PHOT 301: Quantum Photonics

LECTURE 03

Michaël Barbier, Summer (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.	
Week 2	The harmonic oscillator, Creation and annihilation operators. Free particle, 1D Bound states & Scattering/Transmission, Finite well	**Ch. 2 (from Harmonic oscillator)**
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

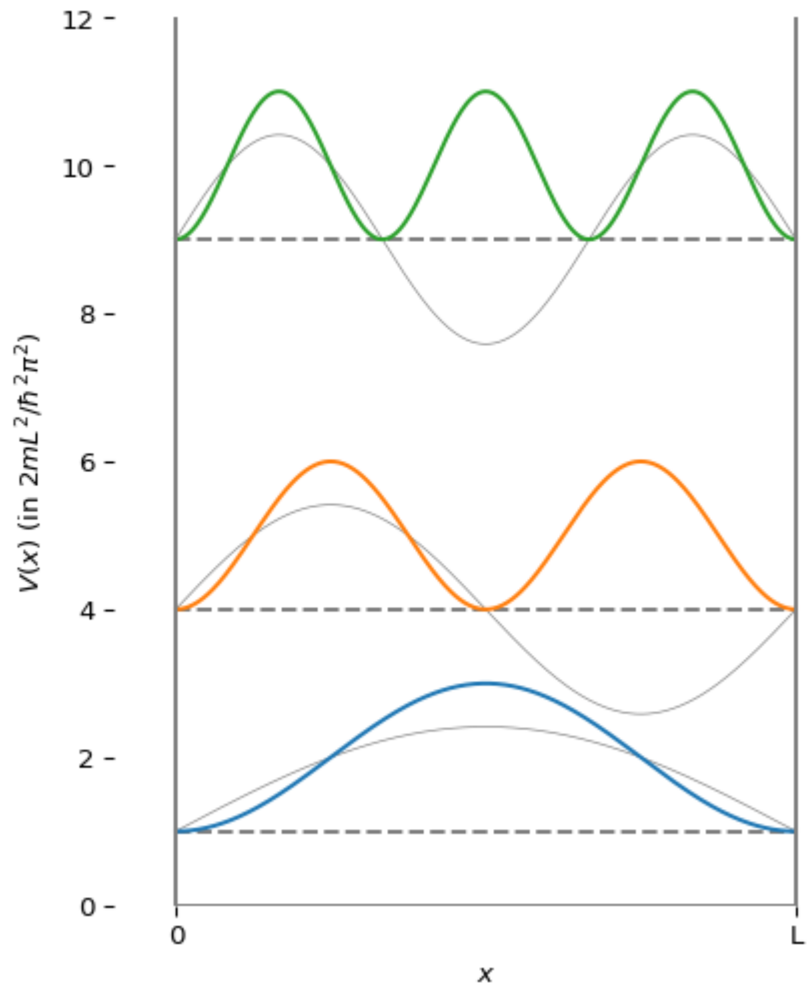
- Textbook Chapter 2: 2.11, 2.13, 2.14, 2.17, 2.18, 2.25, 2.31, 2.34, 2.41, 2.53
- Homework documents:
  - phot301_homework_matrices.pdf
  - phot301_homework_system_of_equations.pdf
  - phot301_homework_eigenvalue_equations.pdf
- Reading (by Thursday 31 July 2025): Chapter 3 of Griffiths

REVIEW: INFINITE WELL

Time-independent solutions:

- Eigenstates and eigenenergies
- Quantum number n

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

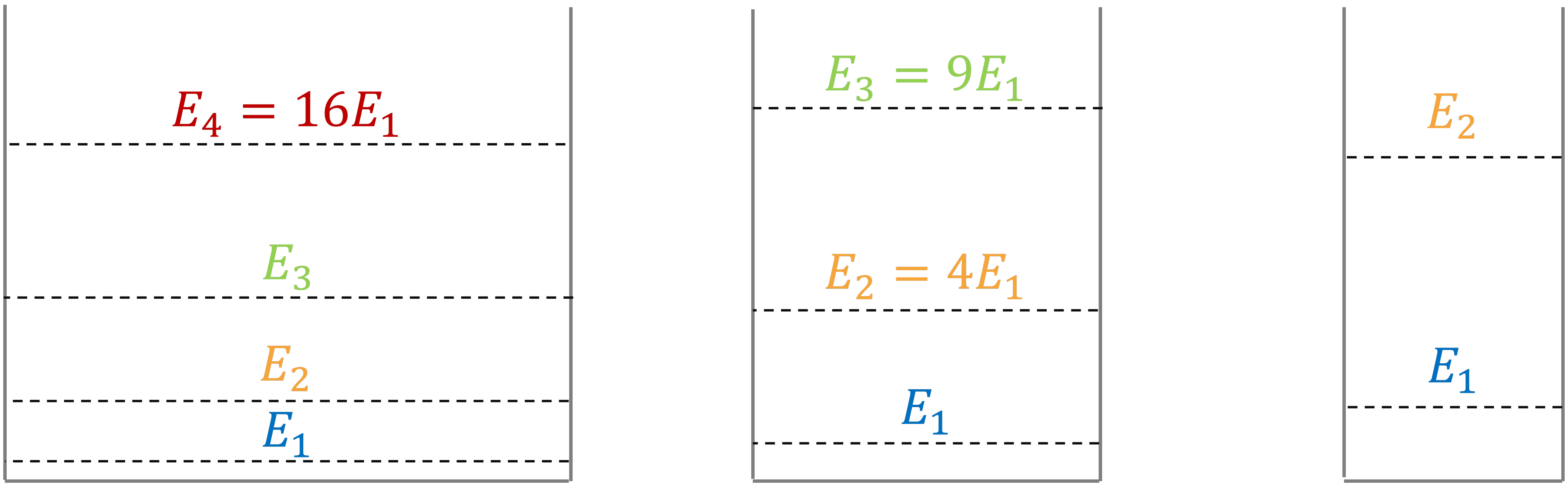


Plot shows the wave function (ψ, grey), probability ($|\psi|^2$, color) for first 3 eigenstates

REVIEW: QUANTIZATION BY SPACIAL CONSTRAINTS

Energy-levels E_n proportional with $\frac{1}{L^2}$ and n^2

$$E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}, \qquad E_1 = \frac{\hbar^2\pi^2}{2mL^2}, \qquad E_n = n^2 E_1$$



