Lecture 23

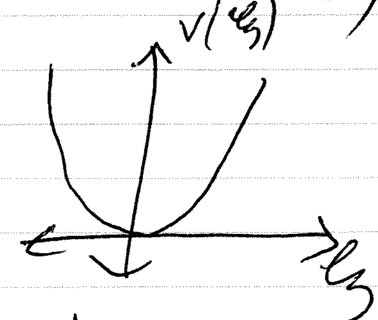
Hermite & Laguerre Polynomials

Consider a 1D quantum simple harmonic oscillator:

$$-\frac{\hbar^2}{2m}\psi''(\xi) + V(\xi)\psi(\xi) = E\psi(\xi)$$

$$V(\xi) = \frac{1}{2}m\omega^2\xi^2 \quad \text{(quadratic potential)}$$

ω - frequency



$$\Rightarrow -\frac{\hbar^2}{2m}\psi'' + \frac{1}{2}m\omega^2\xi^2\psi = E\psi$$

$$\Rightarrow \psi'' - \frac{m^2\omega^2}{\hbar^2}\xi^2\psi + \frac{2m}{\hbar^2}\psi = 0$$

ξ has units of length

& $m\omega\hbar^{-1}$ has units $\frac{1}{[\text{length}]^2}$

then $x = \xi \sqrt{\frac{m\omega}{\hbar}}$ is dimensionless

Define $l = \sqrt{\frac{\hbar}{m\omega}}$

& rescale $x = \xi/l$ & $\frac{dx}{d\xi} = \frac{1}{l}$

$\psi(\xi) = y(x)$

$$\Rightarrow \frac{d\psi}{d\xi} = \frac{dx}{d\xi}\frac{dy}{dx} = \frac{1}{l}\frac{dy}{dx}$$

$$\Rightarrow \psi''(\xi) = \frac{1}{l^2} y''(x)$$

$$\Rightarrow \frac{1}{l^2} y''(x) - \frac{1}{l^2} x^2 y(x) = -\frac{2mE}{\hbar^2} y(x)$$

$$\Rightarrow y''(x) - x^2 y(x) = \frac{-2m}{\hbar^2} E \frac{\hbar}{m\omega}$$

$$= \frac{-2E}{\hbar\omega}$$

define $\varepsilon = \frac{E}{\hbar\omega}$

$\Rightarrow y''(x) - x^2 y(x) = -2\varepsilon y(x)$

- we do not justify, but ~~[illegible]~~ state that energy is quantized, so that $\varepsilon = n + 1/2$ for $n \in \{0, 1, 2, \ldots\}$
- we then have

$$y_n''(x) - x^2 y_n(x) = -2(n + 1/2) y_n(x)$$

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

this is a Hermite diff eq. where $y_n(x)$ are Hermite functions.

- Let $\frac{d}{dx} = D = D_x = \partial_x = \partial$

then $[D - x][D + x] y = [D - x][y'(x) + xy]$

$= y''(x) + y + xy'(x) - xy'(x) - x^2 y$

$$= y''(x) + y - x^2 y$$

Furthermore,

$$[D+x][D-x]y = [D+x](y' - xy)$$

$$= y'' - y - xy' + xy' - x^2 y$$

$$= y'' - y - x^2 y$$

Using this, we can write Hermite diff. eq. as

$$y_n''(x) - x^2 y_n(x) + y_n(x) = -2n\, y_n(x)$$

(1) $\Rightarrow$ $[D-x][D+x]\, y_n(x) = -2n\, y_n(x)$

can also write as

$$y_n''(x) - x^2 y_n(x) - y_n(x) = -2(n+1)\, y_n(x)$$

(2) $\Rightarrow$ $[D+x][D-x]\, y_n(x) = -2(n+1)\, y_n(x)$

Now operate on 1^{st} one w/ $D+x$

& on second one w/ $D-x$

& change n to m

(3) $\Rightarrow$ $[D+x][D-x][D+x]\, y_m(x) = -2m [D+x]\, y_m(x)$

(4) $\Rightarrow$ $[D-x][D+x][D-x]\, y_m(x) = -2(m+1) [D-x]\, y_m(x)$

Compare (1) & (4).

If $y_n(x) = (D-x)\, y_m(x)$ &

$n = m+1$, then

the equations are identical.

Then write

$$y_{m+1}(x) = (D-x)(y_m(x))$$

& can conclude from this development, that if we have a solution $y_m(x)$ for $n=m$, we can obtain

another solution for $n=m+1$
by applying the "raising operator"
$[D-x]$ to $y_m(x)$.

- Similarly, from (2) + (3),
  we find that

$$y_{m-1}(x) = [D+x]\, y_m(x)$$

$[D+x]$ is known as a "lowering operator"

- these operators are also called ladder operators since they allow for going up or down, as in a rung of ladders
- Idea is now to solve Hermite diff. eq. for $n=0$ + then generate all other solutions by using raising operator.

