L19-SHO Frobenius Method

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* Overview: we are going to solve the same problem using the Frobenius method (series solutions). Here are the main steps:

1) dimensionless $\mathcal{H}$: $\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right)\psi = E\psi \Rightarrow \left(-\frac{d^2}{d\xi^2}+\xi^2-K\right)\psi = 0$

2) asymptotic form: $\psi = h(\xi)e^{-\xi^2/2}$ $\quad h'' - 2\xi h' + (K-1)h = 0$

3) power series: $h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j$ $\quad a_{j+2} = \frac{2j+1-K}{(j+1)(j+2)}$

4) B.C.'s (truncation): $E_n = \frac{1}{2}\hbar\omega K_n = \hbar\omega(n+\frac{1}{2})$ $\quad a_{j+2}^{(n)} = \frac{-2(n-j)}{(j+1)(j+2)}$
quantization

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

* Example of Frobenius method: exponential : $f' = f$

analytic solution: $\frac{df}{f} = dx$ $\quad \ln f/f_0 = x$ $\quad f = f_0 e^x$

power series: $f = \sum_{j=0}^{\infty} a_j x^j = a_0 + a_1 x + a_2 x^2 + \ldots \sim \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \end{pmatrix}\begin{matrix} |1\rangle \\ |x\rangle \\ |x^2\rangle \\ \vdots \end{matrix}$

derivative: $f' = \sum_{j=\cancel{0}\,1}^{\infty} j a_j x^{j-1} = \underbrace{\cancel{0}\,0a_0}_{j=0,\ \cancel{j'=-1}} + \underbrace{a_1}_{j=1,\ j'=0} + \underbrace{2a_2 x^1}_{j=2,\ j'=1} + \ldots$

let $j' = j-1$ $\quad = \sum_{j'=0}^{\infty}(j'+1)a_{j'+1}x^{j'}$

note the "matrix" (components) of the derivative operator in the power series basis:

$$\begin{pmatrix} a_1 \\ 2a_2 \\ 3a_3 \\ \vdots \end{pmatrix}\begin{matrix} |1\rangle \\ |x\rangle \\ |x^2\rangle \\ \\ \end{matrix} = \begin{array}{c} \begin{matrix} |1\rangle & |x\rangle & |x^2\rangle & |x^3\rangle \end{matrix} \\ \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 2 & 0 & \cdots \\ 0 & 0 & 0 & 3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \end{array} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix}\begin{matrix} |1\rangle \\ |x\rangle \\ |x^2\rangle \\ |x^3\rangle \\ \\ \end{matrix}$$

relabel "dummy index" $j' \to j$ to match f on powers of x

$$f' - f = \sum_{j=0}^{\infty}\underbrace{\left[(j+1)a_{j+1} - a_j\right]}_{\text{component}}\underbrace{x^j}_{\text{basis}} = (a_1 - a_0)1 + (2a_2 - a_1)x + (3a_3 - a_2)x^2 + \ldots = 0$$

independence of basis: if $f = \sum_{j=0}^{\infty} a_j x^j = 0$ then all $a_j = 0 \Rightarrow (j+1)a_{j+1} = a_j$

1 constant of integration (1st order eq.): $a_0 = $ arbitrary. $a_1 = \frac{a_0}{1}$ $a_2 = \frac{a_1}{2}$ ...

thus $a_j = \frac{a_{j-1}}{j} = \frac{a_{j-1}}{j}\frac{a_{j-2}}{j-1}\cdots a_0 = \frac{a_0}{j!}$ $f = a_0 \sum_{j=0}^{\infty} \frac{1}{j!} x^j = a_0 e^x$

* TISE for SHO : $\hat{H}\Psi = E\Psi$

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right)\Psi(x) = E\,\Psi(x)$$

a) solve ODE
b) apply B.C.'s.

- dimensionless variables:

let $\xi = \sqrt{\frac{m\omega}{\hbar}}\,x$ $K = \frac{2E}{\hbar\omega}$ $\Rightarrow$ $\frac{d^2\Psi}{d\xi^2} - (\xi^2 - K)\Psi = 0$

- asymptotic limit: if $\xi^2 \gg K$ then $\frac{d^2\Psi}{d\xi^2} = \xi^2\Psi$, $\Psi \approx e^{-\xi^2/2}$

$$\frac{d}{d\xi}\left(\frac{d}{d\xi}e^{-\xi^2/2}\right) = \frac{d}{d\xi}\left(-\xi e^{-\xi^2/2}\right) = \underbrace{\cancel{-1}\cdot e^{-\xi^2/2}}_{\text{smaller}} + \underbrace{(-\xi)(-\xi)e^{-\xi^2/2}}_{\text{dominant as } \xi\to\infty} \approx \xi^2 e^{-\xi^2/2}$$

let $\Psi(\xi) = h(\xi)\,e^{-\xi^2/2}$ to factor out this dependence

$$\Psi' = h' e^{-\xi^2/2} + h(-\xi)e^{-\xi^2/2}$$
$$\Psi'' = h'' e^{-\xi^2/2} + 2h'(-\xi)e^{-\xi^2/2} - he^{-\xi^2/2} + h\xi^2 e^{-\xi^2/2}$$
$$\Psi'' - (\xi^2 - K)\Psi = \left(h'' - 2h'\xi + h\xi^2 + (K-1)h\right)e^{-\xi^2/2} = 0$$

thus $h'' - 2\xi h' + (K-1)h = 0$ Hermite ODE with $K-1 \to 2n$

- Power series solution: let $h = \sum_{j=0}^{\infty} a_j \xi^j$ $h' = \sum_{j=0}^{\infty} a_j\, j\, \xi^{j-1}$

plug these into ODE: $h'' = \sum_{j=0}^{\infty} a_j\, j(j-1)\,\xi^{j-2} = \sum_{j=0}^{\infty} (j+1)(j+2)\,a_{j+2}\,\xi^j$