REVIEW: SUPERPOSITION OF STATIONARY SOLUTIONS

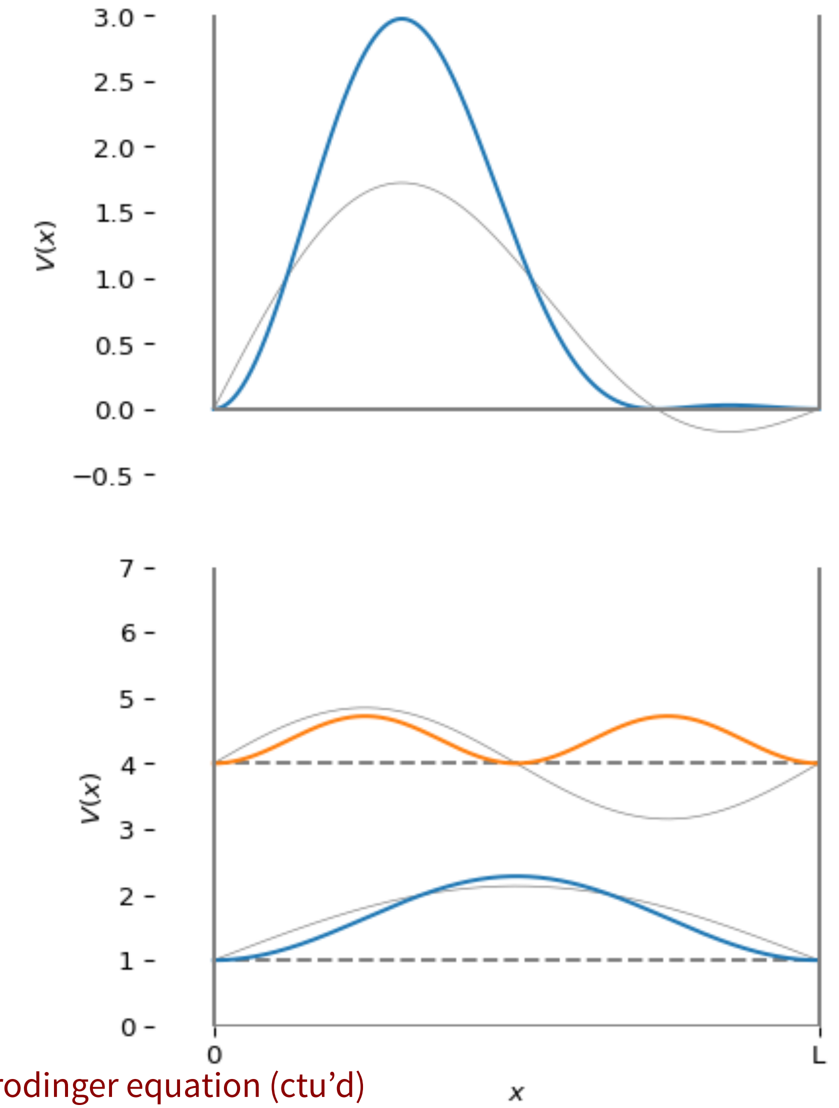
For the infinite well

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

Example state:

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

- What if we let time evolve?



REVIEW: ADDING THE TIME-DEPENDENCY

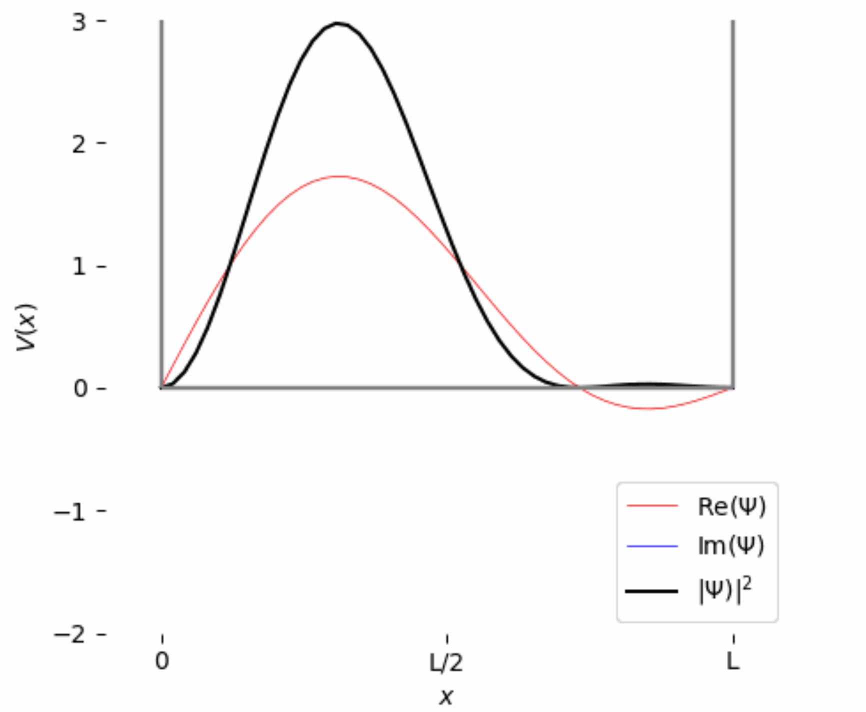
Add $e^{-iE_n/\hbar}$ to each eigenstate:

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

For the infinite well:

$$\Psi(x,t) = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{L}x\right) e^{-iE_n/\hbar}$$

- The wave function $\Psi(x,t)$ is complex-valued
- Probability density $|\Psi(x,t)|^2$ is real-valued



REVIEW: PROPERTIES OF STATIONARY EIGENSTATES

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

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

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

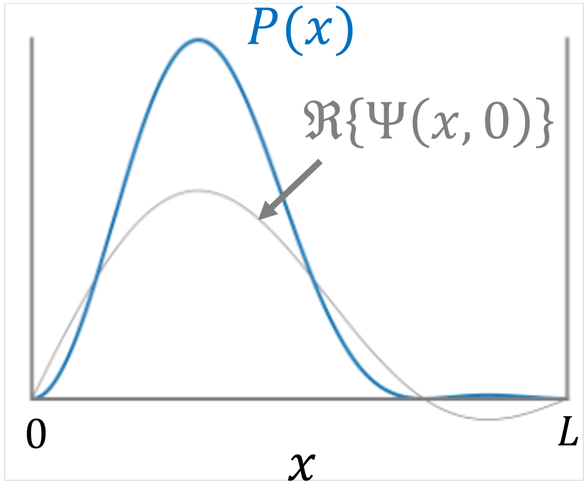
Coefficients $|c_n|^2$ give the probability to measure energy as E_n:

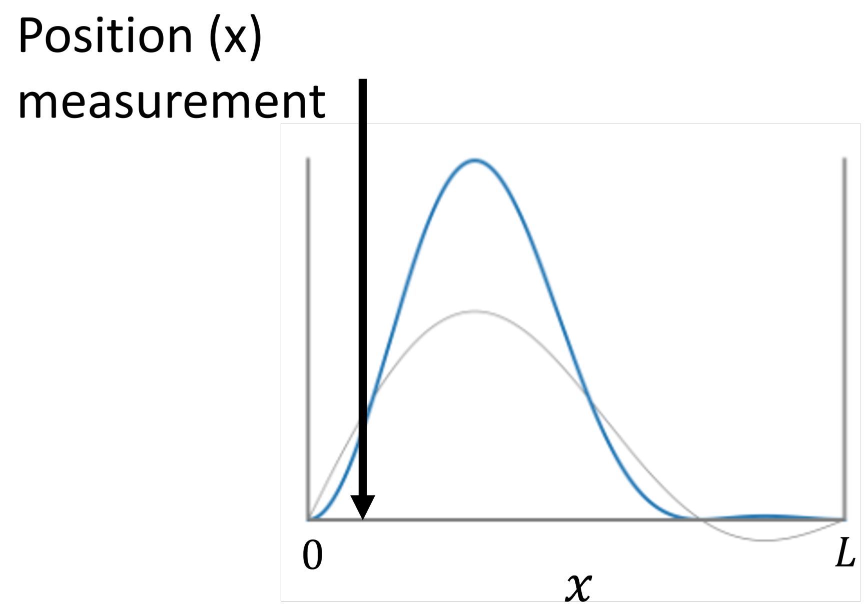
$$\langle \hat{H} \rangle = \int \Psi^* \hat{H} \Psi dx = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

Expectation values for operators $\hat{x}$, $\hat{p}$, etc.

