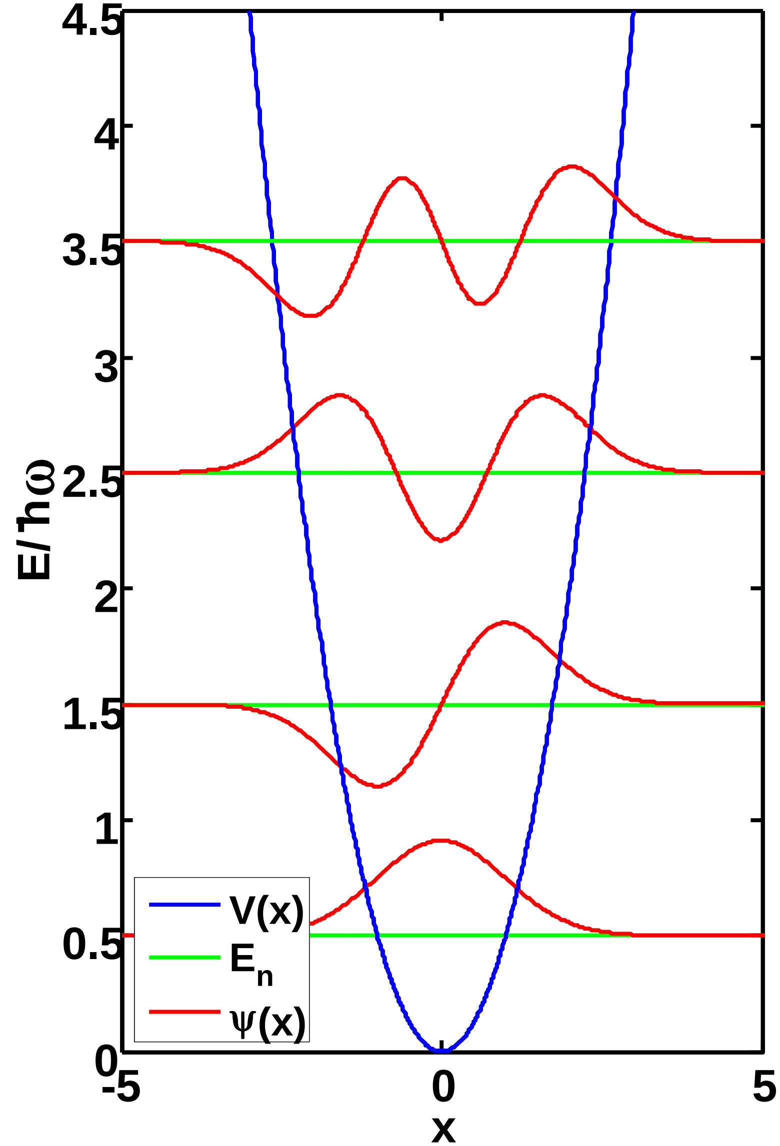
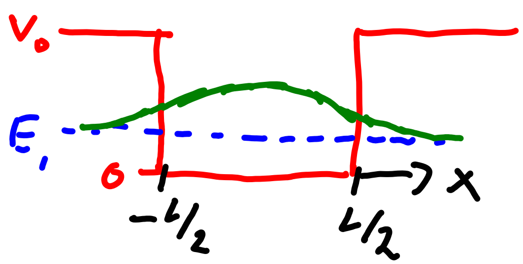
Lecture 19: 03/02/09

- More on the simple harmonic oscillator potential $V(x) = \frac{1}{2} c x^2$



Recap:

$II_{2,4}$ Square Well of Finite Depth, part II :



Boundary conditions at $x = \pm L/2$

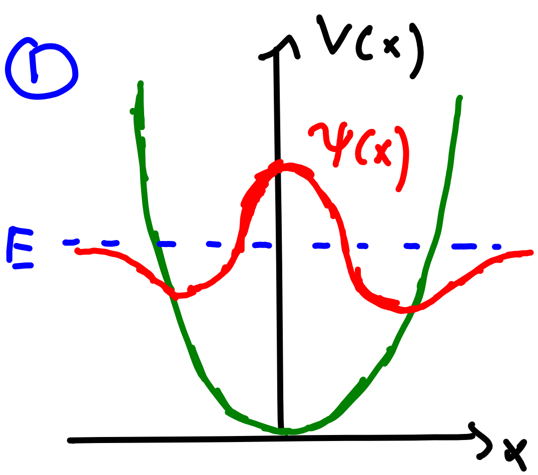
+ normalization ($\psi(x) \xrightarrow[x \to \pm\infty]{} 0$)

