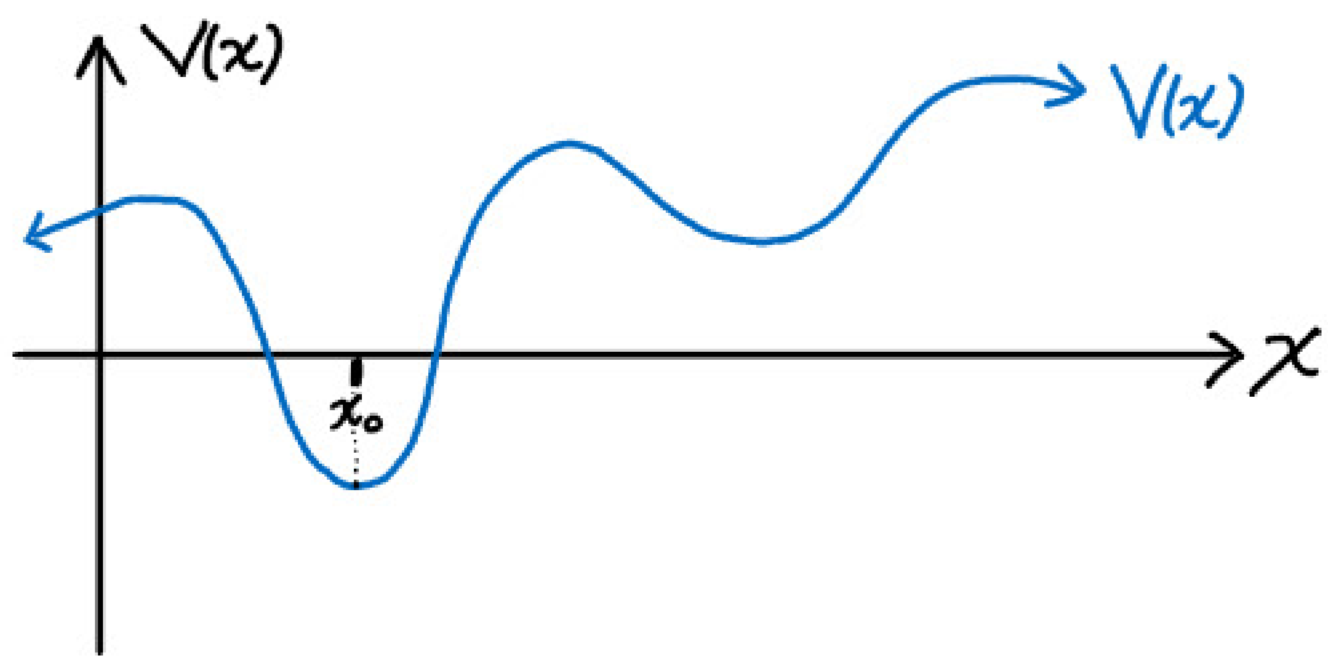
Quantum Simple Harmonic Oscillator

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2} m\omega^2 \hat{X}^2$$

I. Why Study? Consider a Generic Potential in 1D



- Let x_0 denote a Local Stable Minimum of $V(x)$:

$$\left.\frac{dV}{dx}\right|_{x=x_0} = 0 \quad \text{EXTREMUM OF } V(x) \; ; \quad \left.\frac{d^2V}{dx^2}\right|_{x=x_0} \equiv m\omega^2 > 0 \quad \underline{\text{STABLE MINIMUM}}$$

$$\therefore \; V(x) \simeq V(x_0) + (x-x_0)\left.\frac{dV}{dx}\right|_{x=x_0} + \frac{1}{2!}(x-x_0)^2 \left.\frac{d^2V}{dx^2}\right|_{x=x_0} + \mathcal{O}(x-x_0)^3$$

$$= V(x_0) + 0 + \frac{m\omega^2}{2}(x-x_0)^2 + \mathcal{O}(x-x_0)^3$$

$\Longrightarrow$ SHO is generally applicable near any stable potential minimum (as long as $V(x)$ is <u>analytic</u> in the vicinity of x_0)

Another Reason to Study SHO: Modes of Quantum Fields

$$\hat{H} = \sum_{\vec{k}} \underbrace{\hbar\omega_{\vec{k}}}_{\text{Energy of a mode,}} \cdot \hat{n}_{\vec{k}}$$