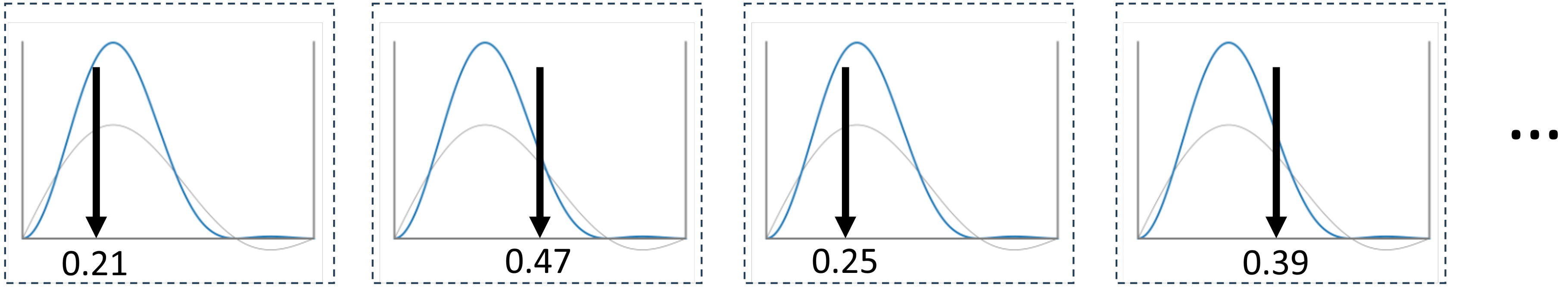
$$\langle \hat{x} \rangle (t) = \int \Psi^* \hat{x} \Psi \, dx = \int x |\Psi|^2 \, dx$$

REVIEW: OBSERVABLES & MEASUREMENTS

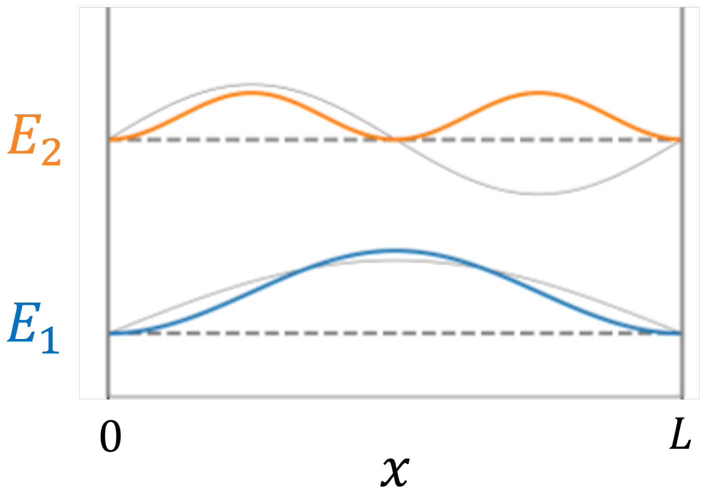




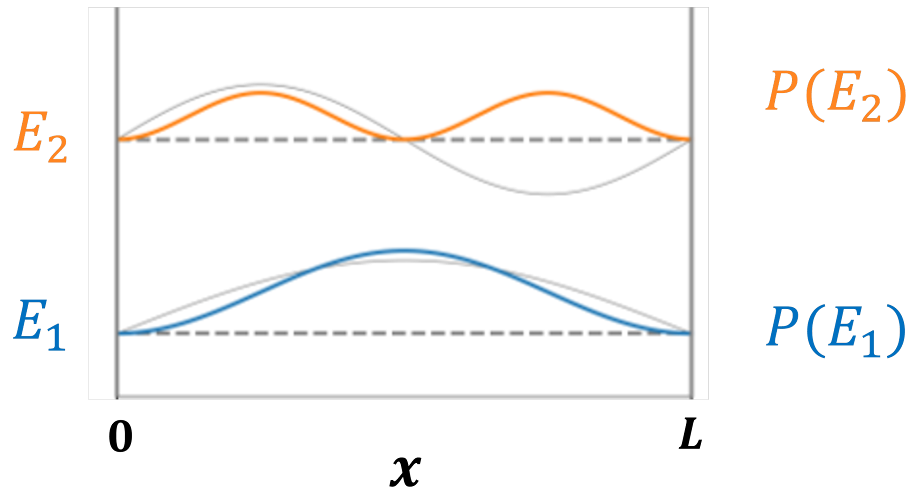
Every measurement probabilistic BUT average position $\langle x \rangle \propto \int_0^L P(x)\, x\, dx$



