College of Science
Department of Physics
Fourth Class
Lecture 18

Quantum Mechanics

2023-2024

Lecture 18: Harmonic oscillator

Preparation

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To solve eq.36 let us make first an attempt to obtain an solution for the case when

$q^2 > \lambda \ \rightarrow \quad \lambda = 0$

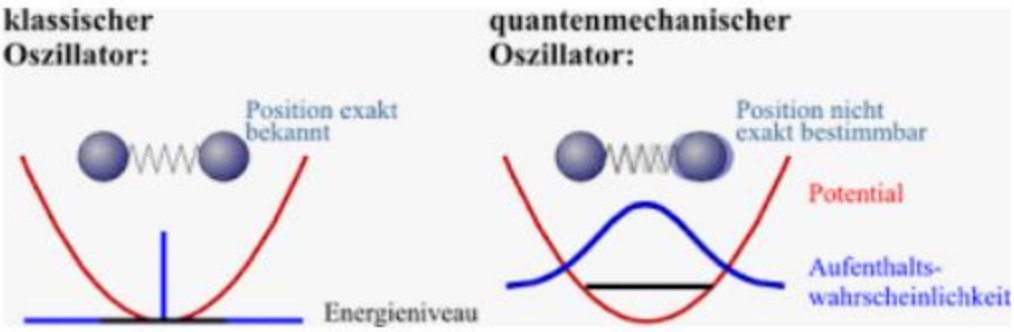
In this case eq.36 becomes

$$\frac{\partial^2 \Psi}{\partial q^2} - q^2 \Psi = 0 \ ----37$$

The solution of this eq. is

$$\Psi = e^{\pm\frac{q^2}{2}} \quad ------38$$

The quantity $|\Psi|^2$ represents the probability of finding the particle along x-axis, therefore it must decrease continuously to zero as x i.e. q approaches $\pm\infty$.



Clearly out of the two possible solutions represented by eq.38

$$\Psi = e^{+\frac{q^2}{2}} \quad and \quad \Psi = e^{-\frac{q^2}{2}} \ ----40$$

The solution $\Psi = e^{+\frac{q^2}{2}}$ is not acceptable (because $e^{+\frac{\infty^2}{2}} = \infty$) since it increases with increasing x, i.e. q , while the solution $\Psi = e^{-\frac{q^2}{2}}$ satisfies the conditions (because $e^{-\frac{\infty^2}{2}} = 0$), and therefore is an asymptotic solution of the waves equation.

From the above consideration it is clear that the solution of eq.36 will contain the term $e^{-\frac{q^2}{2}}$ as a factor, the possible solution may be written as

$$\Psi = e^{-\frac{q^2}{2}} \Phi(q) \ ----41$$

Where $\Phi(q)$ is the function of q , and hence of x. So $\boxed{\frac{\partial^2\Phi}{\partial q^2} - 2q\frac{\partial \Phi}{\partial q} + (\lambda\ - 1)\Phi = 0}$ $----42$

let us assume that the function Φ(q) may be expressed in the form of a power series in q, i.e.

$$\Phi(q) = a_o + a_1 q + a_2 q^2 + a_3 q^3 +\ ---+ a_n q^n$$

$$= \sum_{n=0}^{\infty} a_n q^n ----43$$

$$\therefore \sum_{n=0}^{\infty} q^n[(n+1)(n+2)a_{n+2} - 2na_n + (\lambda\ - 1)a_n] = 0 - 44$$

A power series will be equal to zero if all its coefficients are equal to zero, i.e. eq.44 is only satisfied if the coefficients of various power of q are separately equal zero. Thus, we have

$$(n+1)(n+2)a_{n+2} - (2n + 1 -\ \lambda)a_n = 0$$

Or $\boxed{a_{n+2} = \frac{2n+1-\lambda}{(n+1)(n+2)}a_n}$ $----45$

Where n is an integer or zero. This expression is called recursion formula. From this we calculate the coefficient of q^2, q^4, q^6etc., if that of q^0 is known, similarly we calculate the coefficient of q^3, q^5, q^7 etc, if the coefficient of q^1 is known.

