LINEAR HARMONIC OSCILLATOR

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2}x^2$$

$$H u_n = E_n u_n \,, \quad n = 0, 1, \ldots$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad \omega = 2\pi\nu$$

$$u_n = N_n H_n(\xi) e^{-\frac{1}{2}\xi^2}$$

$$\xi = \alpha x, \quad \alpha = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}$$

$$H_n'' - 2\xi H_n' + 2n H_n = 0$$

H_n is a polynomial of order n and parity of n, $H_n(-\xi) = (-1)^n H_n(\xi)$

1. Energy is quantized, we have bound states only.

2. u_ns have well-defined parity,

$$u_n(-x) = (-1)^n u_n(x)$$

(V is an even function of x)

3. u_n has n nodes (roots of H_n).

4. Each energy level is nondegenerate.

5. $E_{n+1} - E_n = \hbar\omega = h\nu$

(as in the old quantum theory)

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right) \neq \underbrace{\hbar\omega\, n}_{\text{old quantum theory}}$$

$$E_0 = \frac{1}{2}\hbar\omega > 0$$

zero-point energy

HERMITE POLYNOMIALS

(H_n)

H_n is a polynomial of order n and parity of n satisfying

$$H_n'' - 2\xi H_n' + 2nH_n = 0 \quad (\star)$$

We could generate H_ns using recursive relationships

$$a_{\nu+2}(\nu+s+2)(\nu+s+1) = a_\nu(2\nu+2s+\underbrace{1-\lambda}_{-2n})$$

2n+1

$$H_n(\xi) = \xi^s(a_0 + a_2\xi^2 + \cdots + a_{2k}\xi^{2k})$$

$$n = 2k + s \quad , \quad s = 0, 1$$

$s = 0$ (even H_ns):

$$H_0 = a_0$$

$$H_2 = a_0 + a_2\xi^2 = a_0(1 - 2\xi^2)$$

$\ldots$

$s = 1$ (odd H_ns):

$$H_1 = a_0\xi$$

$\ldots$

GENERATING FUNCTION FOR HERMITE POLYNOMIALS

$$S(\xi, s) = e^{\xi^2 - (s-\xi)^2}$$

$$= e^{-s^2 + 2s\xi} \quad \checkmark$$

$$S(\xi,s) = \sum_{m,n} c_{mn}\,\xi^m s^n$$

$$= \sum_n \underbrace{\left(\sum_m c_{mn}\,\xi^m\right)}_{\frac{H_n(\xi)}{n!}} s^n$$

$$\sum_m c_{mn}\,\xi^m = \frac{H_n(\xi)}{n!}$$

$$S(\xi,s) = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n \checkmark$$

We will prove now that

1. H_n is a polynomial of order n.
2. H_n has a parity of n.
3. H_n satisfies Eq. ($\star$).

① + ②:

$$e^{z} = \sum_{k=0}^{\infty} \frac{z^k}{k!}$$

$$S = e^{-s^2+2s\xi}$$

$$= \sum_{k=0}^{\infty} \frac{(-s^2+2s\xi)^k}{k!}$$

$$(a+b)^k = \sum_{l=0}^{k} \binom{k}{l} a^l b^{k-l}$$

$$S = \sum_{k=0}^{\infty} \sum_{l=0}^{k} \binom{k}{l} \frac{1}{k!} (-s^2)^l$$

$$\times (2s\xi)^{k-l}$$

$$S = \sum_{k=0}^{\infty} \sum_{l=0}^{k} \frac{\cancel{k!}}{l!(k-l)!\,\cancel{k!}}$$

$$\times (-1)^l \, s^{2l} \, 2^{k-l} \, s^{k-l} \, \xi^{k-l}$$

$$S = \sum_{k=0}^{\infty} \sum_{l=0}^{k} \frac{(-1)^l \, 2^{k-l} \, \xi^{k-l}}{l! \, (k-l)!}$$

$$\times \, s^{k+l}$$

$n = k+l, \quad k-l = n-2l \geq 0$

$$S = \sum_{n=0}^{\infty} \left[\sum_{l=0}^{[\frac{n}{2}]} \frac{(-1)^l \, 2^{n-2l} \, \xi^{n-2l}}{l! \, (n-2l)!} \right] s^n$$

