Lecture 7

Review. Quantum harmonic oscillator

$$V(x) = \frac{1}{2} m\omega^2 x^2$$

The ground (lowest) solution of time-independent Schrödinger equation for harmonic oscillator is:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$E_0 = \frac{1}{2}\hbar\omega.$$

To find all other functions, we can use $\psi_n(x) = A_n (a_+)^n \psi_0(x)$

The possible energies are: $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$

The ladder operators:

Raising operator $a_+ = \frac{1}{\sqrt{2m\omega\hbar}}(-ip + m\omega x)$

Lowering operator $a_- = \frac{1}{\sqrt{2m\omega\hbar}}(ip + m\omega x)$

Definition of commutator: $[A, B] = AB - BA$

Canonical commutation relation $[x, p] = i\hbar$

Exercise 4

Find the first excited state of the harmonic oscillator.

$$\int_0^\infty x^{2n} e^{-x^2/a^2} dx = \sqrt{\pi} \frac{(2n)!}{n!} \left(\frac{a}{2}\right)^{2n+1}$$

$$\int_0^\infty x^{2n+1} e^{-x^2/a^2} dx = \frac{n!}{2} a^{2n+2}$$

Exercise 4

Find the first excited state of the harmonic oscillator.

Solution:

$$\psi_1(x) = A_1\, a_+ \psi_0(x) = A_1 \frac{1}{\sqrt{2m\hbar\omega}}[-i\overset{-i\hbar\frac{d}{dx}}{p} + m\omega x]\,\psi_0(x)$$

$$= \frac{A_1}{\sqrt{2m\hbar\omega}}\left(-\hbar\frac{d}{dx} + m\omega x\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$= \frac{A_1}{\sqrt{2m\hbar\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left\{+\cancel{\hbar}\left(+\frac{m\omega}{\cancel{2\hbar}}\right)\cancel{2}x\, e^{-\frac{m\omega}{2\hbar}x^2} + m\omega x\, e^{-\frac{m\omega}{2\hbar}x^2}\right\} = A_1\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{2m\omega}{\sqrt{2m\hbar\omega}}\, x\, e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\psi_1(x) = A_1\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}\; x\, e^{-\frac{m\omega}{2\hbar}x^2}$$

$$\int|\psi_1|^2 dx = |A_1|^2\sqrt{\frac{m\omega}{\pi\hbar}}\left(\frac{2m\omega}{\hbar}\right)\int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega}{\hbar}x^2}dx =$$

$$= |A_1|^2\sqrt{\frac{m\omega}{\cancel{\pi}\hbar}}\left(\frac{\cancel{2}m\omega}{\hbar}\right)\cancel{2}\cancel{\sqrt{\pi}}\cdot 2\left(\frac{1}{\cancel{2}}\sqrt{\frac{\hbar}{m\omega}}\right)^3 = |A_1|^2$$

We used:

$$\boxed{\int_0^\infty x^{2n} e^{-x^2/a^2}dx = \sqrt{\pi}\,\frac{(2n)!}{n!}\left(\frac{a}{2}\right)^{2n+1}}\qquad n=1,\quad a=\sqrt{\frac{\hbar}{m\omega}}\qquad \boxed{A_1 = 1}$$

$$\boxed{\psi_1(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}\; x\, e^{-\frac{m\omega}{2\hbar}x^2}}$$

Your can also get normalization algebraically using

$$\boxed{\begin{aligned} a_+ \psi_n &= \sqrt{n+1}\ \psi_{n+1} \\ a_- \psi_n &= \sqrt{n}\ \psi_{n-1} \end{aligned}}$$

← see pages 47-48 of the textbook for proof

Then, $a_+ \psi_0 = \psi_1 \Rightarrow \psi_1 = a_+ \psi_0$

$$a_+ \psi_1 = \sqrt{2}\, \psi_2 \Rightarrow \psi_2 = \frac{1}{\sqrt{2}} a_+ \psi_1 = \frac{1}{\sqrt{2}} (a_+)^2 \psi_0$$

$$a_+ \psi_2 = \sqrt{3}\, \psi_3 \Rightarrow \psi_3 = \frac{1}{\sqrt{3}} a_+ \psi_2 = \frac{1}{\sqrt{3 \cdot 2}} (a_+)^3 \psi_0$$

$$\vdots$$

$$\boxed{\psi_n = \frac{1}{\sqrt{n!}} (a_+)^n \psi_0}$$

Therefore, the normalization constant A_n is

$$A_n = \frac{1}{\sqrt{n!}} \quad (\text{Remember, } A_1 = 1).$$

Other useful formulas:

Since $$a_\pm = \frac{1}{\sqrt{2\hbar m\omega}} (\mp ip + m\omega x) \Rightarrow$$

$$\boxed{\begin{aligned} x &= \sqrt{\frac{\hbar}{2m\omega}} (a_+ + a_-) \\ p &= i\sqrt{\frac{\hbar m\omega}{2}} (a_+ - a_-) \end{aligned}}$$

