder operator:

$$\hat{a}_+\psi_n = \sqrt{n+1}\psi_{n+1}, \qquad \hat{a}_-\psi_n = \sqrt{n}\psi_{n-1}$$

SUMMARY

- Infinite well
  - Eigenstates evolve different in time
  - Pure eigenstates are stationary for finite expectation energy $\langle \hat{H} \rangle$
  - Mixing of eigenstates leads to non-constant $\langle \hat{x} \rangle$, i.e. a nonzero velocity
- Harmonic oscillator
  - Energy levels equally spaced $E_n = \hbar\omega(n + 1/2)$
  - Nonzero ground energy $E_0 = \frac{1}{2}\hbar\omega$
  - Solutions proportional with Hermite polynomials $H_n(x)$
  - Alternative algebraic method
  - Ladder operators (Algebraic method)