FAQs & their solutions for Module 3:
Linear Harmonic Oscillator

Question1: At $t=0$, a linear harmonic oscillator is described by the wave function

$$\Psi(x,0)=\frac{1}{\sqrt{3}}\,\psi_0(x)+i\sqrt{\frac{2}{3}}\,\psi_2(x) \qquad (1)$$

where $\psi_n(x)$ are the normalized eigenfunctions of the Schrodinger equation for the linear harmonic oscillator problem.

(a) Is the wave function normalized???
(b) Write the wave function describing the time evolution of $\Psi\ x,0$.
(c) If we make a measurement of energy, what will be the probabilities of finding it in the ground state (with $E=\frac{1}{2}\hbar\omega$), first excited state (with $E=\frac{3}{2}\hbar\omega$) and the second excited state (with $E=\frac{5}{2}\hbar\omega$),?
(d) Calculate the average energy value.

Solution1:

(a) The eigen functions satisfy the following orthonormality condition

$$\int_{-\infty}^{+\infty}\psi_m^*(x)\,\psi_n(x)\,dx=\delta_{mn} \quad ;\ m,n=0,1,2,\ldots$$

Using the above orthonormality condition, one can easily show that

$$\int_{-\infty}^{+\infty}\left|\Psi(x,0)\right|^2\,dx=1$$

Thus the wavefunction is normalized.

(b) Since $E_n=\left(n+\frac{1}{2}\right)\hbar\omega$, we will have $\exp\left[-\frac{iE_n t}{\hbar}\right]=\exp\left[-i\left(n+\frac{1}{2}\right)\omega t\right]$. Thus the time evolution of the wave function would be given by

$$\Psi(x,t)=\frac{1}{\sqrt{3}}\,\psi_0(x)e^{-i\omega t/2}+i\sqrt{\frac{2}{3}}\,\psi_2(x)e^{-5i\omega t/2}$$

(c) If we make a measurement of energy, there will be $\left(\frac{1}{3}\right)^{\text{rd}}$ probability of finding it in the ground state (with $E = \frac{1}{2}\hbar\omega$), zero probability of finding it in the second excited state (with $E = \frac{3}{2}\hbar\omega$) and $\left(\frac{2}{3}\right)^{\text{rd}}$ probability of finding it in the second excited state (with $E = \frac{5}{2}\hbar\omega$).

(d) The average energy will be given by

$$\begin{aligned}\langle E\rangle &= \frac{1}{3}\left(\frac{1}{2}\hbar\omega\right)+\frac{2}{3}\left(\frac{5}{2}\hbar\omega\right)\\ &= \frac{11}{6}\hbar\omega\end{aligned}$$

Question2: For the linear harmonic oscillator problem, write $\Psi(x,t)$ in the following form

$$\Psi(x,t) = \int_{-\infty}^{+\infty} K(x,\, x',t)\ \Psi(x',0)\ dx' \tag{2}$$

where $K(x,x',t)$ is known as the propagator. Derive an expression for $K(x,\, x',t)$.

Solution 2: The most general solution of the Schrodinger equation for the linear harmonic oscillator problem is given by

$$\psi(x,t) = \sum_{n=0,1,.....}^{\infty} c_n \psi_n\ x\ \exp\left[-\frac{iE_n t}{h}\right] \tag{3}$$

or

$$\Psi\ \ x,t\ \ = \sum_{n=0,1,...}^{\infty}\ c_n\ \psi_n(x)\ e^{-i\left(n+\frac{1}{2}\right)\omega t} \tag{4}$$