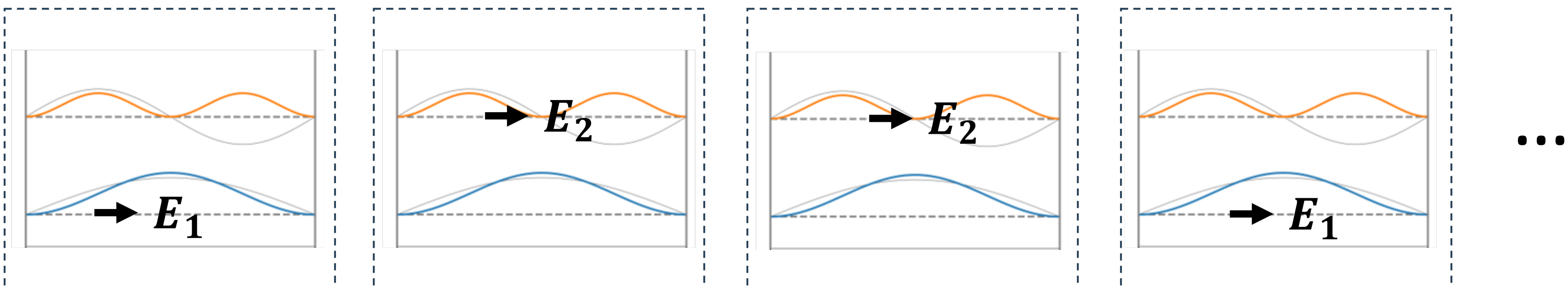
REVIEW: OBSERVABLES & MEASUREMENTS



Energy (E_n) measurement



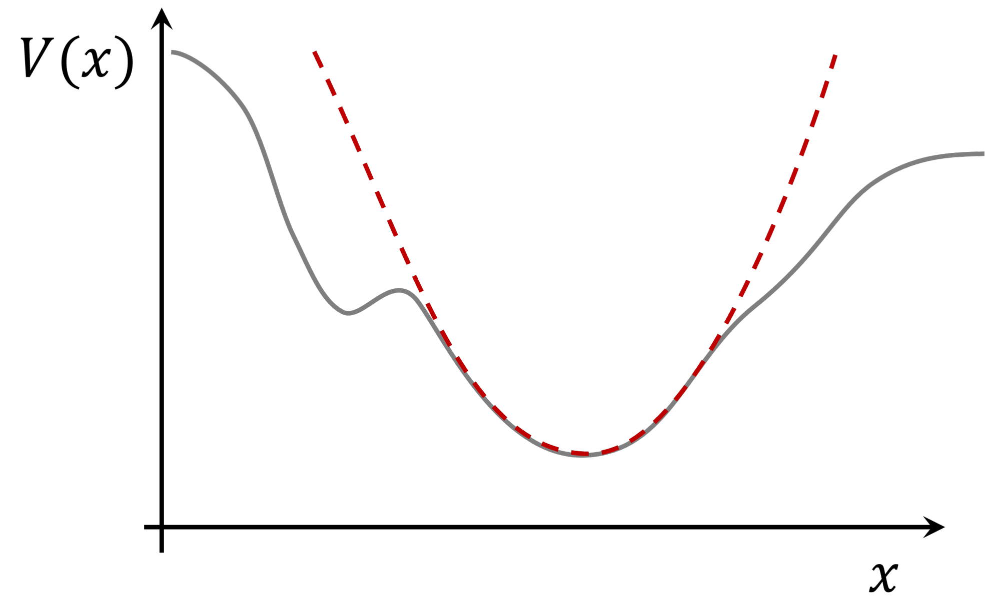
Every measurement probabilistic BUT average energy $\langle H \rangle \propto \sum_n P(E_n) E_n$



HARMONIC OSCILLATOR

INTRODUCTION

- Ball-spring problem
- Analog RCL electric circuit
- Many systems are (approximately) harmonic oscillators
  - Optical cavity
  - **2nd order Taylor approximation** $V(x)$
  - Phonons, vibrations in molecules/ matter
- **Quantization of light: Photons**



CLASSICAL HARMONIC OSCILLATOR: PARABOLIC WELL

- Mass in parabolic well $V(x) = \alpha m g x^2$
- Restoring force: $F = -\frac{dV(x)}{dx} = -2\alpha m g x$
- Motion via Newton's equation $F = ma$:

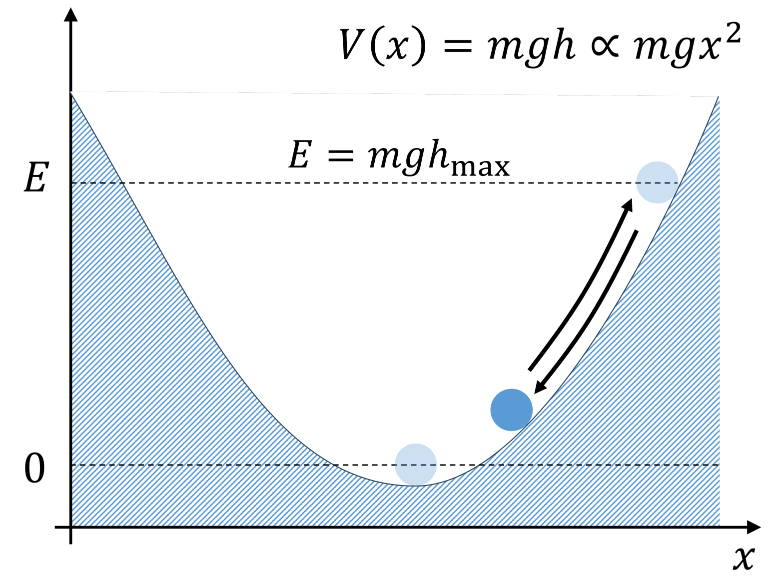
$$ma = m\frac{d^2x}{dt^2} = -2\alpha m g x$$

Linear equation with constant coefficients

$$\frac{d^2x}{dt^2} = -2\alpha g x = -\omega^2 x, \text{ with } \omega = \sqrt{2\alpha g}.$$

Resulting solutions are: $x \propto \sin(\omega t)$

Turning points at $\pm x_{\max}$: $\alpha m g x_{\max}^2 = \frac{1}{2} m v_0^2$



CLASSICAL HARMONIC OSCILLATOR: BALL-SPRING

- mass attached to a spring
- Restoring force: $F = -\frac{dV(x)}{dx} = -kx$
- Motion via Newton's equation $F = ma$:

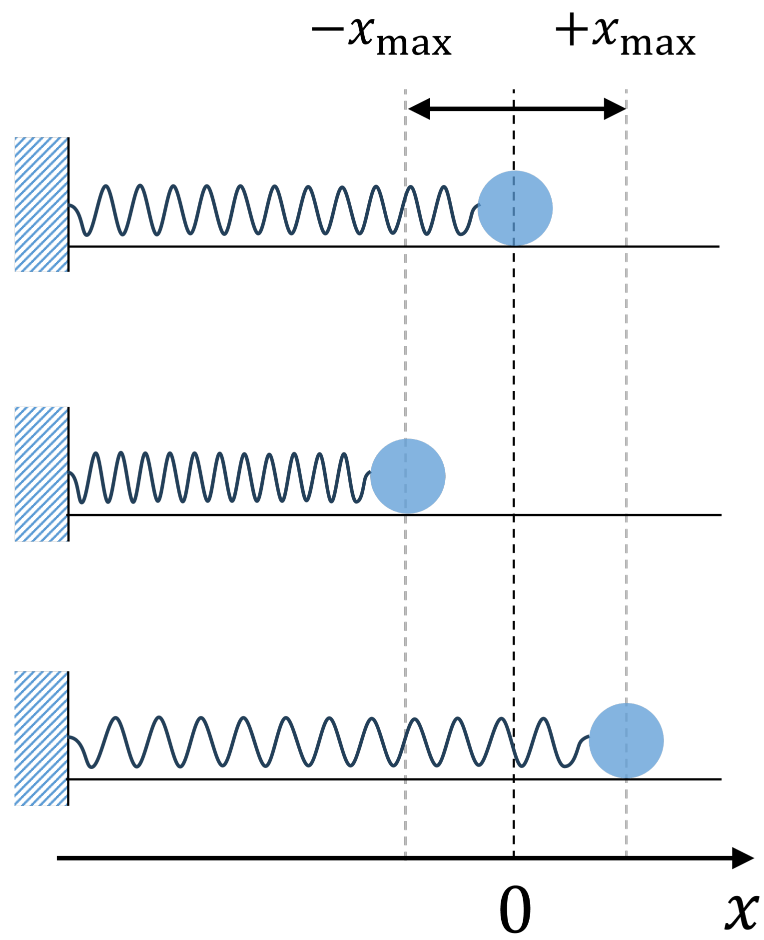
$$ma = m\frac{d^2x}{dt^2} = -k'x$$

Linear equation with constant coefficients

$$\frac{d^2x}{dt^2} = -\frac{k}{m}x = -\omega^2 x, \text{ with } \omega = \sqrt{k'/m}.$$

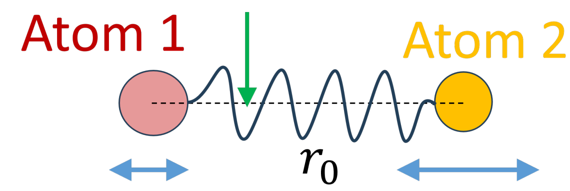
Resulting solutions are: $x \propto \sin(\omega t)$

Turning points at $\pm x_{\max}$: $\frac{1}{2}k' x_{\max}^2 = \frac{1}{2}mv_0^2$



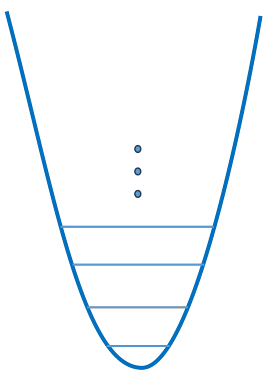
QUANTUM HARMONIC OSC.: DIATOMIC MOLECULE