From above discussion we have seen that in order to obtain a satisfactory wave – function, the series (eq.43) must break off after a finite number of terms. The series will break off after n^{th} term. If we set the numerator in the recursion formula eq.45 equal to zero, i.e

2n + 1 – λ = 0 i.e. λ = 2n + 1

Substituting this value of λ in eq.33

$$2E\sqrt{\frac{m}{\hbar^2 k}} = 2n + 1$$

Or $2E\sqrt{\frac{m}{\hbar^2 4\pi^2\vartheta^2 m}} = 2n + 1$ $\quad or \quad$ $\frac{2E}{2\pi\vartheta\hbar} = 2n + 1$

$$\boxed{E = E_n = (2n+1)\frac{2\pi\vartheta\hbar}{2} = (n + \frac{1}{2})\hbar\omega_o} ----46$$

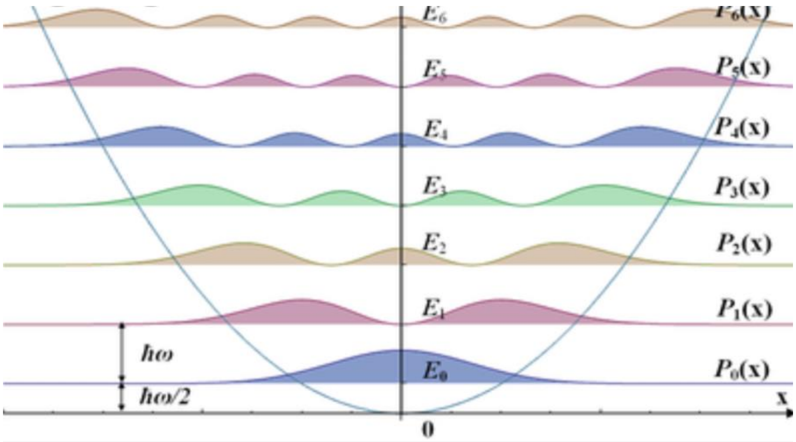
Where $\omega_o = 2\pi\vartheta \rightarrow angular\ frequency,\ n = 0,1,2,3, - - -$

The allowed integer values of n lead to certain discrete values of energy represented by eq.46, known as eigen value of harmonic oscillator. Moreover eq.46 indicates that the energy levels of harmonic oscillator are equally spaced.

Significance of zero-point energy

A comparison with the result $E = n\hbar\omega_o$,obtained by old quantum theory shows that the only difference is that all the equally spaced energy levels are shifted upward by an amount equal to half the separation of energy levels, i.e. $E = \frac{1}{2}\hbar\omega_o$ called the zero-point energy. Thus, even in the lowest state, the H.O. has greater energy than it would have if it were at reset in its equilibrium position. The existence of zero points agrees with experiments and is an important feature of quantum mechanics.

The energy levels of the H.O. according to wave mechanics are represented in Fig.



Eigen function of harmonic oscillator :

We have seen that in order to have a satisfactory solution of wave eq.33 Φ should be restricted in such a manner so as to make it polynomial rather than a power series. Then the eigen function Ψ can be set equal to the product of this polynomial and the factor $e^{-\frac{q^2}{2}}$, i.e.

$$\boxed{\Psi_n(x) = N_n e^{-\frac{q^2}{2}} H_n(q)} - - - -47$$

Where N_n is a normalizing factor. $H_n(q)$ the Hermit polynomial of degree n defined by

$$\boxed{H_n(q) = (-1)^n e^{q^2} \frac{d^n e^{-q^2}}{dq^n}} ----48$$

Values of Hermit polynomial of different orders may be obtained by using above eq.

$$n = 0 \;, \qquad H_o(q) = 1 \;\; Hermit\,polynomial\,of\,order\,zero$$

$$n = 1 \;,\; H_1(q) = 2q \; Hermit\,polynomial\,of\,order\; 1$$

$$n = 2 \;, H_2(q) = 4q^2 - 2 \; Hermit\,polynomial\,of\,order\; 2$$

$$n = 3 \;, H_3(q) = 8q^3 - 12q \;\; Hermit\,polynomial\,of\,order\; 3$$

And so on

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

$$H_0(q) = (-1)^0 e^{q^2} \frac{d^0 e^{-q^2}}{dq^0} = (-1)^0 e^{q^2} e^{-q^2} = 1$$

$$H_1(q) = (-1)^1 e^{q^2} \frac{d^1 e^{-q^2}}{dq^1} = (-1) e^{q^2} \left(-2q e^{-q^2}\right) = (-1)(-2q) = 2q$$