If we know $\Psi\ \ x,0$, we can determine $\Psi(x,t)$ as follows:

$$\Psi\ \ x,0\ \ = \sum_{n=0,1,...}^{\infty}\ c_n\ \ \psi_n\ \ x$$

we multiply the above equation by $\psi_m^*(x)$ and integrate to obtain

$$c_n = \int_{-\infty}^{+\infty} \psi_n^*\ \ x'\ \ \Psi\ \ x',0\ \ dx'$$

where we have used the orthonormality condition. If we substitute the above expression for c_n in

$$\Psi(x,t) = \sum_{n=0,1,\ldots}^{\infty} c_n\, \psi_n(x)\, e^{-i\left(n+\frac{1}{2}\right)\omega t}$$

we may write it in the form:

$$\Psi(x,t) = \int_{-\infty}^{+\infty} K(x, x', t)\, \Psi(x',0)\, dx'$$

where

$$K(x,x',t) = \sum_{n=0,1,\ldots}^{\infty} \psi_n^*(x')\, \psi_n(x) \exp\left[-i\left(n+\frac{1}{2}\right)\omega t\right]$$

$$= \sum_{n=0,1,\ldots}^{\infty} |N_n|^2 H_n(\xi')\, H_n(\xi) \exp\left[-\frac{1}{2}(\xi^2+\xi'^2) - i\left(n+\frac{1}{2}\right)\omega t\right]$$

The above summation can be carried out and the final result is

$$K(x,x',t) = \frac{\gamma}{(2\pi i \sin \omega t)^{1/2}} \exp\left[-\frac{\gamma^2}{2i \sin \omega t}\left\{(x^2 + x'^2)\cos \omega t - 2xx'\right\}\right]$$

<u>Question3:</u> Show that the function

$$\psi(x) = A\, e^{-bx^2}$$

satisfies the Schrodinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2\mu}{\hbar^2}\left[E - \frac{1}{2}\mu\omega^2 x^2\right]\psi(x) = 0$$

for a particular value of *b*; determine the value of *b* and the corresponding value of the energy eigenvalue.

<u>Solution 3:</u>

$$\frac{d^2}{dx^2}\left(e^{-bx^2}\right) = \frac{d}{dx}\left(-2bx\, e^{-bx^2}\right) = \left(4b^2x^2 - 2b\right) e^{-bx^2}$$

Substituting in the Schrodinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2\mu}{\hbar^2}\left[E - \frac{1}{2}\mu\omega^2 x^2\right]\psi(x) = 0$$

we get

$$4b^2x^2 - 2b \ + \frac{2\mu}{\hbar^2}\left[E - \frac{1}{2}\mu\omega^2 x^2\right] = 0$$

For the above equation to be valid for all values of *x*, we must have

$b = \frac{1}{2}\frac{\mu\omega}{\hbar}$ and $E = \frac{b\hbar^2}{\mu} = \frac{1}{2}\hbar\omega$.

Question4: Show that the function e^{-cx^4} can never be an eigenfunction of the Schrodinger equation.

Solution4:

$$\frac{d^2}{dx^2}\ e^{-cx^4} \ = \frac{d}{dx}\ -4cx^3 e^{-cx^4} \ = \ 16c^2x^6 - 12cx^2 \ \ e^{-cx^4}$$

Substituting in the Schrodinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2\mu}{\hbar^2}\left[E - \frac{1}{2}\mu\omega^2 x^2\right]\psi(x) = 0$$

we get

$$16c^2x^6 - 12cx^2 \ + \frac{2\mu}{\hbar^2}\left[E - \frac{1}{2}\mu\omega^2 x^2\right] = 0$$

which can never be satisfied. Thus e^{-cx^4} can never be an eigenfunction of the Schrodinger equation.

Question5: The probability distribution for a coherent state is given by

$$|\Psi(x,t)|^2 = \frac{\gamma}{\sqrt{\pi}} \ \exp\left[- \ \xi \ - \ \xi_0 \ \cos \ \omega \ t \ ^2\right]$$

Calculate $\langle x \rangle$, $\langle x^2 \rangle$ and $\Delta x = \sqrt{< x^2 > - < x >^2}$.