<u>Number Operator</u>: $\hat{n}|n\rangle = n|n\rangle$, $n \in \{0, 1, 2, 3, \dots\}$

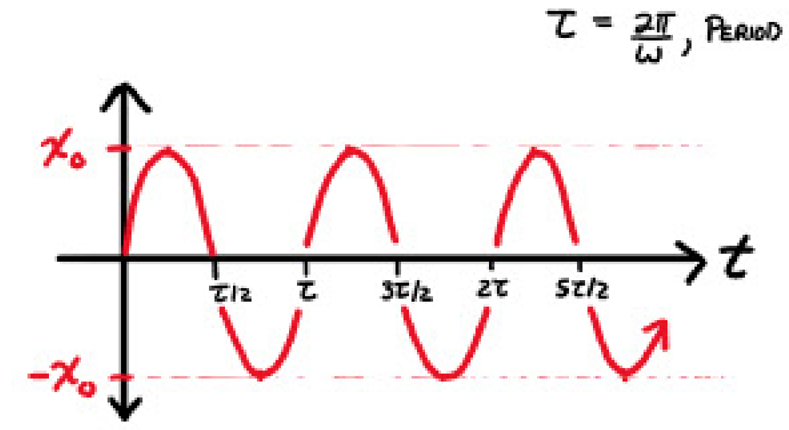
n = # Quanta (e.g. photons) in a mode.

... We will see the SHO is a single-mode version of this Hamiltonian

---

II. Classical Version

$\tau = \frac{2\pi}{\omega}$, Period



$$\cancel{m}\ddot{x} = -\cancel{m}\omega^2 x \Rightarrow x(t) = x_0 \cos(\omega t + \phi_0), \quad \pm x_0 : \text{"Classical Turning Points"}$$

<u>Energy</u>: $E = \frac{P^2}{2m} + \frac{m}{2}\omega^2 x^2 = \frac{m}{2}(\dot{x}^2 + \omega^2 x^2) = \frac{m\omega^2}{2} x_0^2 \left[\sin^2(\omega t + \phi_0) + \cos^2(\omega t + \phi_0)\right] = \frac{m\omega^2 x_0^2}{2}$

$$\Longrightarrow \sqrt{\frac{2E}{m} - \omega^2 x^2} = |\dot{x}| \; ; \quad \text{Speed vanishes at } x = \pm x_0$$

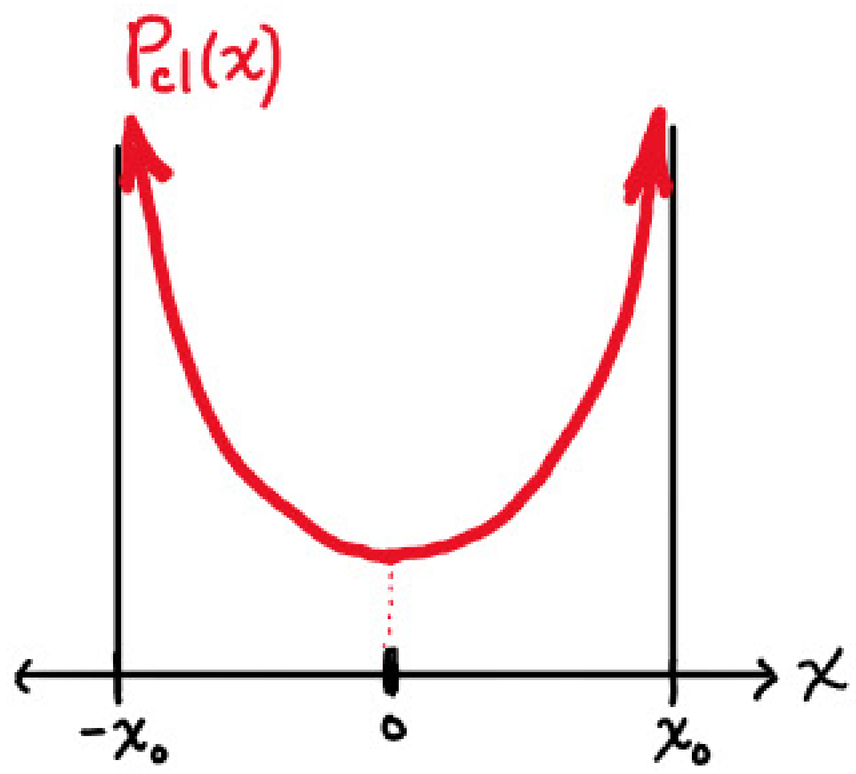
$$\therefore \; x_0 = \frac{1}{\omega}\sqrt{\frac{2E}{m}}$$