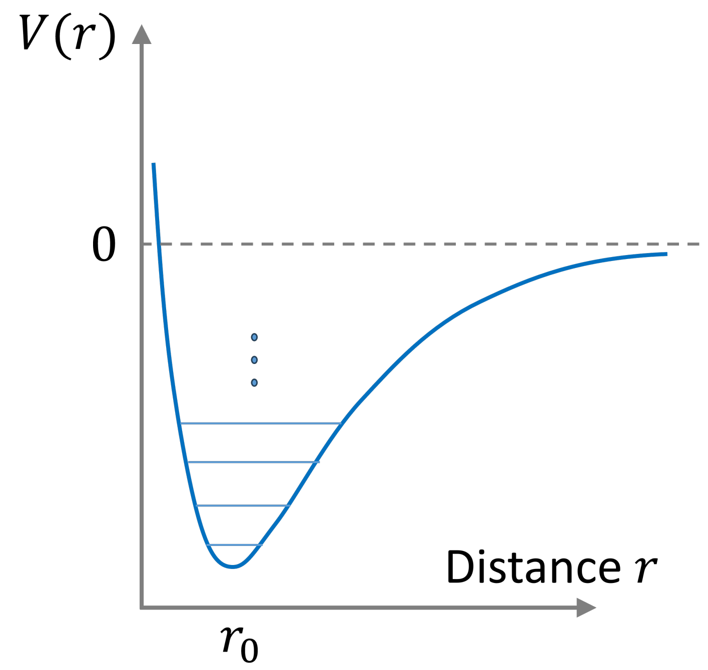
- **Vibrations** approximate harmonic oscillator
- Restoring force: $F = -\frac{dV(x)}{dx} = -k'x$
- Schrodinger equation with potential:



$$V(x) = -\frac{1}{2}k'x^2$$

$$\begin{cases} \text{Quantization energy-levels} \\ \text{Groundstate nonzero energy} \\ \text{Time-evolution} \quad \rho(x,t) = |\Psi(x,t)|^2 \end{cases}$$





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

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

Standard method to solve differential equation

STEP 1: Try to find asymptotic solutions

$$\lim_{\xi \longrightarrow \infty} \quad \Rightarrow \quad \frac{E}{\hbar\omega} \ll \frac{1}{2}\xi^2$$

$$\Rightarrow \frac{\partial^2}{\partial \xi^2}\psi(\xi) \approx \xi^2\psi(\xi) \qquad \Rightarrow \qquad \psi \propto \exp(-\xi^2/2)$$

STEP 2: Trial solution to **hopefully simplify** the equation

$$\psi(x) = \exp(-\xi^2/2)H(\xi), \qquad \text{where solutions } H(\xi) \text{ are yet unknown}$$

SOLVING THE QM HARMONIC OSCILLATOR

STEP 2: Trial solution to **hopefully simplify** the equation

Fill in trial solution $\psi = \exp(-\xi^2/2)H(\xi)$ in the original equation.

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

(and we multiply equation by 2)

$$\frac{\partial^2}{\partial\xi^2}\left[e^{-\xi^2/2}H(\xi)\right] - \xi^2 e^{-\xi^2/2}H(\xi) = -\frac{2E}{\hbar\omega}e^{-\xi^2/2}H(\xi)$$

Then calculate 2nd derivative ($f'(x) = \partial f(x)/\partial x$):

$$\left[e^{-\xi^2/2}H(\xi)\right]'' = \left[-\xi e^{-\xi^2/2}H(\xi) + e^{-\xi^2/2}H(\xi)\right]'$$

$$= -e^{-\xi^2/2}H(\xi) + \xi^2 e^{-\xi^2/2}H(\xi) - 2\xi e^{-\xi^2/2}H'(\xi) + e^{-\xi^2/2}H''(\xi)$$

SOLVING THE QM HARMONIC OSCILLATOR

STEP 2: Trial solution to **hopefully simplify** the equation

$$e^{-\xi^2/2}H''(\xi) - 2\xi e^{-\xi^2/2}H'(\xi) = \left(1 - \frac{2E}{\hbar\omega}\right) e^{-\xi^2/2}H(\xi)$$

Divide by $e^{-\xi^2/2}$

$$H''(\xi) - 2\xi H'(\xi) = \left(1 - \frac{2E}{\hbar\omega}\right) H(\xi)$$

Define dimensionless $K \equiv \frac{2E}{\hbar\omega}$

$$H''(\xi) - 2\xi H'(\xi) + (K-1)\ H(\xi) = 0$$

New differential equation: **Simpler?**

SOLVING THE QM HARMONIC OSCILLATOR

STEP 3: Solve by power series expansion

$$H''(\xi) - 2\xi H'(\xi) + (K-1)\ H(\xi) = 0$$

Assume $H(\xi) = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + \cdots = \sum_n a_{j=0}^{\infty} a_j \xi^j$

$$\begin{cases} H(\xi) = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + \cdots = \displaystyle\sum_{j=0}^{\infty} a_j \xi^j \\ H'(\xi) = a_1 + 2a_2\xi + 3a_3\xi^2 + \cdots = \displaystyle\sum_{j=0}^{\infty} (j+1) a_{j+1} \xi^j \\ H''(\xi) = 2a_2 + 6a_3\xi + \cdots = \displaystyle\sum_{j=0}^{\infty} (j+2)(j+1) a_{j+2} \xi^j \end{cases}$$

Then fill in the power series in the equation

SOLVING THE QM HARMONIC OSCILLATOR

STEP 3: Solve by power series expansion

$$H''(\xi) - 2\xi H'(\xi) + (K-1)\ H(\xi) = 0$$

$$\begin{cases} H(\xi) = a_0 + a_1\xi + a_2\xi^2 + a_3\xi^3 + \cdots = \sum_{j=0}^{\infty} a_j \xi^j \\ H'(\xi) = a_1 + 2a_2\xi + 3a_3\xi^2 + \cdots = \sum_{j=0}^{\infty} (j+1) a_{j+1} \xi^j \\ H''(\xi) = 2a_2 + 6a_3\xi + \cdots = \sum_{j=0}^{\infty} (j+2)(j+1) a_{j+2} \xi^j \end{cases}$$

Then fill in the power series in the equation:

$$\sum_{j=0}^{\infty} \left[(j+2)(j+1)a_{j+2} - 2ja_j + (K-1)\ a_j\right] \xi^j = 0$$

SOLVING THE QM HARMONIC OSCILLATOR

STEP 3: Solve by power series expansion

$$\sum_{j=0}^{\infty} \left[(j+2)(j+1)a_{j+2} - 2ja_j + (K-1)\ a_j\right] \xi^j = 0$$

For every power of ξ equation needs to be zero

$$(j+2)(j+1)a_{j+2} - 2ja_j + (K-1)\ a_j = 0$$

Solve for coefficients:

$$a_{j+2} = \frac{2j+1-K}{(j+2)(j+1)}\, a_j = 0$$

If we know a_0 (even series) and a_1 (odd series) we know all a_n

SOLVING THE QM HARMONIC OSCILLATOR

STEP 3: Solve by power series expansion

One problem: we require

$$\lim_{\xi \longrightarrow \infty} e^{\xi^2/2} H(\xi) = 0$$

This is not the case for our infinite series.