<u>The normalizing condition</u> is

$$\int_{-\infty}^{\infty} |\Psi_n(x)|^2 \, dx = 1 \qquad , \qquad \frac{|N_n|^2}{\alpha} \int_{-\infty}^{\infty} H_n^2(q) e^{-q^2} dq = 1$$

but $\int_{-\infty}^{\infty} H_n^2(q) e^{-q^2} dq = 2^n (n!) \sqrt{\pi}$

$$\therefore \; \frac{|N_n|^2}{\alpha} 2^n (n!) \sqrt{\pi} = 1 \quad , \qquad \boxed{N_n = \left[\frac{\alpha}{2^n (n!) \sqrt{\pi}}\right]^{\frac{1}{2}}}$$

Thus, the normalized wave functions of harmonic oscillator are

$$\boxed{\Psi_n(x) = \left[\frac{\alpha}{2^n (n!) \sqrt{\pi}}\right]^{\frac{1}{2}} e^{-\frac{q^2}{2}} H_n(q) = \left[\frac{\alpha}{2^n (n!) \sqrt{\pi}}\right]^{\frac{1}{2}} e^{-\frac{\alpha^2 x^2}{2}} H_n(\alpha x)}$$

Where α is given by equation 33 is $\alpha^2 = \sqrt{\frac{mk}{\hbar^2}}$

The wave function corresponding to the lowest state of energy is

$$\boxed{\Psi_o(x) = [\frac{\alpha}{\sqrt{\pi}}]^{\frac{1}{2}} e^{-\frac{\alpha^2 x^2}{2}}}$$

As $H_o(q) = H_o(\alpha x) = 1$

Problem 8.1:

Find the expectation value of the energy when the state of the harmonic oscillator is described by the following wave function

$$\Psi(x,t) = \frac{1}{\sqrt{2}}[\Psi_o(x,t) + \Psi_1(x,t)]$$

Where $\Psi_o(x,t) \& \Psi_1(x,t)$ are the waves for the ground state and the first excited state respectively.

Solution:

the expectation value of energy is given by

$$\langle E \rangle = \int \Psi^*(x,t)\, \hat{\mathrm{H}}\, \Psi(x,t)\, dx$$

Here

$$\Psi(x,t) = \frac{1}{\sqrt{2}}[\Psi_o(x,t) + \Psi_1(x,t)]$$

$$\therefore \Psi^*(x,t) = \frac{1}{\sqrt{2}}[\Psi_o^*(x,t) + \Psi_1^*(x,t)]$$

But $\boxed{\Psi_o(x,t) = [\frac{\alpha}{\sqrt{\pi}}]^{\frac{1}{2}} e^{-\frac{\alpha^2 x^2}{2}}}$ and $\boxed{\Psi_1(x,t) = [\frac{\alpha}{2\sqrt{\pi}}]^{\frac{1}{2}} e^{-\frac{\alpha^2 x^2}{2}}.2\alpha x}$

So $\Psi_o^*(x,t) = [\frac{\alpha}{\sqrt{\pi}}]^{\frac{1}{2}} e^{-\frac{\alpha^2 x^2}{2}} = \Psi_o(x,t)$

And $\Psi_1^*(x,t) = [\frac{\alpha}{2\sqrt{\pi}}]^{\frac{1}{2}} e^{-\frac{\alpha^2 x^2}{2}}.2\alpha x = \Psi_1(x,t)$

$$\Psi^*(x,t)\, \Psi(x,t) = \frac{1}{\sqrt{2}}[\Psi_o^*(x,t) + \Psi_1^*(x,t)].\frac{1}{\sqrt{2}}[\Psi_o(x,t) + \Psi_1(x,t)]$$

$$= \frac{1}{2}[\Psi_o(x,t) + \Psi_1(x,t)]^2 = \frac{1}{2}[\Psi_o^2 + \Psi_1^2 + 2\Psi_o.\Psi_1]$$