Classical Probability to observe oscillator between positions x and $x+dx$:

$$P_{cl}(x)\,dx = \frac{\text{Time interval spent in spatial interval } \{x, x+dx\}}{\text{Total period}} = \frac{2\,dx}{|\dot{x}|}\frac{1}{\tau}$$

Rightward undulation, leftward undulation

$$= \frac{2\,dx}{\omega\sqrt{x_0^2 - x^2}}\,\frac{\omega}{2\pi} = \frac{dx}{\pi\sqrt{x_0^2-x^2}}$$



- Maximum classical probability near turning points, where velocity goes (momentarily) to zero.
- Minimum at $x=0$, where $|\dot{x}|$ is maximum.

III. Position Space

$\hat{H}|E\rangle = E|E\rangle$; $\hat{H} = \frac{\hat{P}^2}{2m} + \frac{m}{2}\omega^2\hat{X}^2$

$$\Rightarrow \left(\frac{2}{\hbar\omega}\right)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m}{2}\omega^2 x^2\right]\psi_E(x) = \left(\frac{2}{\hbar\omega}\right)E\,\psi_E(x)$$

; define $\varepsilon \equiv \frac{E}{\hbar\omega}$ (dimensionless energy)

$$\Big(\underbrace{-\frac{\hbar}{m\omega}\frac{d^2}{dx^2}}_{\text{Must be dimensionless!}} + \frac{m\omega}{\hbar}x^2\Big)\psi_\varepsilon(x) = 2\varepsilon\,\psi_\varepsilon(x)$$

Introduce length scale $b \equiv \sqrt{\frac{\hbar}{m\omega}}$; $[b] = \left(\frac{\text{Energy} \times \text{Time}}{\text{Energy} \times \frac{\text{Time}^2}{\text{Length}^2} \times \frac{1}{\text{Time}}}\right)^{\frac{1}{2}}$ = Length ✓

- $x \equiv b\,y$; $y = x/b$ is dimensionless

$$\therefore \boxed{\left[\frac{d^2}{dy^2} - y^2 + 2\varepsilon\right]\psi_\varepsilon(y) = 0.}$$

This is a linear, homogeneous ODE with non-constant coefficients.

How to Solve? General Strategy: Examine small, large-y behavior

① $|y| \ll 1$: $\left(\frac{d^2}{dy^2} + 2\varepsilon\right)\psi_\varepsilon(y) \simeq 0 \Rightarrow \psi_\varepsilon(y) = A\sin(\sqrt{2\varepsilon}\,y) + B\cos(\sqrt{2\varepsilon}\,y)$

$= a + by + cy^2 + \ldots$ (analytic power series)

② $|y| \gg 1$: $\left(\frac{d^2}{dy^2} - y^2\right)\psi_\varepsilon(y) \simeq 0 \Rightarrow \psi_\varepsilon(y) = A\,e^{-\frac{y^2}{2}} + \cancel{B\,e^{+\frac{y^2}{2}}}$

Not physical — state should be confined in parabolic well.

Natural "Ansatz":

$$\psi_\varepsilon(y) \equiv h(y)\,e^{-\frac{y^2}{2}}, \quad h(y) = \sum_{p=0}^{\infty} h_p\,y^p$$

Note: $\frac{d^2}{dy^2}\left(y^m e^{-\frac{y^2}{2}}\right)$

$= y^2 \cdot \left(y^m e^{-y^2/2}\right)\left[1 + \mathcal{O}(y^{-2})\right]$

Same large-y behavior for any $m \geq 0$.

$$\left(\frac{d^2}{dy^2} - y^2 + 2\varepsilon\right)\psi_\varepsilon(y) = 0 \quad ; \quad \psi_\varepsilon(y) \equiv h(y)\cdot e^{-\frac{y^2}{2}} \quad ; \quad h(y) \equiv \sum_{p=0}^{\infty} h_p\, y^p$$