UNLESS the series terminates: $\exists j : \quad 2j + 1 - K = 0$

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

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

HARMONIC OSCILLATOR SOLUTIONS

$$\begin{cases} \psi_n = A_n \exp(-\xi^2/2) H_n(\xi), \\ E_n = \left(n + \frac{1}{2}\right) \hbar\omega \ \text{ with } n = 0, 1, 2, \ldots \\ A_n = \sqrt{\frac{1}{\sqrt{\pi} 2^n n!}} \qquad \xi = \sqrt{\frac{m\omega}{\hbar}} \end{cases}$$

Hermite polynomials $H_n(\xi)$ (our even/odd power series)

$$\begin{aligned} H_0 &= 1 \\ H_1 &= 2\xi \\ H_2 &= 4\xi^2 - 2 \\ H_3 &= 8\xi^3 - 12\xi \\ &\vdots \end{aligned}$$

$$H_n(\xi) = 2\xi H_{n-1}(\xi) - 2(n-1) H_{n-2}(\xi)$$

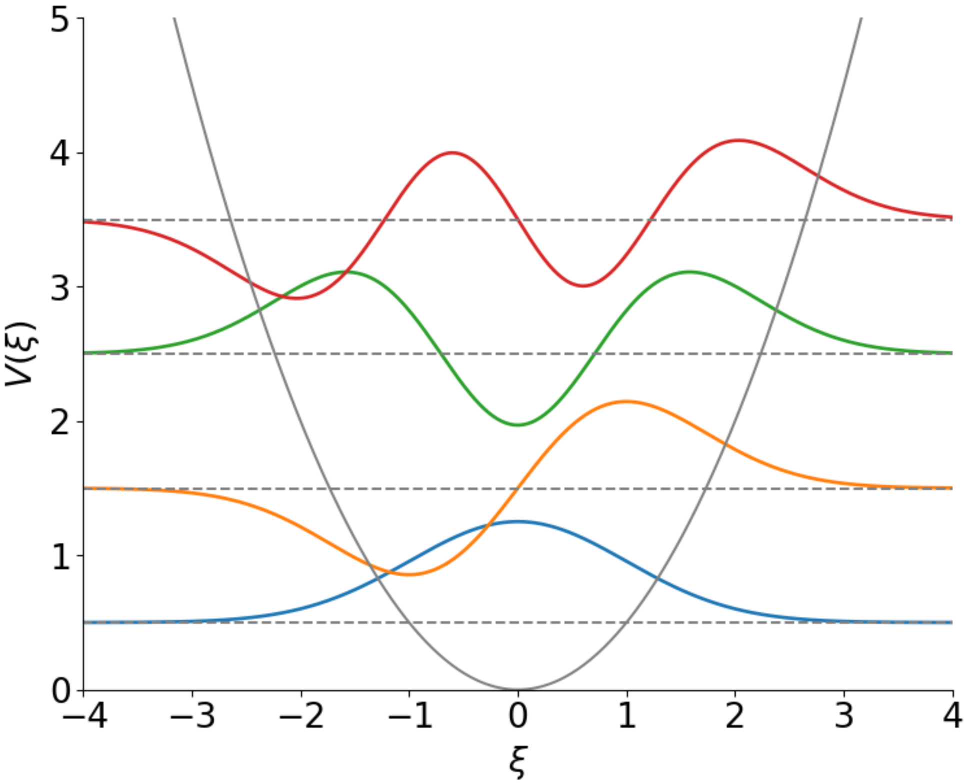
HARMONIC OSCILLATOR SOLUTIONS

Solutions for the wave function:

$$\psi_n(x) = \frac{1}{\sqrt{2^n\, n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-\frac{m\omega}{2\hbar}\, x^2}$$

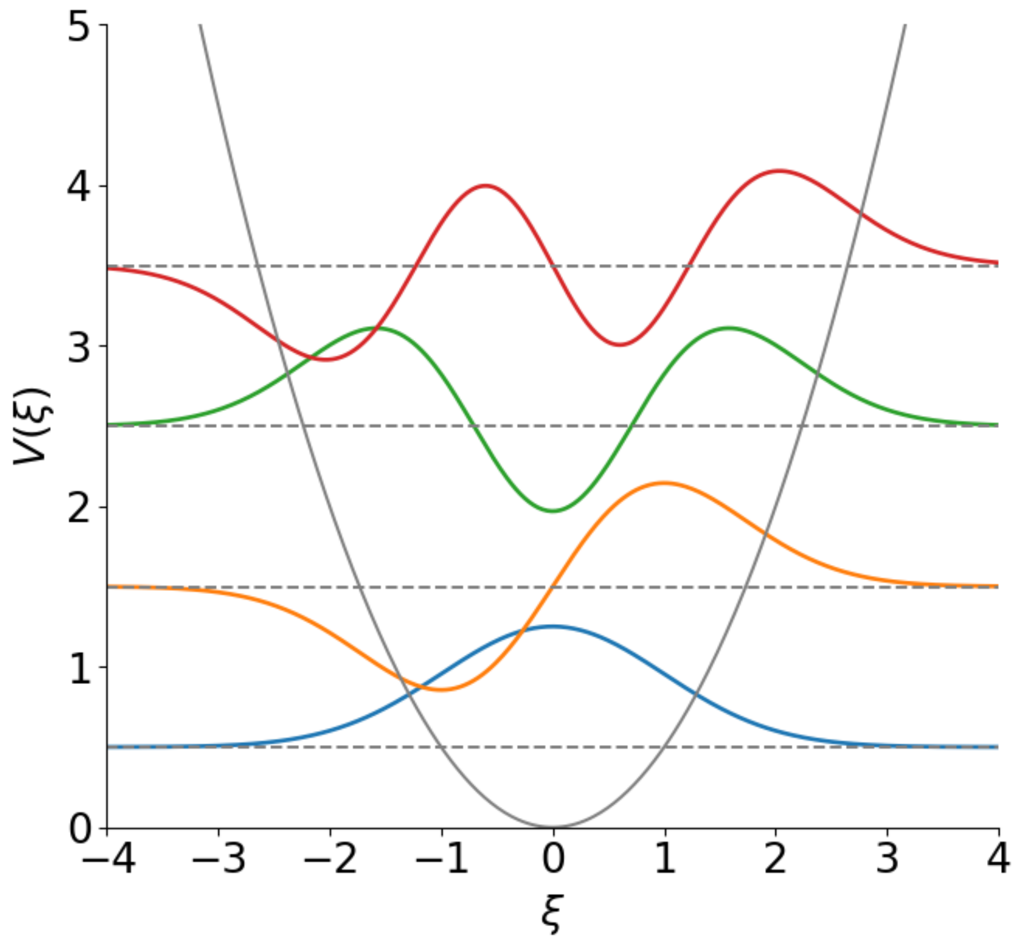
- Gaussian
- Normalization
- Hermite polynomials $H_n(\xi)$

$$H_0 = 1$$
$$H_1 = 2\xi$$
$$H_2 = 4\xi^2 - 2$$
$$H_3 = 8\xi^3 - 12\xi$$
$$\vdots$$

