Lecture #9 Harmonic Osc. Cont.

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

$$V = \frac{1}{2} k x^2 \qquad \omega = \sqrt{k/m}$$

Dimensionless variables

$$\xi = \sqrt{\frac{m\omega}{\hbar}}\, x \qquad K = \frac{E}{\left(\frac{1}{2}\hbar\omega\right)}$$

$$\boxed{\frac{d^2\psi}{d\xi^2} = \left(\xi^2 - K\right)\psi(\xi)}$$

Last time

(a) Pull out asym. behavior $e^{\pm \xi^2/2}$

Chose $e^{-\xi^2/2}$ to be normalizable

(b) Guess $\psi(\xi) = h(\xi)\, e^{-\xi^2/2}$

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

(c) Expand $h = \sum_i a_i \xi^i$

$$a_{i+2} = \frac{2i+1-K}{(i+1)(i+2)}\, a_i$$

(d) Impose b.c. $h(\xi)$ can't blow up to much as $\xi \to \infty$ otherwise $\psi(\xi)$ will not be normalizable

$\Rightarrow$ Series must terminate

$$K = 2n+1 \qquad n = 0, 1, 2 \ldots$$

$$\boxed{E = K \tfrac{1}{2}\hbar\omega = \left(n + \tfrac{1}{2}\right)\hbar\omega}$$

with this choice of K a_{n+2} and all higher $n \equiv 0$

Numerical solution to see how b.c. determines allowed E

$$\frac{d\psi}{dx} \simeq \frac{1}{2h}\left(\psi(x+h) - \psi(x-h)\right)$$

$$\frac{d^2\psi}{dx^2} \simeq \frac{1}{h^2}\left[\psi(x+h) + \psi(x-h) - 2\psi(x)\right]$$

Calculate ψ on grid $\psi_i \equiv \psi(ih)$

can see formulas for 2^{nd} der. as follows

$$\frac{d^2\psi}{dx^2} \approx \frac{1}{h}\left[\frac{d\psi}{dx}\bigg|_{x+\frac{1}{2}h} - \frac{d\psi}{dx}\bigg|_{x-\frac{1}{2}h}\right]$$

and $$\frac{d\psi}{dx}\bigg|_{x+\frac{1}{2}h} \approx \frac{1}{h}\left(\psi(x+h) - \psi(x)\right)$$

$$\frac{d\psi}{dx}\bigg|_{x-\frac{1}{2}h} \approx \frac{1}{h}\left[\psi(x) - \psi(x-h)\right]$$

$$\psi'' = (x^2 - K)\psi(x)$$

$$\frac{1}{h^2}\left(\psi_{i+1} + \psi_{i-1} - 2\psi_i\right) \approx (x_i^2 - K)\psi_i$$

$$x_i = ih$$

Solve for ψ_{i+1}

$$\boxed{\psi_{i+1} = h^2(x_i^2 - K)\psi_i + 2\psi_i - \psi_{i-1}}$$

Consider odd solution. These have

$$\psi(0) = 0 \Rightarrow \psi_0 = 0$$

guess $\psi_1 = \epsilon$ $\qquad$ ϵ = any small #

go back and normalize later

$$\psi_2 = h^2 (x_1^2 - K)\epsilon + 2\epsilon - 0$$

etc. then get ψ_3 from ψ_2 and ψ_1

Procedure (a) Guess K

(b) Integrate out to large x

(c) Repeat and adjust K so $\psi(x) \to 0$ as $x \to 0$ to be normalizable.

basic code HOSC.bas See course Web site Folder Computer programs in course lectures.

PSIP = h2*(X^2 - K)*PSI + 2*PSI - PSIM

PSIP = ψ_{i+1} , PSIM = ψ_{i-1}

Shooting method, adjust K till wave function behaves as $x \to \infty$

$$E = (n + \tfrac{1}{2})\hbar\omega \quad \text{with } n \text{ odd}$$

note n even does not have $\psi(0) = 0$

Example of power series

$n = 2 \Rightarrow K = 5$

$$a_2 = \frac{1 - 5}{1 \cdot 2} a_0$$

$$a_2 = -2 a_0$$

$$a_4 = \frac{5 - 5}{3 \cdot 4} a_2 = 0 = a_6 \ldots$$

$$\psi_2(\xi) = a_0 (1 - 2\xi^2) e^{-\xi^2/2}$$

Can find a_0 by normalization

Finite polynomials $h(\xi)$ are related to Hermite polynomials $H_n(x)$.

$H_n(x)$ is polynomial of order n with 1^{st} coef 2^n

$H_0 = 1, \quad H_1 = 2x, \quad H_2 = 4x^2 - 2$

$H_3 = 8x^3 - 12x \quad \ldots$

Note $\quad H_{n+1}(x) = 2x\, H_n(x) - 2n\, H_{n-1}(x)$

$$\psi_2(\xi) = \left(\frac{a_0}{-2}\right) H_2(\xi)\, e^{-\xi^2/2}$$

Normalization integral can ~~be~~ done

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

Normalized Harmonic osc. wave function

For low n quantum osc. very different from classical. Most prob. place to find particle in ground state $x=0$ quantum

turning points classical

$$\frac{1}{2} k x_{turn}^2 = E = V(x_{turn}) + (T=0)$$

$$x_{turn} = \pm \left(\frac{2E}{k}\right)^{1/2} = \pm\sqrt{\frac{2\left(n+\frac{1}{2}\right)\hbar\omega}{k}}$$

Correspondance principle

In limit $n \rightarrow \infty$ expect to recover classical behavior.

Use code Harmonic.bas to plot wave functions.