Plug into Diff. Eq.: $h' \equiv \frac{dh}{dy}$

$$\left(\frac{d^2}{dy^2} + (2\varepsilon - y^2)\right) h(y)\, e^{-\frac{y^2}{2}} = (2\varepsilon - y^2)\, h\, e^{-\frac{y^2}{2}} + \frac{d}{dy}\left[h' e^{-\frac{y^2}{2}} - h y\, e^{-\frac{y^2}{2}}\right] = (2\varepsilon - \cancel{y^2})\, h\, e^{-\frac{y^2}{2}} + h'' e^{-\frac{y^2}{2}} - y h' e^{-\frac{y^2}{2}} - h' y\, e^{-\frac{y^2}{2}} - h\, e^{-\frac{y^2}{2}} + \cancel{h y^2 e^{-\frac{y^2}{2}}}$$

$$\therefore \quad \boxed{\left[\frac{d^2}{dy^2} - 2y\frac{d}{dy} + (2\varepsilon - 1)\right] h(y) = 0}$$

$\Rightarrow$ Traded initial ODE $\left[\frac{d^2}{dy^2} - y^2 + 2\varepsilon\right]\psi_\varepsilon(y) = 0$ for another one. But: expect dominant $|y| \to \infty$ behavior $\left(e^{-\frac{y^2}{2}}\right)$ has been "extracted" from $\psi_\varepsilon(y)$; try power series solution for $h(y)$

$$h(y) = \sum_{p=0}^{\infty} h_p\, y^p \quad \Rightarrow \quad \text{Plug into ODE:}$$

$$\sum_{p=2}^{\infty} p(p-1)\, h_p\, y^{p-2} - 2\sum_{p=1}^{\infty} p\, h_p\, y^p + (2\varepsilon - 1)\sum_{p=0}^{\infty} h_p\, y^p = 0$$

$p' \equiv p - 2 \,;\; p = p' + 2$

Can extend to $p = 0$, since $p\, h_p\, y^p\big|_{p=0} = 0$.

$$\therefore \quad \sum_{p=0}^{\infty}\left[(p+2)(p+1)\, h_{p+2} - 2p\, h_p + (2\varepsilon - 1) h_p\right] y^p = 0$$

The functions $\{1, y, y^2, y^3, \ldots\}$ are linearly indep. (This is the basis for any power or Taylor series)

$$\therefore \quad h_{p+2} = \left[\frac{2p - (2\varepsilon - 1)}{(p+1)(p+2)}\right] h_p \qquad \text{Recursion Relation for Coefficients}$$

$\therefore$ if $h_0 \neq 0,\ h_1 = 0$ (Even Parity!) $\Rightarrow$ Determines $\{h_2, h_4, h_6, \ldots\}$

$(h_3 = h_5 = h_7 = \ldots = 0)$

if $h_0 = 0,\ h_1 \neq 0$ (Odd Parity!) $\Rightarrow$ Determines $\{h_3, h_5, h_7, \ldots\}$

$(h_2 = h_4 = h_6 = \ldots = 0)$

Large-p Behavior:

$$\lim_{p\to\infty} \frac{h_{p+2}}{h_p} \simeq \frac{2p}{p^2} = \frac{2}{p}$$

Consider
$$e^{+y^2} = \sum_{n=0}^{\infty} \frac{y^{2n}}{n!} \equiv \sum_{k=0}^{\infty} b_k\, y^k \; ; \qquad b_k = \begin{cases} 0\,, & k = 1, 3, 5, \ldots \quad \text{(Even Parity)} \\ \dfrac{1}{(k/2)!}\,, & k \in 0, 2, 4, 6, \ldots \end{cases}$$

$$\Rightarrow \quad \frac{b_{k+2}}{b_k} = \frac{(k/2)!}{(k/2 + 1)!} = \frac{1}{k/2 + 1} \quad \Rightarrow \quad \lim_{k\to\infty} \frac{b_{k+2}}{b_k} = \frac{2}{k}$$

Same as $h(y)$!!

$\therefore \quad \lim_{y\to\infty} h(y) \simeq e^{y^2}$ IF WE KEEP THE ENTIRE (INFINITE) SERIES.