← Very useful in calculating averages

Analytic method

We now solve the Schrödinger equation for the harmonic oscillator directly

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi$$

Change variables for convenience $\quad \xi \equiv \sqrt{\frac{m\omega}{\hbar}}\, x$

$$K \equiv \frac{2E}{\hbar\omega}$$

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

For very large ξ : $\quad \frac{d^2\psi}{d\xi^2} \approx \xi^2\psi$

Approximate solution:

$$\psi(\xi) \approx A e^{-\xi^2/2} + \boxed{B e^{+\xi^2/2}}$$

Not normalizable since $\psi \to \infty$ at $\xi \to \infty$

Discard

Therefore, we look for solutions in the form $\psi(\xi) = h(\xi)\, e^{-\xi^2/2}$

$$\frac{d\psi}{d\xi} = \frac{dh}{d\xi} e^{-\xi^2/2} - \xi h(\xi) e^{-\xi^2/2}$$

$$\frac{d^2\psi}{d\xi^2} = \frac{d^2h}{d\xi^2} e^{-\xi^2/2} \underbrace{- \xi \frac{dh}{d\xi} e^{-\xi^2/2} - h e^{-\xi^2/2} - \xi \frac{dh}{d\xi} e^{-\xi^2/2}}$$

$$+ \xi^2 h e^{-\xi^2/2}$$

$$\frac{d^2\psi}{d\xi^2} = \left(\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\xi^2-1)h\right)e^{-\xi^2/2}$$

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

$$\Downarrow$$

$$\boxed{\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (K-1)h = 0}$$

Hermit's differential equation

We look for solution in the form of power series

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \dots = \sum_{j=0}^{\infty} a_j \xi^j$$

plug in

$$h'(\xi) = a_1 + 2a_2\xi + 3a_3\xi^2 + \dots = \sum_{j=0}^{\infty} j a_j \xi^{j-1}$$

$$h''(\xi) = 2a_2 + 2\cdot 3 a_3 \xi + \dots = \sum_{j=0}^{\infty} (j+1)(j+2)a_{j+2}\xi^j$$

$$\Downarrow$$

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

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

The coefficient of each power of ξ must vanish

$$(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j = 0$$

Recursion formula: $$\boxed{a_{j+2} = \frac{2j+1-K}{(j+1)(j+2)} a_j}$$

a_0: $a_2 = \frac{1-K}{2} a_0$, $a_4 = \frac{5-K}{12} a_2 \dots$ (EVEN)

a_1: $a_3 = \frac{3-K}{6} a_1$, $a_5 = \frac{7-K}{20} a_3, \dots$ (ODD)

$$h(\xi) = h_{even}(\xi) + h_{odd}(\xi)$$

$h_{even} = a_0 + a_2 \xi^2 + \dots$ $h_{odd} = a_1 + a_3 \xi^3 + \dots$

Problem: not all solutions are normalizable

If j is very large $\Rightarrow$ $a_{j+2} \approx \frac{2j}{j^2} a_j = \frac{2}{j} a_j$

and $a_j \approx \frac{c}{(j/2)!}$ $h(\xi) \approx c \sum \frac{1}{(j/2)!} \xi^j \approx c \sum \frac{1}{j!} \xi^{2j}$

$\approx c e^{\xi^2}$

Again $\psi \to \infty$ at $\xi \to \infty$ $\Rightarrow$ we must terminate the power series at some point $\Rightarrow$

for some j_{max} we have to get

$$a_{j_{max}+2} = 0$$

(we call this $j_{max} \equiv n$)

$j_{max} = n$

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

$$a_{n+2} = \frac{\overbrace{2n+1-K}^{=0}}{(n+1)(n+2)} a_n = 0$$

$$\boxed{K = 2n+1} \qquad K \equiv \frac{2E}{\hbar\omega} \; ; \; E = \frac{1}{2}\hbar\omega K$$

$$\Downarrow$$

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

for $n = 0, 1, 2, \ldots$

We recovered our previous result!

Note: the condition above will terminate either odd or even power series, the other must be zero from the start.

How to generate the wave functions?

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)} a_j$$

If $n=0 \Rightarrow$ odd series is zero $a_1 = 0$, $a_3 = 0, \ldots$

start with $j=0$ for even series

$a_2 = 0 \Rightarrow$ there is only one term $a_0 = 0$

$h_0(\xi) = a_0 \Rightarrow \psi_0(\xi) = a_0 e^{-\xi^2/2}$

as we obtained before.

If $n = 1 \Rightarrow a_0 = 0$ and even series is zero

The recursion formula gives $a_3 = 0 \Rightarrow$

$h_1(\xi) = a_1 \Rightarrow \psi_0(\xi) = a_1 \xi e^{-\xi^2/2}$

as we proved earlier by another method.

For $n=2$, $j=0$ gives $a_2 = -2a_0$
$j=2$ gives $a_4 = 0$ $\Rightarrow$
(odd series is zero)

$$h_2(\xi) = a_0(1 - 2\xi^2)\, e^{-\xi^2/2}$$

Apart from overall factor (a_0 or a_1) these polynomials are called Hermite polynomials.

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