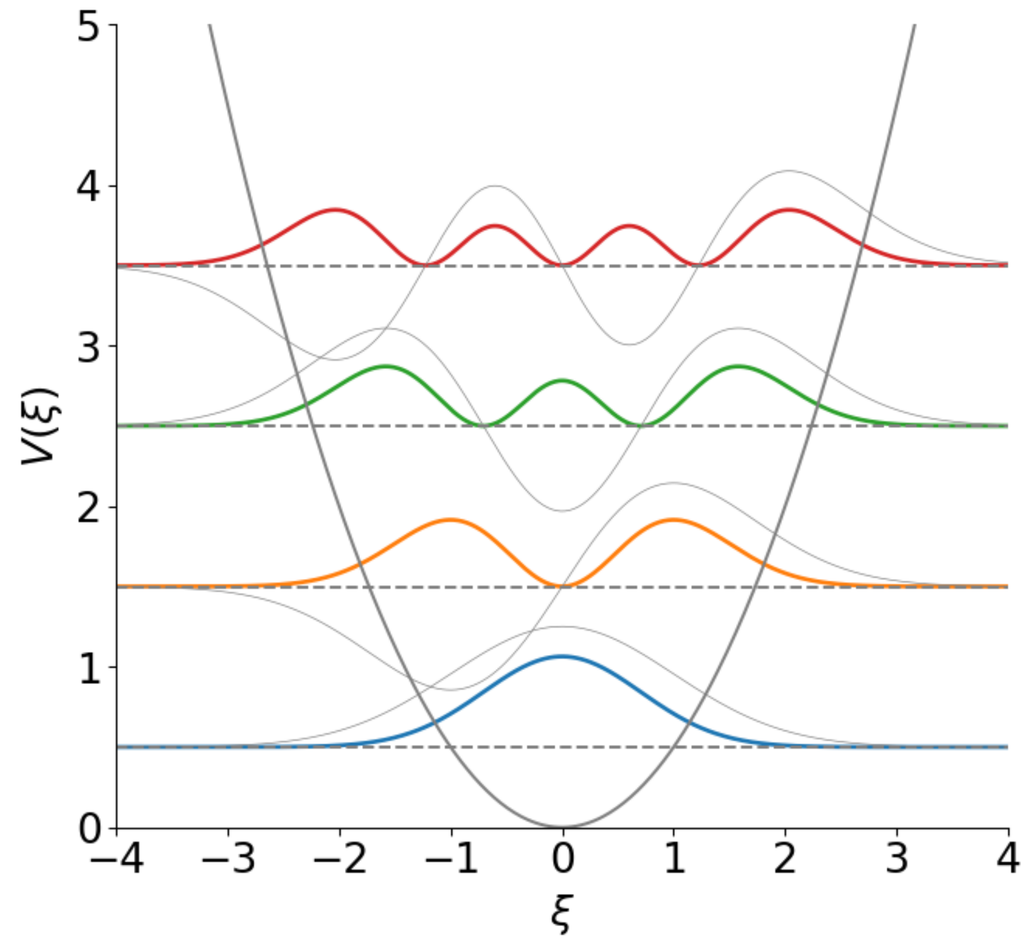


HARMONIC OSCILLATOR SOLUTIONS

Wave function $\psi(\xi)$



Probability density function $|\psi(\xi)|^2$



HIGH ENERGY SOLUTIONS

Classically $x \in \left[-\sqrt{\frac{2E}{m\omega^2}}, \sqrt{\frac{2E}{m\omega^2}}\right]$ and $|\psi_n|^2 \rightarrow \rho_{\text{class.}}(x) = \frac{1}{T}\frac{1}{v(x)}$

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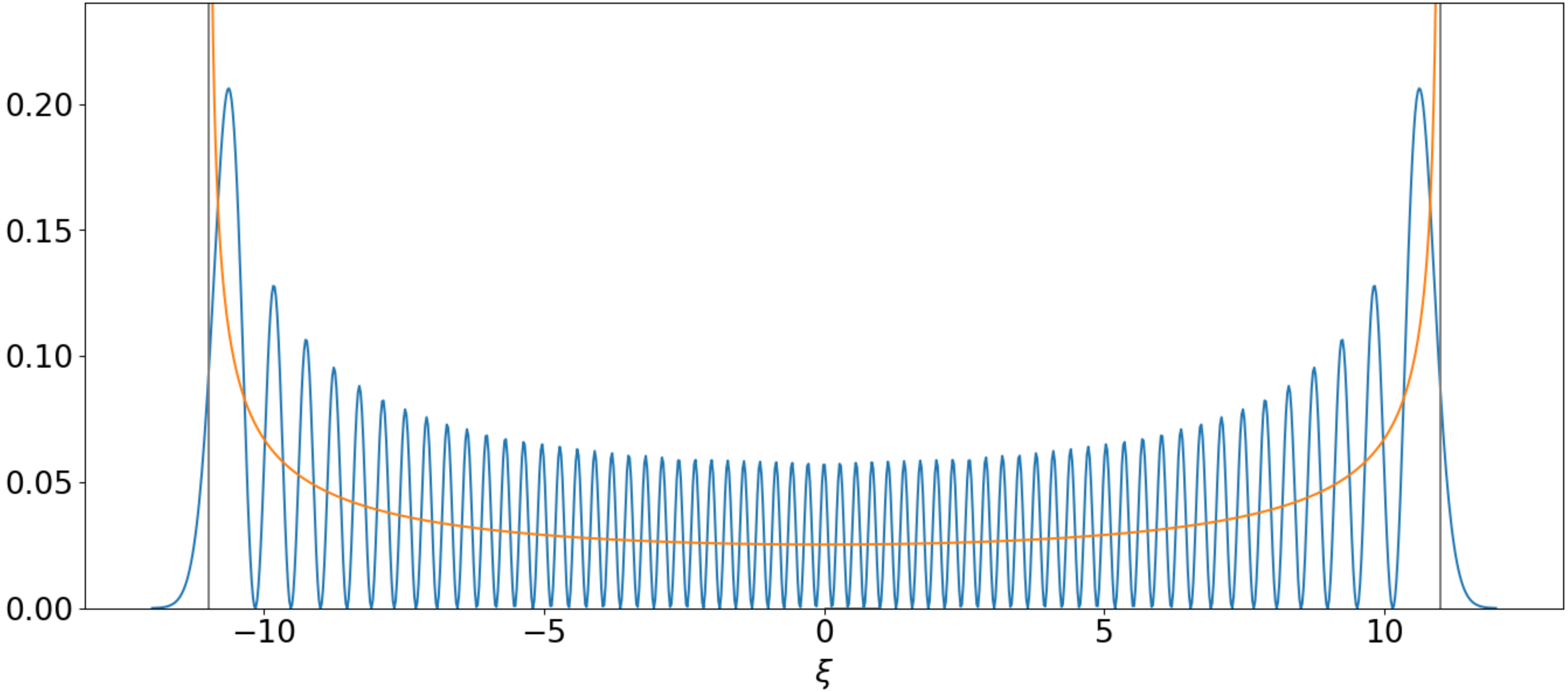
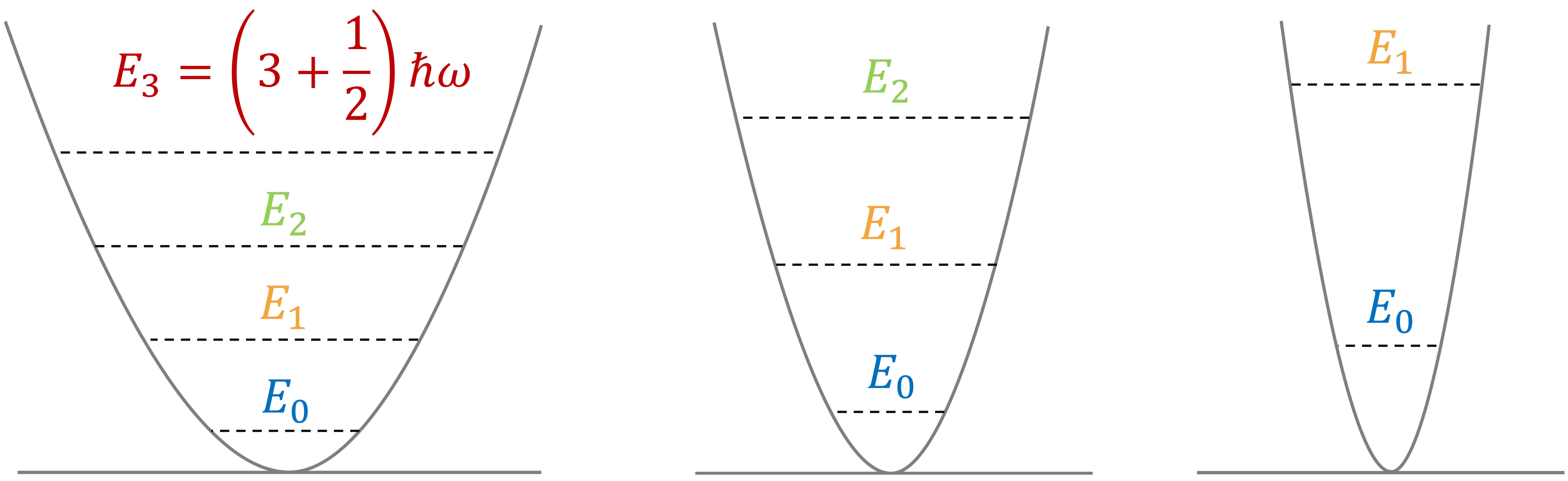