THIS WOULD IMPLY THAT $\lim_{y\to\infty} \psi_\varepsilon(y) = \lim_{y\to\infty} h(y)\, e^{-\frac{y^2}{2}} \simeq e^{+\frac{y^2}{2}}$ ⇐ THE LARGE-y BEHAVIOR THAT WE ALREADY REJECTED!

$$h(y) = \sum_{p=0}^{\infty} h_p\, y^p \quad ; \quad h_{p+2} = \left[\frac{2p - (2\varepsilon - 1)}{(p+1)(p+2)}\right] h_p$$

HOW TO RESOLVE BAD LARGE-y BEHAVIOR OF $h(y)$? SERIES MUST TERMINATE

$$h_n(y) \equiv \sum_{p=0}^{n} h_p^{(n)}\, y^p \quad ; \quad h_{n+2}^{(n)} = 0 \;\Rightarrow\; 2n = 2\varepsilon - 1 \;\text{ or }\; \varepsilon_n = n + \tfrac{1}{2}$$

$\therefore \quad \psi_n(y) \equiv h_n(y)\, e^{-\frac{y^2}{2}}$ HAS QUANTIZED EIGENENERGY $E_n = \hbar\omega\,\varepsilon_n = \hbar\omega\,(n+\tfrac{1}{2})$

$n \in \{0, 1, 2, \ldots\}$

$$h_{p+2}^{(n)} = \left[\frac{2p - 2n}{(p+1)(p+2)}\right] h_p^{(n)} \;\Rightarrow\; h_n(y) \text{ is an } n^{\text{th}} \text{ order Polynomial in } y$$

IN PARTICULAR

① EVEN PARITY : $h_1 = h_3 = h_5 = \cdots = 0$; $h_n(y) = h_0^{(n)} + h_2^{(n)} y^2 + h_4^{(n)} y^4 + \cdots + h_n^{(n)} y^n$, n = even

② ODD PARITY : $h_0 = h_2 = h_4 = \cdots = 0$; $h_n(y) = h_1^{(n)} y + h_3^{(n)} y^3 + h_5^{(n)} y^5 + \cdots + h_n^{(n)} y^n$, n = odd

THESE POLYNOMIALS ARE COMPLETELY DETERMINED BY n AND THE VALUE OF h_0 or h_1

- (ARBITRARY) VALUES OF h_0 or h_1 ARE CHOSEN ACCORDING TO A STANDARD CONVENTION
- WITH THIS CONVENTION, $H_n(y)$ "n^{TH} ORDER HERMITE POLYNOMIAL"

EVEN PARITY	ODD PARITY
① $H_0(y) = 1$	① $H_1(y) = 2y$
② $H_2(y) = -2(1 - 2y^2)$	② $H_3(y) = -12(y - \frac{2}{3}y^3)$
③ $H_4(y) = 12(1 - 4y^2 + \frac{4}{3}y^4)$	③ $H_5(y) = 120(y - \frac{4}{3}y^3 + \frac{4}{15}y^5)$

"HermiteH[n,y]" IN MATHEMATICA

Summary: Solution to SHO in Coordinate Basis

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m}{2}\omega^2 x^2\right]\psi_n(x) = E_n\,\psi_n(x)$$

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

Energy is linear in n
$\Rightarrow$ View n as counting the Number of Excitations with energy $\hbar\omega$
$\uparrow$
"Quanta"

"Zero-Point Energy": $E_0 = \frac{\hbar\omega}{2}$

State with $n=0$ Quanta (Ground State) has positive $E_0 > 0$, due to Parabolic Confinement $(\omega > 0)$

WaveFunctions:

$$\psi_n(x) = C_n\, H_n\!\left(\frac{x}{b}\right) e^{-\frac{1}{2}\left(\frac{x}{b}\right)^2},$$

where

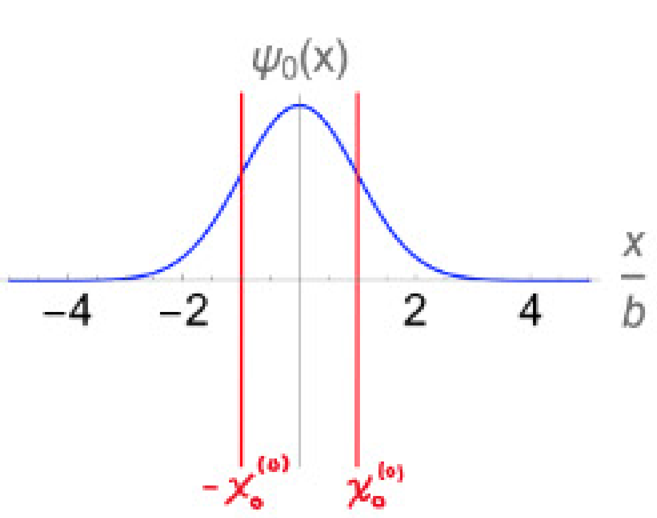
- C_n is a normalization constant
- $H_n(y)$ is the Hermite Polynomial of order n, which has
  - Even Parity, $n \in \{0, 2, 4, \ldots\}$
  - Odd Parity, $n \in \{1, 3, 5, \ldots\}$