The expectation value of energy is given by

$$\langle E\rangle = \frac{1}{2}\int_{-\infty}^{\infty} \Psi_o^2 E_o\, dx + \frac{1}{2}\int_{-\infty}^{\infty} \Psi_1^2 E_1\, dx + \frac{1}{2}.2\int_{-\infty}^{\infty} \Psi_o.\Psi_1 E\, dx$$

$$E_o = \frac{1}{2}\hbar\omega \rightarrow \left(n+\frac{1}{2}\right)\hbar\omega = \left(0+\frac{1}{2}\right)\hbar\omega = \frac{1}{2}\hbar\omega$$

$$E_1 = \frac{3}{2}\hbar\omega \rightarrow \left(n+\frac{1}{2}\right)\hbar\omega = \left(1+\frac{1}{2}\right)\hbar\omega = \frac{3}{2}\hbar\omega$$

$$\int_{-\infty}^{\infty} \Psi_o.\Psi_1 E\, dx = \int_{-\infty}^{\infty} [\frac{\alpha}{\sqrt{\pi}}]^{\frac{1}{2}} e^{-\frac{\alpha^2x^2}{2}}.[\frac{\alpha}{2\sqrt{\pi}}]^{\frac{1}{2}} e^{-\frac{\alpha^2x^2}{2}}.2\alpha x E\, dx$$

$$= \frac{2\alpha^2 E}{\sqrt{2}\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-\alpha^2x^2}\ x\, dx = zero$$

Product of two functions symmetric about origin, one is even and the other is odd integration $-\infty \rightarrow \infty is\ zero.$

$$\langle E\rangle = \frac{1}{2}\int_{-\infty}^{\infty}\frac{1}{2}\hbar\omega\Psi_o^2\, dx + \frac{1}{2}\int_{-\infty}^{\infty}\frac{3}{2}\hbar\omega\Psi_1^2\, dx + zero$$

$$\langle E\rangle = \frac{1}{4}\hbar\omega\int_{-\infty}^{\infty}\frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2x^2}\, dx + \frac{3}{4}\hbar\omega\int_{-\infty}^{\infty}\frac{\alpha}{2\sqrt{\pi}} e^{-\alpha^2x^2} 4\alpha^2x^2\, dx$$

$$\langle E\rangle = \frac{1}{4}\hbar\omega.\frac{\alpha}{\sqrt{\pi}}\frac{\sqrt{\pi}}{\alpha} + \frac{3}{4}\hbar\omega\frac{\alpha}{2\sqrt{\pi}}4\alpha^2\frac{1}{2}\frac{\sqrt{\pi}}{\alpha^3}$$

$$\langle E\rangle = \frac{1}{4}\hbar\omega + \frac{3}{4}\hbar\omega = \hbar\omega$$

Problem 8.2

Normalize the ground state wave function for the one-dimensional H.O. $\Psi_o = Aexp(-\frac{m\omega x^2}{2\hbar})$ .So that the total probability of finding the particle is unity. You may need the following integral $\int_0^{\infty} e^{-kx^2}dx = \frac{1}{2}\frac{\sqrt{\pi}}{\sqrt{k}}$

Solution:

$$1 = \int_{-\infty}^{\infty}|\Psi_o|^2\, dx = \int_{-\infty}^{\infty}|A|^2 exp(-\frac{m\omega x^2}{\hbar})\mathrm{dx}$$

$$1 = 2|A|^2 \int_0^{\infty} exp(-\frac{m\omega x^2}{\hbar})\mathrm{dx} \ = 2|A|^2 . \frac{1}{2} \frac{\sqrt{\pi}}{\sqrt{\frac{m\omega}{\hbar}}}$$

$$1 = |A|^2 \sqrt{\frac{\pi\hbar}{m\omega}} \quad \rightarrow \quad A = (\frac{m\omega}{\pi\hbar})^{\frac{1}{4}}$$

$$\Psi_o = (\frac{m\omega}{\pi\hbar})^{\frac{1}{4}} exp(-\frac{m\omega x^2}{2\hbar})$$

Problem 8.3

The wave function Ψ(x,t) for the lowest energy state of a S.H.O. consisting of mass m acted on by a restoring force of force constant C , can be expressed as

$$\Psi(x,t) = A\, e^{-\frac{\sqrt{Cm}}{2\hbar}x^2}\ e^{-\frac{i}{2}\sqrt{\frac{C}{m}}\,t}$$

Where the real constant A can have any value. Verify that this expression is a solution to the schrӧedinger eq. for the appropriate potential.

Solution:

The expression applies to the case in which the equilibrium point of the oscillator is at the origin of the x-axis (x=0).