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

solution: $h(\xi) = \left[\underbrace{a_0}_{\text{normalization}} + \underbrace{a_2\xi^2 + a_4\xi^4 + \ldots}_{\text{by recursion}}\right] + \left[\underbrace{a_1}_{\text{norm}}\xi + \underbrace{a_3\xi^3 + \ldots}_{\text{recursion}}\right] = a_0 h_{even} + a_1 h_{odd}$

- quantization: $a_{j+2} \approx \frac{1}{j/2} a_j \approx \frac{a_0}{(j/2)!}$ exponential growth!

$$h(\xi) \approx a_0 \sum_{j=0}^{\infty} \frac{1}{(j/2)!} \xi^j \approx a_0 \sum_j \frac{1}{j!} \xi^{2j} \approx a_0 e^{+\xi^2} \text{ blows up.}$$

only get normalized solution if series terminates

if $K_n = 2n+1$ then $a_{n+2} = a_{n+4} = \dots = 0$. K_n satisfies B.C.

thus $E_n = \frac{\hbar\omega}{2}(2n+1) = \hbar\omega(n+\frac{1}{2})$ $\quad a_{j+2}^{(n)} = \frac{-2(n-j)}{(j+1)(j+2)}$

- Hermite polynomials: "standardized" so $a_n^{(n)} = 2^n$

$h_0(\xi) = a_0^{(0)} = 1$ $\quad \boxed{H_0(\xi) = 1}$ $\quad h_1(\xi) = a_1^{(1)} = \xi$ $\quad \boxed{H_1(\xi) = 2\xi}$

$h_2(\xi) = a_0^{(2)} + a_2^{(2)}\xi^2 \propto 1 - 2\xi$ $\quad h_3(\xi) = a_1^{(3)}\xi + a_3^{(3)}\xi^3 \propto \xi - \frac{2}{3}\xi^3$

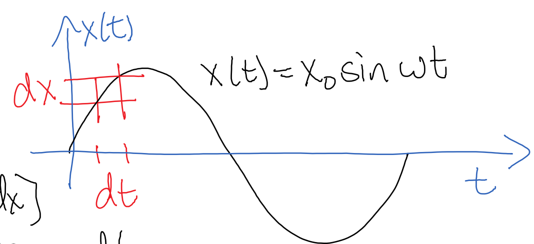
$\boxed{H_2(\xi) = 4\xi^2 - 2}$ $\quad \boxed{H_3(\xi) = 8\xi^3 - 12\xi}$

- Normalized wavefunctions:

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

$$\int_{-\infty}^{\infty} \psi_n(x)\psi_m(x)\,dx = \frac{1}{\sqrt{\pi 2^n n! 2^m m!}} \int_{-\infty}^{\infty} \underbrace{e^{-\xi^2}}_{\text{weight } w(\xi)} d\xi \, H_n(\xi) H_m(\xi) = \delta_{nm}$$

* Classical probability density:



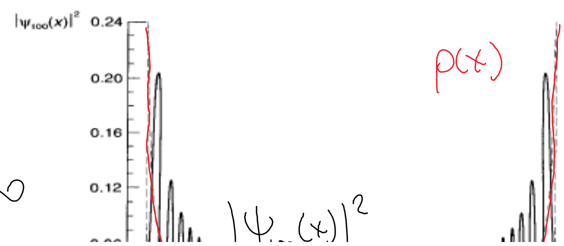
$\rho\, dx$ = probability that $x \in [x, x+dx]$
$\propto$ time spent in this region dt.

thus $\rho(x) \propto \frac{1}{dx/dt} = \frac{1}{\cos(\omega t)} = \frac{1}{\sqrt{1-\sin^2\omega t}} = \frac{1}{\sqrt{1-(x/x_0)^2}}$

$$\int_{-x_0}^{x_0} \rho(x)\,dx = \int_{-x_0}^{x_0} \frac{k\,dx}{\sqrt{1-(x/x_0)^2}} = k x_0 \int_{-1}^{1} \frac{du}{\sqrt{1-u^2}} = k x_0 \frac{\pi}{2} = 1 \qquad u = x/x_0$$

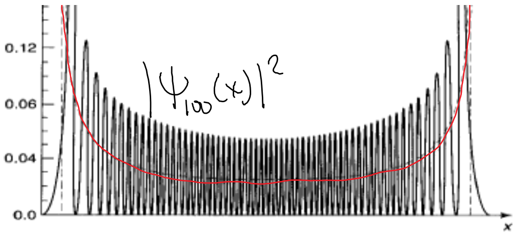
thus $\rho(x) = \frac{2/\pi}{\sqrt{x_0^2 - x^2}}$

Compare with $|\psi_{100}(x)|^2$ to



Compare with $|\psi_{100}(x)|^2$ to see classical limit.

(Griffiths)



(b)

Figure 2.5: (a) The first four stationary states of the harmonic oscillator. (b) Graph of $|\psi_{100}|^2$, with the classical distribution (dashed curve) superimposed.