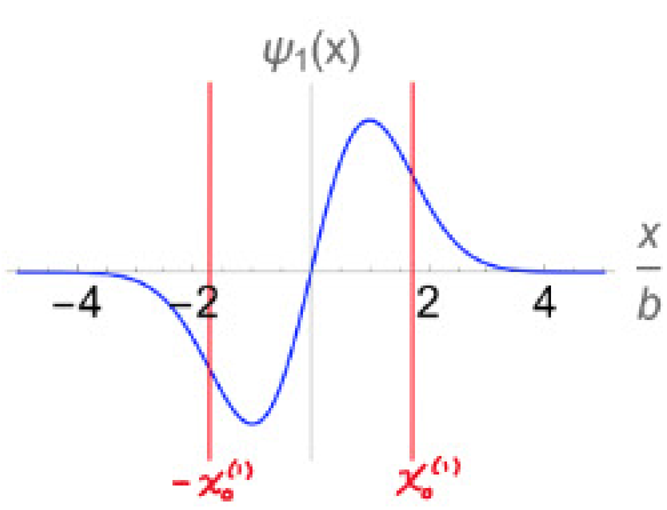
$b \equiv \sqrt{\frac{\hbar}{m\omega}}$, intrinsic length scale.

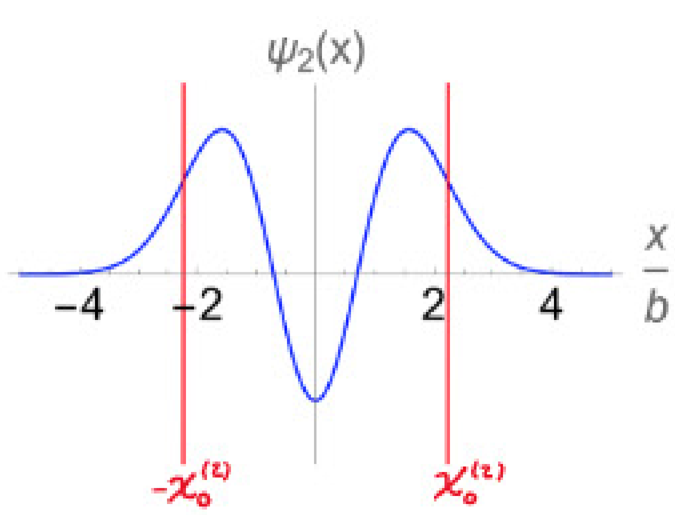
Plots: SHO Wavefunctions, Probability Densities

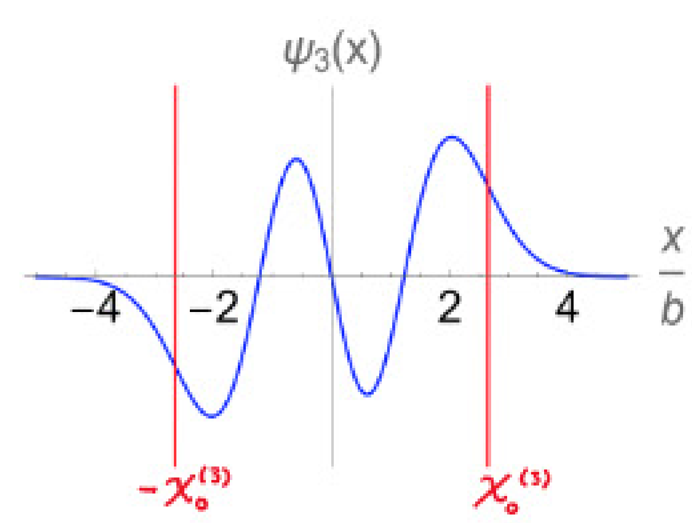
p. 1: Classical Turning Points $\pm x_0 = \pm\frac{1}{\omega}\sqrt{\frac{2E}{m}} \Rightarrow \pm\sqrt{\frac{2\hbar\cancel{\omega}\left(n+\frac{1}{2}\right)}{m\omega^{\cancel{2}}}}$