$[\frac{n}{2}] \rightarrow$ the largest integer not exceeding $\frac{n}{2}$

$$S(\xi, s) = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n \quad \checkmark$$

$\rightarrow$ at s^n

$$H_n(\xi) = \sum_{l=0}^{[\frac{n}{2}]} \frac{(-1)^l \, 2^{n-2l} \, n!}{l! \, (n-2l)!} \xi^{n-2l} \quad \checkmark$$

H_n is a polynomial of order n (contains powers of ξ up to ξ^n)

H_n is also a polynomial of parity of n:

$\xi^n, \; \xi^{n-2}, \; \xi^{n-4}, \ldots$

We must prove now that H_n satisfies Eq. (☆).

$$\frac{\partial S}{\partial \xi} = \frac{\partial}{\partial \xi} e^{-s^2+2s\xi}$$

$$= 2s\, e^{-s^2+2s\xi} = 2s\, S$$

$$S = \sum_{n=0}^{\infty} \frac{H_n}{n!} s^n \quad \checkmark$$

$$\frac{\partial S}{\partial \xi} = \sum_{n=0}^{\infty} \frac{2s^{n+1}}{n!} H_n \quad \checkmark$$

$$\frac{\partial S}{\partial \xi} = \sum_{n=0}^{\infty} \frac{H_n'}{n!} s^n \quad \checkmark$$

At s^n:

$$\frac{H_n'}{n!} = \frac{2H_{n-1}}{(n-1)!} \quad / \times n!$$

$$H_n' = 2n H_{n-1} \quad \checkmark$$

$$\frac{\partial S}{\partial s} = \frac{\partial}{\partial s} e^{-s^2+2s\xi}$$

$$= (-2s+2\xi) e^{-s^2+2s\xi}$$

$= S$

$$= \sum_{n=0}^{\infty} \frac{(-2s+2\xi)H_n}{n!} s^n$$

$$= -\sum_{n=0}^{\infty} \frac{2s^{n+1}}{n!} H_n$$

$$+ \sum_{n=0}^{\infty} \frac{2s^n}{n!} \xi H_n$$

$$\frac{\partial S}{\partial s} = \frac{\partial}{\partial s} \sum_{n=0}^{\infty} \frac{H_n}{n!} s^n$$

$$= \sum_{n=1}^{\infty} \frac{H_n}{n!} n s^{n-1}$$

$$= \sum_{n=1}^{\infty} \frac{H_n}{(n-1)!} s^{n-1}$$

At s^n:

$$\frac{H_{n+1}}{n!} = \frac{2\xi H_n}{n!} - \frac{2H_{n-1}}{(n-1)!} \Big/ \times n!$$

$$H_{n+1} = 2\xi H_n - 2n H_{n-1}$$

$$H_{n+1} = 2\xi H_n - 2n H_{n-1} \quad \checkmark$$

$$H_n' = 2n H_{n-1} \quad \checkmark$$

$$\frac{d}{d\xi} \Big/ \quad H_{n+1} = 2\xi H_n - H_n'$$

$$2(n+1)H_n = H_{n+1}' = 2H_n + 2\xi H_n' - H_n''$$

$$2nH_n + \cancel{2H_n} = \cancel{2H_n} + 2\xi H_n' - H_n''$$

$$H_n'' - 2\xi H_n' + 2nH_n = 0$$

$$\therefore$$

$$S(\xi,s)=\sum_{n=0}^{\infty}\frac{H_n(\xi)}{n!}s^n$$

$$f(x)=\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{d^nf}{dx^n}\right)_{x=0}x^n$$

$$H_n(\xi)=\left(\frac{\partial^n S(\xi,s)}{\partial s^n}\right)_{s=0}$$

$$\frac{\partial^n S}{\partial s^n}=\frac{\partial^n}{\partial s^n}e^{\xi^2-(s-\xi)^2}$$