Solution5: The probability distribution is given by

$$|\Psi(x,t)|^2 = \frac{\gamma}{\sqrt{\pi}} \ \exp\left[- \ \xi \ - \ \xi_0 \ \cos \ \omega \ t \ ^2\right] \qquad (5)$$

Notice that

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 \ dx \ = \ 1 \qquad (6)$$

for all values of *t*, as it indeed should be. Now

$$\langle x \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t)\, x\, \Psi(x,t)\; dx = \int_{-\infty}^{+\infty} x\, |\Psi(x,t)|^2\; dx$$

Simple integrations will give us

$$\langle x \rangle = x_0 \cos \omega t \qquad (7)$$

where

$$x_0 = \frac{1}{\gamma_0} \xi$$

Further

$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2\, |\Psi(x,t)|^2\; dx = x_0^2 \cos^2 \omega t + \frac{1}{2\gamma^2} \qquad (8)$$

$$\Delta x = \sqrt{< x^2 > - < x >^2} = \sqrt{\frac{\hbar}{2\mu\omega}} \qquad (9)$$

Question6: The Schrodinger equation for the linear harmonic oscillator can be written as

$$\frac{d^2\psi}{d\xi^2} + \left[\Lambda - \xi^2 \right] \psi\;\; \xi\;\; = 0$$

where $\xi = \gamma x$ and $\gamma = \sqrt{\frac{\mu\omega}{\hbar}}$. Make the transformation $\eta = \xi^2$ and look for the solution as $\eta \to \infty$ and obtain solutions in terms of confluent hypergeometric functions.

Solution6: We will obtain the solution of the following equation

$$\frac{d^2\psi}{d\xi^2} + \left[\Lambda - \xi^2 \right] \psi\;\; \xi\;\; = 0 \qquad (10)$$

We introduce the variable

$$\eta = \xi^2 \qquad (11)$$

Thus

$$\frac{d\psi}{d\xi} = \frac{d\psi}{d\eta}\frac{d\eta}{d\xi} = \frac{d\psi}{d\eta} 2\xi \qquad (12)$$

and

$$\frac{d^2\psi}{d\xi^2} = 4\eta \frac{d^2\psi}{d\eta^2} + 2\frac{d\psi}{d\eta} \tag{13}$$

Substituting in Eq. (8), we obtain

$$\frac{d^2\psi}{d\eta^2} + \frac{1}{2\eta}\frac{d\psi}{d\eta} + \left[\frac{\Lambda}{4\eta} - \frac{1}{4}\right]\psi(\eta) = 0 \tag{14}$$

In order to determine the asymptotic form, we let $\eta \to \infty$ so that the above equation takes the form

$$\frac{d^2\psi}{d\eta^2} - \frac{1}{4}\psi(\eta) = 0$$

the solution of which would be $e^{\pm\frac{1}{2}\eta}$. This suggests that we try out the following solution

$$\psi \;\; \eta \;\; = y \;\; \eta \;\; e^{-\frac{1}{2}\eta} \tag{15}$$

Thus

$$\frac{d\psi}{d\eta} = \left[\frac{dy}{d\eta} - \frac{1}{2}y\right]e^{-\frac{1}{2}\eta} \tag{16}$$

and

$$\frac{d^2\psi}{d\eta^2} = \left[\frac{d^2y}{d\eta^2} - \frac{dy}{d\eta} + \frac{1}{4}y(\eta)\right]e^{-\frac{1}{2}\eta} \tag{17}$$

Substituting the above equations in Eq. (12) we get

$$\eta\frac{d^2y}{d\eta^2} + \left(\frac{1}{2} - \eta\right)\frac{dy}{d\eta} + \frac{\Lambda - 1}{4}y(\eta) = 0 \tag{18}$$