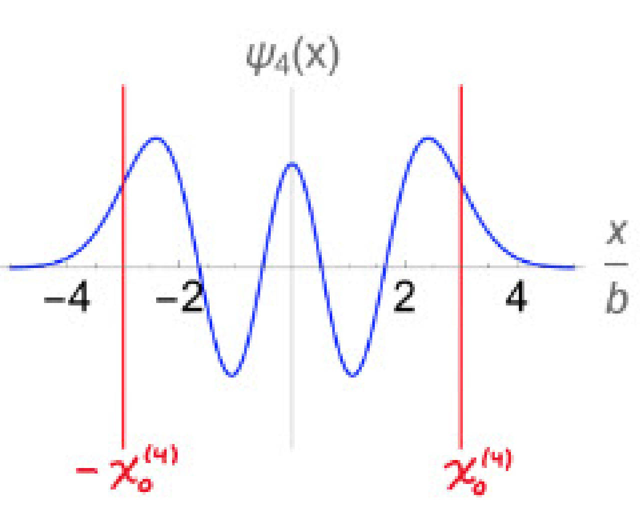
$$\pm x_0^{(n)} = \pm\, b\sqrt{2\left(n+\tfrac{1}{2}\right)}$$

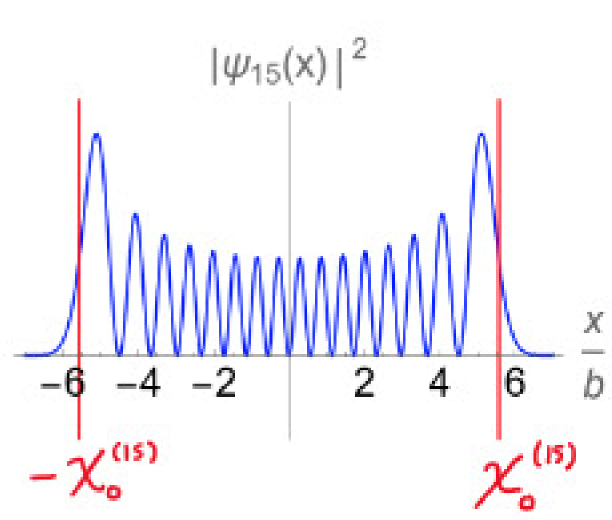












$\Leftarrow$ For $n \gg 1$, Probability Density begins to resemble Classical Result, $P_{cl}(x)$ on page 2.

Dynamics: $$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \Rightarrow |\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$$

Position Basis Propagator: $$U(x,x';t) = \langle x| e^{-i\frac{\hat{H}t}{\hbar}} |x'\rangle$$

(Response Function — Lec. 17, p.4)

$$= \sum_{n=0}^{\infty} \psi_n(x)\, \psi_n^*(x')\, e^{-i\omega(n+\frac{1}{2})t}$$

Not easy to evaluate; Closed-Form Solution can be obtained using Path Integral Method

Operator Expectations: $$\langle\hat{\Omega}\rangle(t) \equiv \langle\psi(t)|\hat{\Omega}|\psi(t)\rangle$$

Lec. 16, P.S:

① $$\frac{d\langle\hat{X}\rangle}{dt} = \frac{1}{m}\langle\hat{P}\rangle$$; ② $$\frac{d\langle\hat{P}\rangle}{dt} = -\left\langle \frac{d\hat{V}}{d\hat{X}} \right\rangle$$

$$= -m\omega\langle\hat{X}\rangle$$

Classical E.O.M.!

(special to potential of form $V(x) = V_0 + xV_1 + x^2V_2$)

$$\therefore \langle\hat{X}\rangle(t) = \langle\hat{X}\rangle(0)\cos(\omega t) + \frac{\langle\hat{P}\rangle(0)}{m}\sin(\omega t)$$

Note however for a stationary (eigen) state

$$|\psi(t)\rangle = e^{-i\omega(n+\frac{1}{2})t}|\psi_n\rangle, \quad \langle\hat{X}\rangle(t) = \langle\hat{X}\rangle(0) = 0;$$

$$\langle\hat{P}\rangle(t) = \langle\hat{P}\rangle(0) = 0.$$