$$=e^{\xi^2}\frac{\partial^n}{\partial s^n}\underbrace{e^{-(s-\xi)^2}}_{\text{function of }(s-\xi)} \checkmark$$

$$f(s-\xi),\quad \frac{\partial f}{\partial s}=-\frac{\partial f}{\partial \xi}$$

$$\frac{\partial^n f}{\partial s^n} = (-1)^n \frac{\partial^n f}{\partial \xi^n}$$

$$\frac{\partial^n S}{\partial s^n} = e^{\xi^2} (-1)^n \frac{\partial^n}{\partial \xi^n} e^{-(s-\xi)^2}$$

$$H_n(\xi) = \left(\frac{\partial^n S}{\partial s^n}\right)_{s=0}$$

$$= (-1)^n e^{\xi^2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2}$$

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2} \checkmark$$

$$H_0(\xi) = 1,$$
$$H_1(\xi) = 2\xi$$
$$H_2(\xi) = 4\xi^2 - 2$$
$$\dots$$

$$H u_n = E_n u_n, \quad n = 0, 1, \dots$$

$$\alpha = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

$$u_n = N_n H_n(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2}$$

↑ normalization

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{\partial^n}{\partial \xi^n} e^{-\xi^2}$$

We will now learn how to determine $\langle u_n | F | u_m \rangle$.

Normalization:

$$\langle u_n | u_m \rangle = \delta_{nm}$$

$$\langle u_n | u_m \rangle = \int_{-\infty}^{\infty} u_n^*(x)\, u_m(x)\, dx$$

$$= N_n N_m \int_{-\infty}^{\infty} H_n(\alpha x) H_m(\alpha x)$$

$$\times e^{-\alpha^2 x^2} dx$$

$$\langle u_n | u_m \rangle \overset{\xi = \alpha x}{\underset{d\xi = \alpha dx}{=}} \frac{N_n N_m}{\alpha}$$

$$\times \underbrace{\int_{-\infty}^{\infty} H_n(\xi) H_m(\xi) e^{-\xi^2} d\xi}_{I_{nm}}$$

$S(\xi, s)$ $\qquad$ $S(\xi, t)$

$$A = \int_{-\infty}^{\infty} S(\xi, s)\, S(\xi, t)\, e^{-\xi^2}\, d\xi$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{s^n t^m}{n!\, m!} \times$$

$$\times \int_{-\infty}^{\infty} H_n(\xi)\, H_m(\xi)\, e^{-\xi^2}\, d\xi$$

$$A = \sum_{n,m=0}^{\infty} \frac{I_{nm}}{n!\, m!} s^n t^m \checkmark$$

$$A = \int_{-\infty}^{\infty} e^{-s^2+2s\xi}\, e^{-t^2+2t\xi}\, e^{-\xi^2}\, d\xi$$

$$(\xi - s - t)^2 = \xi^2 + s^2 + t^2$$
$$-2s\xi - 2t\xi + 2st$$

$$A = \int_{-\infty}^{\infty} e^{-(s^2+t^2+\xi^2-2s\xi-2t\xi)}\, d\xi$$

$$= \int_{-\infty}^{\infty} e^{-(\xi-s-t)^2} e^{2st}\, d\xi$$

$$= e^{2st} \int_{-\infty}^{\infty} e^{-(\xi-s-t)^2}\, d\xi$$

$z = \xi - s - t$

$dz = d\xi$

$$= e^{2st} \underbrace{\int_{-\infty}^{\infty} e^{-z^2}\, dz}_{\sqrt{\pi}}$$

$$A = \sqrt{\pi}\, e^{2st}$$

$n=m$

$$= \sqrt{\pi} \sum_{n=0}^{\infty} \frac{2^n s^n t^n}{n!} \quad ✓$$

$$A = \sum_{n,m=0}^{\infty} \frac{I_{nm}}{n!\,m!} s^n t^m$$

At $s^n t^m$:

$$\frac{I_{nm}}{n!\,m!} = \frac{2^n \sqrt{\pi}}{n!} \delta_{nm}$$

$n=m$:

$$\frac{I_{nn}}{(n!)^2} = \frac{2^n \sqrt{\pi}}{n!} \Big/ \times (n!)^2$$

$$I_{nn} = 2^n n! \sqrt{\pi}$$

$n \neq m$:

$$I_{nm} = 0$$

$$\langle u_n | u_m \rangle = \frac{N_n N_m}{\alpha} I_{nm} \checkmark$$

$n = m$:

$$1 = \langle u_n | u_n \rangle = \frac{N_n^2}{\alpha} I_{nn}$$

$$= \frac{N_n^2}{\alpha} 2^n n! \sqrt{\pi}$$

$$N_n = \left(\frac{\alpha}{2^n n! \sqrt{\pi}} \right)^{\frac{1}{2}}$$

$n \neq m$:

$$\langle u_n | u_m \rangle = 0.$$

$$u_n(x) = N_n H_n(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2},$$

$$N_n = \left(\frac{\alpha}{2^n n! \sqrt{\pi}} \right)^{\frac{1}{2}}.$$

Example:

$$\langle u_n|\hat{V}|u_n\rangle = \frac{1}{2}k\langle u_n|\hat{x}^2|u_n\rangle$$

$$\langle u_n|\hat{x}^2|u_n\rangle = \int_{-\infty}^{\infty} u_n^*(x)\, x^2\, u_n(x)\, dx$$

$\xi = \alpha x$

$d\xi = \alpha dx$

$$= \frac{N_n^2}{\alpha^3}\int_{-\infty}^{\infty} H_n(\xi)^2\, \xi^2 e^{-\xi^2} d\xi$$

$$A = \int_{-\infty}^{\infty} S(\xi,s)\, S(\xi,t)\, \xi^2 e^{-\xi^2} d\xi$$

$$= \sum_{n,m=0}^{\infty} \frac{s^n t^m}{n!\,m!} \times \int_{-\infty}^{\infty} H_n(\xi) H_m(\xi)\, \xi^2 e^{-\xi^2} d\xi$$

$$I_{nm} = \int_{-\infty}^{\infty} H_n(\xi) H_m(\xi) \xi^2 e^{-\xi^2} d\xi$$

$$A = \sum_{n,m=0}^{\infty} \frac{s^n t^m}{n!\,m!} I_{nm} \quad \checkmark$$

$$\langle u_n | \hat{x}^2 | u_n \rangle = \frac{N_n^2}{\alpha^3} I_{nn} \quad \checkmark$$

$$A = \int_{-\infty}^{\infty} e^{-s^2+2s\xi} e^{-t^2+2t\xi} \times \xi^2 e^{-\xi^2} d\xi$$

$$A = e^{2st} \int_{-\infty}^{\infty} e^{-(s^2+t^2+\xi^2-2s\xi-2t\xi+2st)} \times \xi^2 d\xi$$

$$A = e^{2st}\int_{-\infty}^{\infty} e^{-(\xi-s-t)^2}\xi^2\,d\xi$$

$z = \xi - s - t$

$dz = d\xi$

$$= e^{2st}\int_{-\infty}^{\infty} e^{-z^2}(z+s+t)^2\,dz$$

$$= e^{2st}\int_{-\infty}^{\infty} e^{-z^2}\big(z^2+s^2+t^2 + 2zs + 2zt + 2st\big)\,dz$$

$$= e^{2st}\left\{\int_{-\infty}^{\infty} \underbrace{e^{-z^2}z^2\,dz}_{n=1}\right.$$

$$\left(\int_{-\infty}^{\infty} e^{-z^2}z\,dz = 0,\ e^{-z^2}z \to \text{odd}\right)$$

$$\left. + (s^2+t^2+2st)\int_{-\infty}^{\infty} \underbrace{e^{-z^2}dz}_{n=0}\right\}$$