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$$y_{m+1}(x) = [D - x]\, y_m(x)$$

Consider $n=0$. then equation is

$$y_0'' - x^2 y_0 = -y_0$$

$$\Rightarrow \quad y_0'' + (1-x^2) y_0 = 0$$

Consider $y_0(x) = e^{-x^2/2}$

take $y_0'(x) = e^{-x^2/2} \cdot (-x)$

$$= -x\, y_0(x)$$

$$y_0''(x) = -y_0(x) + x^2 y_0(x)$$

$$= -(1-x^2)\, y_0(x)$$

$\Rightarrow$ $y_0(x)$ is a solution to

$$y_0''(x) + (1-x^2)\, y_0(x) = 0.$$

So then the solutions are given by

$$y_n(x) = \left[D - x\right]^n e^{-x^2/2}$$

for $n \in \{0, 1, 2, \dots\}$.

called Hermite functions

can also write this more simply as

$$y_n(x) = e^{x^2/2} \left[\frac{d}{dx}\right]^n e^{-x^2}$$

Proof: Consider that

$$e^{x^2/2} D\left[e^{-x^2/2} f\right]$$

$$= e^{x^2/2}\left[-x e^{-x^2/2} f + e^{-x^2/2} f'\right]$$

$$= -x f + f'$$

$$= \left[D - x\right] f$$

So then for the base step, we get

$$[D-x]^2 e^{-x^2/2} =$$

$$[D-x][D-x]\left(e^{-x^2/2}\right)$$

$$= [D-x]\left(e^{x^2/2} D \left[e^{-x^2} \right] \right)$$

$$= e^{x^2/2} D \left[e^{-x^2/2} \left(e^{x^2/2} D \left[e^{-x^2} \right] \right) \right]$$

$$= e^{x^2/2} D D e^{-x^2}$$

$$= e^{x^2/2} D^2 e^{-x^2}$$

Now for inductive step:

Suppose that

$$[D-x]^n e^{-x^2/2} = e^{x^2/2} D^n e^{-x^2}$$

then

$$[D-x]^{n+1} e^{-x^2/2} = [D-x][D-x]^n e^{-x^2}$$

$$= [D-x]\left(e^{x^2/2} D^n e^{-x^2}\right)$$

$$= e^{x^2/2} D\left[e^{-x^2/2}\left(e^{x^2/2} D^n e^{-x^2}\right)\right]$$

$$= e^{x^2/2} D \circ D^n e^{-x^2}$$

$$= e^{x^2/2} D^{n+1} e^{-x^2}$$

QED.

multiplying Hermite functions by $(-1)\, e^{x^2/2}$ gives <u>Hermite polynomials</u>, defined as

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$$

formula always gives rise to a polynomial of degree n.

$$H_0(x) = (-1)^0 e^{x^2} D^0 e^{-x^2} = 1$$

$$H_1(x) = (-1)^1 e^{x^2} D^1 e^{-x^2}$$
$$= (-1)\, e^{x^2} (-2x)\, e^{-x^2}$$
$$= 2x$$

$$H_2(x) = (-1)^2\, e^{x^2} D^2 e^{-x^2}$$
$$= (-1)^2 e^{x^2} D\left[-2x\, e^{-x^2}\right]$$
$$= e^{x^2}\left[-2e^{-x^2} + 4x^2 e^{-x^2}\right]$$
$$= 4x^2 - 2$$

Hermite polynomials satisfy the Hermite equation

$$y'' - 2xy' + 2n\, y = 0$$

they are also orthogonal on $(-\infty, \infty)$ w.r.t weight function e^{-x^2}

$$\int_{-\infty}^{\infty} dx\; e^{-x^2} H_n(x)\, H_m(x) = \delta_{nm} \sqrt{\pi}\; 2^n n!$$

The solution to the original Hermite diff. eq. is

$$y_n(x) = (-1)^n e^{-x^2/2} H_n(x)$$

Putting in units of length, we get

$$\psi_n(\xi) = y_n(x) \cdot c_n$$

↑ normalization

$$\Rightarrow \psi_n(\xi) = c_n (-1)^n e^{-(\xi/l)^2/2} H_n(\xi/l)$$

where $l = \sqrt{\frac{\hbar}{m\omega}}$ & c_n is a normaliz

To compute c_n, calculate

$$1 = \int_{-\infty}^{\infty} |\psi_n(\xi)|^2 d\xi$$

$$= |c_n|^2 \, l \int_{-\infty}^{\infty} e^{-(\xi/l)^2/2} H_n^2(\xi/l) \frac{d\xi}{dl}$$

$$= |c_n|^2 \ell \int_{-\infty}^{\infty} e^{-x^2} H_n^2(x)\, dx$$

$$= |c_n|^2 \ell \sqrt{\pi}\, 2^n n!$$

$$\Rightarrow \quad c_n = \left[\ell \sqrt{\pi}\, 2^n n!\right]^{-1/2}$$

$$= \left(\frac{m\omega}{\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}}$$

So then

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

choose units s.t. $\ell = 1$ & plot

$$\Psi_n = \varepsilon_n + \psi_n$$