⇒ allowed energies $E_n \lesssim \frac{h^2 n^2}{8 m L^2}$ for large V_0

⇒ prefactors A_n (B_n) D_n of $\psi(x)$

$II_{2,5}$ The simple harmonic oscillator potential $V(x)=1/2cx^2$:

①



- Potential: $V(x) = \frac{1}{2} c x^2 = \frac{1}{2} m \omega^2 x^2$
- Introduce: $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x \qquad K = \frac{E}{\frac{1}{2}\hbar\omega}$

⇒ S.E.: $\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\,\psi(\xi)$

- Solve in 4 steps:

1) Quantitative $\psi(x)$

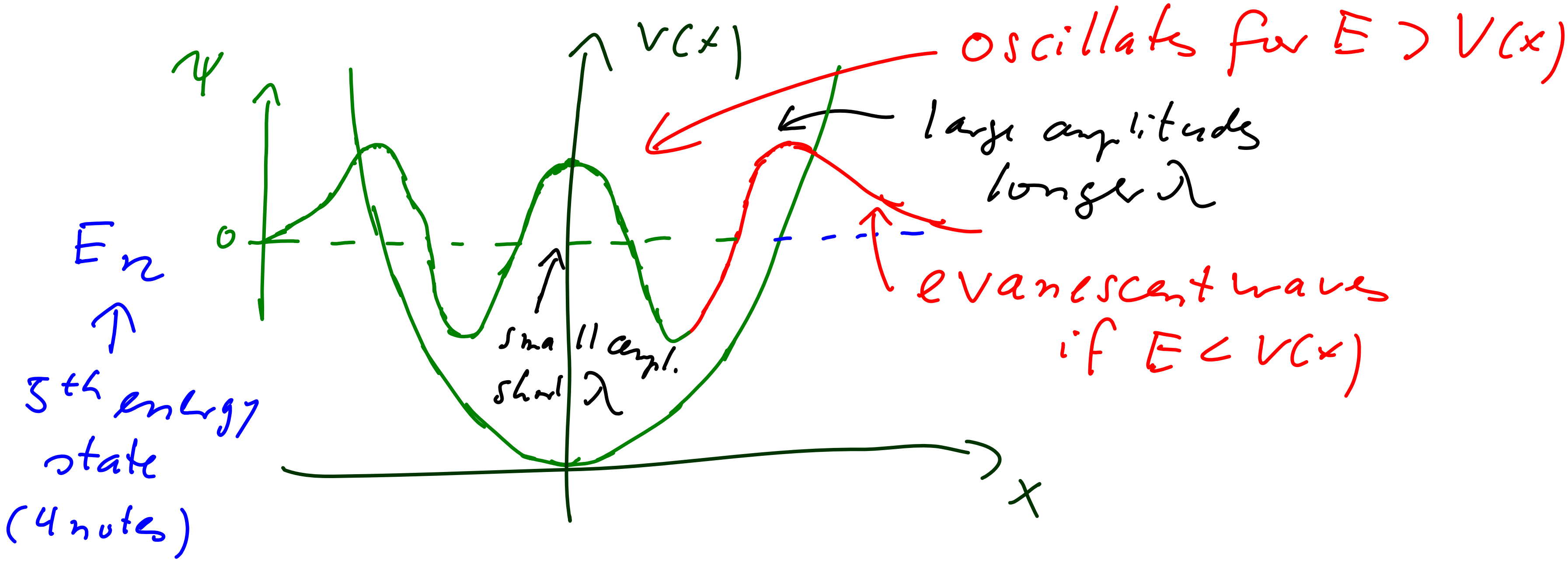
2) Consider large x i.e large ξ

3) Solve at all x i.e all ξ

4) Make sure $\psi(\xi)$ can be normalized

$\Rightarrow$ require $\psi(\xi) \xrightarrow[\xi \to \pm\infty]{} 0$ $\Rightarrow$ quantized allowed energy E_n

1) Quantitative $\psi(x)$



$\Rightarrow$ one region : $-\infty < x < \infty$

$\Rightarrow$ only boundary conditions at

$x = \pm\infty$: $\psi(\pm\infty) \to 0$

2) Consider large ξ:

$\Rightarrow \frac{1}{2}\left(x^2\right) \gg E \Rightarrow \xi^2 \gg K$

$$\Rightarrow \text{S.E.}: \quad \frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi \approx \xi^2\psi(\xi)$$

Note: $\psi \propto e^{-\alpha\xi}$ is no longer a solution here

Try: $\psi(\xi) = \xi^n e^{-\xi^2/2}$ $\quad \left[\psi(\xi) \xrightarrow[\xi \to \pm\infty]{} 0 \text{ good!}\right]$

$$\Rightarrow \frac{d\psi}{d\xi} = n\xi^{n-1} e^{-\xi^2/2} - \xi^{n+1} e^{-\xi^2/2}$$

$$\Rightarrow \frac{d^2\psi}{d\xi^2} = n(n-1)\xi^{n-2} e^{-\xi^2/2} - n\xi^n e^{-\xi^2/2} - (n+1)\xi^n e^{-\xi^2/2} + \underbrace{\xi^{n+2} e^{-\xi^2/2}}_{\text{this term dominates for large } \xi}$$

$$\Rightarrow \xi^{n+2} e^{-\xi^2/2} = \overbrace{\frac{d^2\psi}{d\xi^2} \approx \xi^2 \psi(\xi)}^{\text{S.E.}} = \xi^{n+2} e^{-\xi^2/2} \quad \checkmark$$

$\Rightarrow$ approximate solution at large ξ

3) Solve S.E. for all ξ:

from (2): at large ξ, all solutions have asymptotic form: $\psi(\xi) \longrightarrow \xi^n e^{-\xi^2/2}$ at large ξ

$\Rightarrow$ use: $\psi(\xi) = \underbrace{H(\xi)}_{\text{function of } \xi} \cdot e^{-\xi^2/2}$

$\Rightarrow$ Taylor's Theorem: Any resonable well behaved function can be expressed as a power series

$$H(\xi) = \sum_{j=0}^{\infty} a_j \xi^j$$

Note:
- $V(x)$ is symmetric
  - $\Rightarrow$ even $\psi(\xi)$: $a_j = 0$ for all odd j
  - $\Rightarrow$ odd $\psi(\xi)$: $a_j = 0$ for all even j
- will see later: $\psi(\xi)$ is only normalizable, if power series terminats; i.e. if $a_j = 0$ for all $j >$ some number n $\Rightarrow$ quantized energies

- Easiest example: $\underline{n=0}$

$$\Rightarrow \psi_0(\xi) \propto e^{-\xi^2/2}$$ no nodes $\Rightarrow$ candidate for ground state!

$$\Rightarrow \frac{d\psi_0}{d\xi} \propto -\xi e^{-\xi^2/2} \Rightarrow \frac{d^2\psi}{d\xi^2} \propto -e^{-\xi^2/2} + \xi^2 e^{-\xi^2/2}$$

– Insert into S.E.: $\frac{d^2\psi}{d\xi^2} = (\xi^2 - \mathcal{K})\psi(\xi)$

$$\Rightarrow -e^{-\xi^2/2} + \xi^2 e^{-\xi^2/2} = \xi^2 e^{-\xi^2/2} - \mathcal{K} e^{-\xi^2/2}$$

$\Rightarrow$ solution, if $\mathcal{K} = 1$!

$\Rightarrow$ recall: $\mathcal{K} = \frac{E}{\frac{1}{2}\hbar\omega}$ $\Rightarrow \underline{E_0 = \frac{1}{2}\hbar\omega}$

$\Rightarrow \psi_0(\xi)$ is the ground state wave function with particle energy $E_0 = \frac{1}{2}\hbar\omega$!

- **Same with full power series:**

$$\psi(\xi) = H(\xi)\, e^{-\xi^2/2} = e^{-\xi^2/2}\left(\sum_{j=0}^{\infty} a_j \xi^j\right)$$

$$\Rightarrow \frac{d\psi}{d\xi} = -e^{-\xi^2/2}\sum_{j=0}^{\infty} a_j \xi^{j+1} + e^{-\xi^2/2}\sum_{j=1}^{\infty} j a_j \xi^{j-1}$$

$$\Rightarrow \frac{d^2\psi}{d\xi^2} = e^{-\xi^2/2}\sum_{j=0}^{\infty} a_j \xi^{j+2} - e^{-\xi^2/2}\sum_{j=0}^{\infty}(j+1) a_j \underline{\xi^j}$$