$$\int_{-\infty}^{\infty} e^{-ax^2} x^{2n}\,dx = \frac{(2n)!}{2^{2n} n!}\sqrt{\frac{\pi}{a^{2n+1}}}$$

$$A = e^{2st}\left\{\frac{2!}{2^2 1!}\sqrt{\pi}\right.$$

$$\left. + (s^2+t^2+2st)\sqrt{\pi}\right\}$$

$$A = \sqrt{\pi}\, e^{2st}\left(\frac{1}{2}+s^2+t^2+2st\right)$$

$$A = \sum_{n,m=0}^{\infty} \frac{s^n t^m}{n!\,m!} I_{nm}$$

$$A = \sqrt{\pi}\left\{\sum_{n=0}^{\infty} \frac{2^{n-1} s^n t^n}{n!}\right.$$

$$+\sum_{n=0}^{\infty}\frac{2^n s^{n+2} t^n}{n!}$$

$$+\sum_{n=0}^{\infty}\frac{2^n s^n t^{n+2}}{n!}$$

$$+\sum_{n=0}^{\infty}\frac{2^{n+1} s^{n+1} t^{n+1}}{n!}\Bigg\}$$

$$=\sum_{n,m=0}^{\infty}\frac{s^n t^m}{n!\,m!} I_{nm}$$

At $s^n t^n$:

$$\sqrt{\pi}\left\{\frac{2^{n-1}}{n!}+\frac{2^n}{(n-1)!}\right\}$$

$$=\frac{I_{nn}}{(n!)^2} \quad / \times (n!)^2$$

$$I_{nn} = \sqrt{\pi}\left\{\frac{2^{n-1}}{\cancel{n!}}(n!)^{\cancel{2}} + \frac{2^n}{\cancel{(n-1)!}}\, n!\, \cancel{n!}^{\,n}\right\}$$

$$I_{nn} = 2^n n! \sqrt{\pi}\left(n+\frac{1}{2}\right)$$

$$\langle u_n|\hat{x}^2|u_n\rangle = \frac{N_n^2}{\alpha^3} I_{nn}$$

$$\langle u_n|\hat{x}^2|u_n\rangle = \frac{1}{\alpha^{\cancel{3}\,2}}\left(\frac{\cancel{\alpha}}{\cancel{2^n}\,\cancel{n!}\,\cancel{\sqrt{\pi}}}\right)$$

$$\times\, \cancel{2^n}\, \cancel{n!}\, \cancel{\sqrt{\pi}}\left(n+\frac{1}{2}\right)$$

$$\langle u_n | \hat{x}^2 | u_n \rangle = \frac{1}{\alpha^2}\left(n+\frac{1}{2}\right)$$

$$\langle u_n | \hat{V} | u_n \rangle = \frac{1}{2\alpha^2} k \left(n+\frac{1}{2}\right)$$

$$= \underbrace{\frac{\hbar}{2\cancel{m}\cancel{\omega}}}_{=\frac{1}{\alpha^2}} \underbrace{\cancel{m}\omega^{\cancel{2}}}_{k} \left(n+\frac{1}{2}\right)$$

$$\alpha = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}$$

$$\langle u_n | \hat{V} | u_n \rangle = \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right)$$

$$\langle u_n | \hat{V} | u_n \rangle = \frac{1}{2}E_n$$

Because of this,

$$\langle u_n|\hat{T}|u_n\rangle = \frac{1}{2}E_n$$

$$\langle u_n|\hat{T}|u_n\rangle = \langle u_n|\hat{V}|u_n\rangle = \frac{1}{2}E_n$$

(virial theorem)

We can show (HW7, Problem 2) that

$$\Delta x \Delta p_x = \left(n+\frac{1}{2}\right)\hbar .$$

In particular,

$$\Delta x \Delta p_x = \frac{\hbar}{2} \quad (n=0)$$

The ground state of the

harmonic oscillator is
a minimum wavepacket,

$$u_0(x) = \frac{\alpha^{\frac{1}{2}}}{\pi^{\frac{1}{4}}} e^{-\frac{1}{2}\alpha^2 x^2}$$