In this case the time independent potential energy is

$V(x,t) = V(x) = \frac{1}{2}Cx^2$

As can be verified by noting that the corresponding force, $F = -\frac{d}{dx}V(x) = -Cx$, is a linear restoring force of force constant C. The sch. eq. for this pot. is

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + \frac{1}{2}Cx^2\Psi = i\hbar\frac{\partial \Psi}{\partial t}$$

To check the validity of the solution we evaluate its derivatives, we find

right side $\quad \frac{\partial \Psi}{\partial t} = -\frac{i}{2}\sqrt{\frac{C}{m}}\ \Psi$

$$\therefore\ i\hbar\frac{\partial \Psi}{\partial t} = i\hbar\left(-\frac{i}{2}\right)\sqrt{\frac{C}{m}}\ \Psi = \frac{\hbar}{2}\sqrt{\frac{C}{m}}\ \Psi$$

Left side $\frac{\partial\Psi}{\partial x} = -\frac{\sqrt{Cm}}{2\hbar}2x\Psi = -\frac{\sqrt{Cm}}{\hbar}x\Psi$

$$\frac{\partial^2\Psi}{\partial x^2} = -\frac{\sqrt{Cm}}{\hbar}\Psi - \frac{\sqrt{Cm}}{\hbar}x(-\frac{\sqrt{Cm}}{\hbar}x\Psi) = -\frac{\sqrt{Cm}}{\hbar}\Psi + \frac{Cm}{\hbar^2}x^2\Psi$$

$$\therefore\ -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{1}{2}Cx^2\Psi = \frac{\hbar^2}{2m}\frac{\sqrt{Cm}}{\hbar}\Psi - \frac{\hbar^2}{2m}\frac{Cm}{\hbar^2}x^2\Psi + \frac{1}{2}Cx^2\Psi$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{1}{2}Cx^2\Psi = \frac{\hbar}{2}\sqrt{\frac{C}{m}}\ \Psi$$

Left side = right side = $\frac{\hbar}{2}\sqrt{\frac{c}{m}}$. The solution must be valid.

Example 8.4

Show that the ground state wavefunction of the harmonic oscillator

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

is normalized. If a harmonic oscillator is in this state, find the probability that the particle can be found in the range $0 \le x \le 1$.

SOLUTION

To check normalization, we begin by squaring the wavefunction

$$\psi_0^2 = \sqrt{\frac{m\omega}{\pi\hbar}} \exp\left(-\frac{m\omega}{\hbar}x^2\right)$$

Recalling that

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

we now set $z^2 = \frac{m\omega}{\hbar}x^2$. Then we have

$$z = \sqrt{\frac{m\omega}{\hbar}}x, \quad \Rightarrow dz = \sqrt{\frac{m\omega}{\hbar}}\,dx$$

We invert this relation to give

$$dx = \sqrt{\frac{\hbar}{m\omega}}\,dz$$

Using these substitutions, the normalization integral becomes

$$\begin{aligned}
\int_{-\infty}^{\infty} \psi_0^2(x)\, dx &= \int_{-\infty}^{\infty} \sqrt{\frac{m\omega}{\pi\hbar}} \exp\left(-\frac{m\omega}{\hbar}x^2\right) dx \\
&= \sqrt{\frac{\hbar}{m\omega}} \int_{-\infty}^{\infty} \sqrt{\frac{m\omega}{\pi\hbar}} \exp\left(-z^2\right) dz \\
&= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-z^2}\, dz = \frac{\sqrt{\pi}}{\sqrt{\pi}} = 1
\end{aligned}$$

Therefore the state is normalized. The probability that the particle is found in the range $0 \le x \le 1$ is given by

$$\int_0^1 \psi_0^2(x)\, dx = \sqrt{\frac{m\omega}{\pi\hbar}} \int_0^1 \exp\left(-\frac{m\omega}{\hbar}x^2\right) dx$$

This integral is nearly in the form of the error function

$$erf(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-u^2}\, du$$

Following the procedure used in checking normalization, we set

$$u^2 = \frac{m\omega}{\hbar}x^2$$

and obtain

$$\sqrt{\frac{m\omega}{\pi\hbar}} \int_0^1 \exp\left(-\frac{m\omega}{\hbar}x^2\right) dx = \sqrt{\frac{m\omega}{\pi\hbar}}\sqrt{\frac{\hbar}{m\omega}} \int_0^1 \exp\left(-u^2\right) du$$

$$= \frac{1}{\sqrt{\pi}} \int_0^1 \exp\left(-u^2\right) du = \frac{1}{2}erf(1) \approx \frac{1}{2}(0.84) = 0.42$$