Now the confluent hypergeometric equation is given by

$$x\frac{d^2y}{dx^2} + \;\; c - x \;\; \frac{dy}{dx} - a\,y(x) = 0 \tag{19}$$

where a and c are constants. For $c \neq 0, \pm 1, \pm 2, \pm 3, \pm 4, ...$ the two independent solutions of the above equation are

$$y_1(x) = {}_1F_1 \;\; a, c, x \tag{20}$$

and

$$y_2(x) = x^{1-c}\ {}_1F_1\ a-c+1, 2-c, x \qquad (21)$$

where ${}_1F_1\ a,c,x$ is known as the confluent hypergeometric function and is defined by the following equation

$$ {}_1F_1\ a,c,x\ = 1 + \frac{a}{c}\frac{x}{1!} + \frac{a(a+1)}{c(c+1)}\frac{x^2}{2!} + \frac{a(a+1)(a+2)}{c(c+1)(c+2)}\frac{x^3}{3!} + ... \qquad (22)$$

Obviously, for $a = c$ we will have

$$ {}_1F_1\ a,a,x\ = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + ... = e^x \qquad (23)$$

Thus although the infinite series in Eq. (20) is convergent for all values of *x*, it would blow up at infinity. Indeed the asymptotic form of ${}_1F_1\ a,c,x$ is given by

$$ {}_1F_1\ a,c,x\ \underset{x\to\infty}{\to} \frac{\Gamma(c)}{\Gamma(a)}\, x^{a-c}\, e^x \qquad (24)$$

The confluent hypergeometric series ${}_1F_1\ a,c,x$ is very easy to remember and its asymptotic form is easy to understand. Returning to Eq. (16), we find that $y(\eta)$ satisfies the confluent hypergeometric equation with

$$a = \frac{1-\Lambda}{4} \text{ and } c = \frac{1}{2} \qquad (25)$$

Thus the two independent solutions of Eq.(8) are

$$\psi_1(\eta) = {}_1F_1\left(\frac{1-\Lambda}{4}, \frac{1}{2}, \eta\right) e^{-\frac{1}{2}\eta} \qquad (26)$$

and

$$\psi_2(\eta) = \sqrt{\eta}\ {}_1F_1\left(\frac{3-\Lambda}{4}, \frac{3}{2}, \eta\right) e^{-\frac{1}{2}\eta} \qquad (27)$$

We must remember that $\eta = \xi^2$. Using the asymptotic form of the confluent hypergeometric function, one can readily see that if the series does not become a polynomial then, as $\eta \to \infty$, $\psi(\eta)$ will blow up as $e^{\frac{1}{2}\eta}$. In order to avoid this, the series must become a polynomial. Now $\psi_1(\eta)$ becomes a polynomial for Λ= 1,5, 9, 13,… and $\psi_2(\eta)$ becomes a polynomial for Λ= 3, 7, 11, 15. Thus only when

$$\Lambda = 1, 3, 5, 7, 9, \ldots \qquad (28)$$

we will have a well behaved solution of Eq. (8) – these are the eigenvalues of the Schrodinger equation. The corresponding wavefunctions are the Hermite Gauss functions:

$$\psi(\xi) = N\, H_m(\xi)\, \exp\left(-\frac{1}{2}\,\xi^2\right) \;\; ; \quad m = 0, 1, 2, 3, \ldots \qquad (29)$$

Indeed

$$H_n(\xi) = (-1)^{n/2} \frac{n!}{\left(\frac{n}{2}\right)!}\, {}_1F_1\left(-\frac{n}{2}\,,\, \frac{1}{2}\,, \xi^2\right) \text{ for } n = 0,\, 2, 4, \ldots \qquad (30)$$

and

$$H_n(\xi) = (-1)^{(n-1)/2} \frac{n!}{\left(\frac{n-1}{2}\right)!}\, 2\xi\, {}_1F_1\left(-\frac{n-1}{2}\,,\, \frac{3}{2}\,, \xi^2\right) \text{ for } n = 1,\, 3, 5, \ldots \qquad (31)$$