$$- e^{-\xi^2/2}\sum_{j=1}^{\infty} j a_j \underline{\xi^j} + e^{-\xi^2/2}\sum_{j=2}^{\infty} j(j-1) a_j \xi^{j-2}$$

$$= e^{-\xi^2/2}\left\{\underbrace{\sum_{j=2}^{\infty} j(j-1) a_j \xi^{j-2}} - \sum_{j=0}^{\infty}(2j+1) a_j \xi^j + \sum_{j=0}^{\infty} a_j \xi^{j+2}\right\}$$

same as: $\displaystyle\sum_{j=0}^{\infty}(j+2)(j+1)a_{j+2}\xi^j$

• insert into S.E. for harmonic oscillator:

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\,\psi(\xi)$$

$$\Rightarrow \cancel{e^{-\xi^2/2}}\left\{\sum_{j=0}^{\infty}(j+2)(j+1)a_{j+2}\,\xi^j - (2j+1)a_j\,\xi^j + \cancel{a_j\,\xi^{j+2}}\right\}$$

$$= \cancel{e^{-\xi^2/2}}\left\{\underbrace{\cancel{\xi^2\sum_{j=0}^{\infty}a_j\,\xi^j}}_{H(\xi)} - K\sum_{j=0}^{\infty}a_j\,\xi^j\right\}$$

$\Rightarrow$ bring everything to one side:

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

$\Rightarrow$ needs to be true for all ξ $\Rightarrow$ $\{\ \} \overset{!}{=} 0$

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

recursion formula

- even $\psi(\xi)$: start with $a_0 \neq 0,\ a_1 = 0$
- odd $\psi(\xi)$: start with $a_1 \neq 0,\ a_0 = 0$

④ $\psi(\xi)$ needs to be normalizable

Problem: depending on choice of $\mathcal{K}$ (i.e. energy E), not all solutions are normalizable!

- Example: even solution: $H_{even}(\xi) = \sum_{j=0}^{\infty} a_{2j} \cdot \xi^{2j}$

$$a_{j+2} = \frac{2j+1-\mathcal{K}}{(j+2)(j+1)} a_j \xrightarrow[\text{large } j]{} a_{j+2} \simeq \frac{2}{j} a_j$$

$\Rightarrow$ approximate solution: $a_j \simeq \dfrac{\text{const}}{(j/2)!} \Rightarrow a_{2j} \simeq \dfrac{\text{const}}{j!}$

$$\Rightarrow H_{even}(\xi) \simeq \text{const} \sum_{j=0}^{\infty} \frac{1}{j!} \xi^{2j} = \text{const}\, e^{\xi^2}$$

Taylor series

$$\Rightarrow \psi_{even} = H_{even}(\xi) e^{-\xi^2/2} \simeq \text{const}\, e^{\xi^2} \cdot e^{-\xi^2/2} = \text{const}\, \underline{e^{+\xi^2/2}}$$

$$\Rightarrow \psi_{even}(\xi) \xrightarrow[\xi \to \pm\infty]{} \infty \Rightarrow \text{not physical}$$

(cannot be normalized!)

→ Solution: terminate power series!

⇒ highest j (call it "n"), such that

$$a_{n+2} = 0$$

$$a_{j+2} = \frac{2j+1-\mathcal{K}}{(j+2)(j+1)} a_j \quad \Rightarrow \text{ need } 2j+1-\mathcal{K} = 0 \text{ for } j=n$$

$$\Rightarrow \quad 2n+1-\mathcal{K} = 0 \quad \Rightarrow \quad \mathcal{K}_n = 2n+1$$

$$\Rightarrow \quad E_n = \frac{1}{2}\hbar\omega\mathcal{K}_n = \frac{1}{2}\hbar\omega(2n+1)$$

⇒ allowed energies of particle in SHO potential

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega \qquad n = \underline{0}, 1, 2, 3, \dots$$

note!

<u>Note:</u>
- equally spaced energy levels (spacing $= \hbar\omega$)
- recall Planck $\Delta E = \hbar\omega$
- ground state energy: $E_0 = \frac{1}{2}\hbar\omega > 0$
- got quantization of energy from boundary cond. $\psi(x) \xrightarrow[x \to \pm\infty]{} 0$