POTENTIAL PARAMETERS & SOLUTIONS

- Energy-levels $E_n \propto \omega$, *Width parabola* scales with $1/\omega$

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

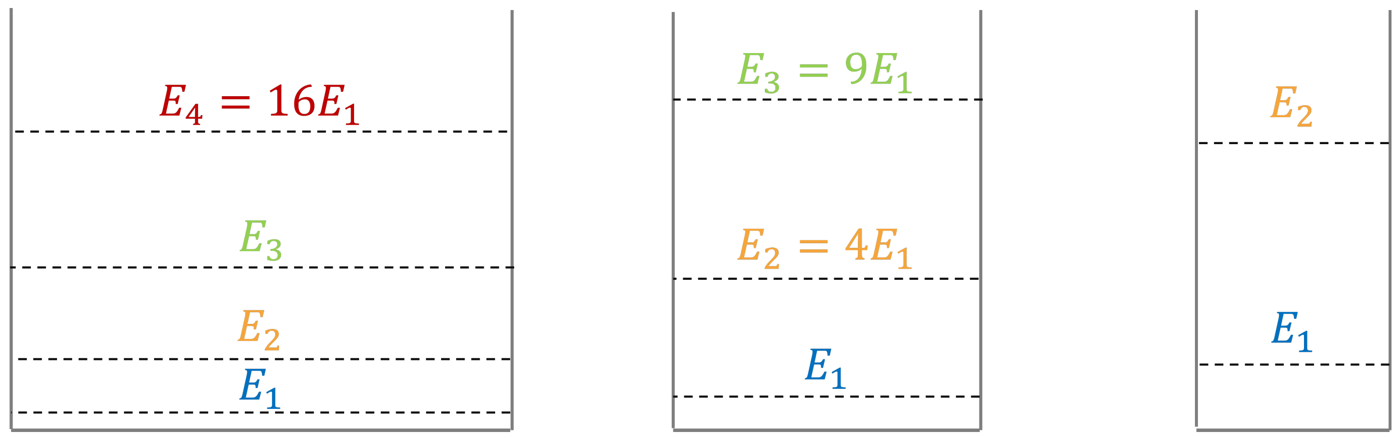


ENERGY INFINITE WELL VS. HARMONIC OSCILLATOR

Infinite well:

- $E_n \propto n^2$
- $E_n \propto 1/L^2$

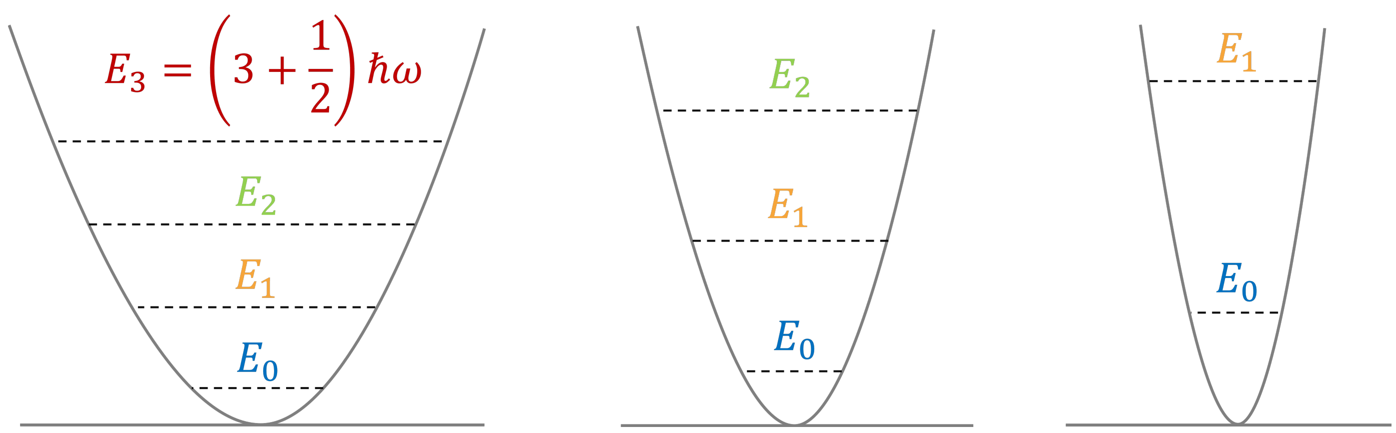
$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$



Quantum H.O.:

- equidistant E_n
- $E_n \propto \omega$
- width $\propto 1/\omega$

$$E_n = (n + 1/2)\hbar\omega$$



ALTERNATIVE (ALGEBRAIC) DERIVATION

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:

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

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

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

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

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:

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

The normalization factor A_n can be calculated

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

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
  - Single eigenstates are stationary for finite expectation energy $\langle \hat{H} \rangle$
  - Superposition 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)

SUMMARY

So far we looked at bound states

- Infinite well
- Linear potential well (Electrical field, not seen yet)
- Harmonic oscillator

Different well potentials lead to different allowed energy levels

Narrower wells $\longrightarrow$ less energy levels (more spread)