UNIT 16 HERMITE AND LAGUERRE POLYNOMIALS

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16.1 INTRODUCTION

You have studied the properties of the Legendre polynomials, and the Bessel functions in Units 14 and 15, respectively. In this unit, you will learn the properties of Hermite polynomials and Laguerre polynomials. These polynomials are useful in studying the behaviour of a harmonic oscillator and the hydrogen atom using quantum mechanics. In fact, these polynomials enable us to describe the microscopic world of molecules, atoms, and sub-atomic particles in a mathematical language. A study of the properties of these polynomials and a knowledge of their zeros is also helpful in developing numerical methods.

Like Legendre and Bessel polynomials, the Hermite and Laguerre polynomials are solutions of linear second order ordinary differential equations (ODE) known as the Hermite and the Laguerre differential equations. You will come across these ODEs and the two polynomials in Sec. 16.2 and 16.6, respectively. The generating function and the recurrence relations for Hermite polynomials are given in Sec. 16.3. You have already seen the importance of the generating functions for Legendre and Bessel polynomials in the last units. You will now learn how the generating function for Hermite polynomials is helpful in obtaining many of their properties. The recurrence relations connecting Hermite polynomials of different orders and their derivatives are derived from the generating function in the same section. In Sec. 16.7 we have introduced the generating function for Laguerre polynomials and discussed their recurrence relations. One very important property of the orthogonal polynomials of different orders is that their integrals with suitable weight polynomials over specified ranges of integrations are zero. We have derived these orthogonality properties of Hermite and Laguerre polynomials in Sec. 16.4 and 16.8, respectively.

Objectives

After studying this unit, you will be able to:

- identify Hermite's and Laguerre's differential equations;
- obtain expressions for Hermite and Laguerre polynomials;
- write generating functions of Hermite and Laguerre polynomials; and
- obtain recurrence relations as well as orthogonality properties of Hermite and Laguerre polynomials.

16.2 HERMITE'S DIFFERENTIAL EQUATION AND HERMITE POLYNOMIALS

You first came across **Hermite's differential equation** and its solutions while working out an SAQ in Unit 3 of the PHE-05 course. We rewrite this ODE as:

$$\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + 2vy(x) = 0 \tag{16.1}$$

The general solution of Hermite's differential equation is

$$y = a_0\left[1 + \frac{(-2)v}{2!}x^2 + \frac{(-2)^2 v(v-2)}{4!}x^4 + \frac{(-2)^3 v(v-2)(v-4)}{6!}x^6 + \ldots\right]$$

$$+ a_1\left[x + \frac{(-2)(v-1)}{3!}x^3 + \frac{(-2)^2(v-1)(v-3)}{5!}x^5 + \ldots\right] \tag{16.2}$$

The constants a_0 and a_1 may take arbitrary values.

Since $x = 0$ is an ordinary point of Hermite's differential equation, its solution in the form of a power series in x is given by

$$y = \sum_{j=0}^{\infty} a_j x^j \qquad \text{(i)}$$

with

$$a_{j+2} = -\frac{2(v-j)}{(j+1)(j+2)}a_j \qquad \text{(ii)}$$

This relation tells us that for even positive integral values of j, the coefficients a_j can be expressed in terms of a_0 and the coefficients for odd positive integral values of j ($j > 1$) can be expressed in terms of a_1:

$$a_2 = -\frac{2v}{1\times 2}a_0$$

$$a_4 = -\frac{2(v-2)}{3\times 4}\times a_2 = \frac{(-2)^2 v(v-2)}{1\times 2\times 3\times 4}a_0$$

and

$$a_3 = -\frac{2(v-1)}{2\times 3}a_1$$

$$a_5 = -\frac{2(v-3)}{4\times 5}a_3 = \frac{(-2)^2 v(v-1)(v-3)}{2\times 3\times 4\times 5}a_1$$

Substituting these results in Eq. (i) above, we obtain Eq. (16.2).

If v is a non-zero negative integer, the series given in Eq. (16.2) will be an infinite series. You may now like to know: What happens if v is zero or an even positive integer? To understand this, let us consider the case corresponding to $v = 6$. You will readily note that the fifth and all subsequent terms of the series (not explicitly shown) in the first square bracket in Eq. (16.2) will be zero as their numerator will have a factor $(v - 6)$. It means that for $v = 6$, the first series will terminate at $\frac{(-2)^3 6\times 4\times 2}{6!}x^6$.

To extend this discussion for the general case, let us write $v = 2\ell$; $\ell = 0,1,2,\ldots$ Then the series in the first square bracket of Eq. (16.2) will terminate at the term

$$\frac{(-2)^\ell (2\ell)(2\ell-2)..\times 2}{(2\ell)!}x^{2\ell} = \frac{(-1)^\ell \ell!}{(2\ell)!}(2x)^{2\ell}$$

and all subsequent terms will have their numerators equal to zero. The series in the second square bracket of Eq. (16.2) will however, remain an infinite series. But if we choose $a_1 = 0$, we will obtain a particular solution of Eq. (16.1) — a polynomial of degree 2ℓ in x. However, you should note that such a polynomial will contain only even powers of x and the coefficient a_0 is still arbitrary. For the series to appear more systematic, we choose the constant a_0 to be

$$a_0 = \frac{(-1)^\ell (2\ell)!}{\ell!}$$

The polynomial so obtained goes by the name of **Hermite polynomial of degree 2ℓ** and is denoted by the symbol $H_{2\ell}(x)$:

$$H_{2\ell}(x) = \frac{(-1)^\ell (2\ell)!}{\ell!} \frac{(-1)^{\ell-1}(2\ell)!}{2!(\ell-1)!} + \ldots + \frac{(-1)(2\ell)!}{(2\ell-2)!}(2x)^{2\ell-2} + (2x)^{2\ell} \tag{16.3}$$

Any solution of Eq. (16.1) can be multiplied by an arbitrary constant to obtain another solution. Then the question arises: Why are we taking the constants a_0 and a_1 in a particular manner? This is because Hermite polynomial of degree n is defined in such a way that the term containing the highest power of x is $(2x)^n$.

Note that the term containing the highest power of x is $(2x)^{2\ell}$.

Similarly when v is a positive odd integer, say $2\ell+1$; $\ell = 0,1,2,\ldots$, the second series in Eq. (16.2) will terminate at

$$\frac{(-1)^\ell \ell!}{(2\ell+1)!}\frac{(2x)^{2\ell+1}}{2}$$

and the first series remains an infinite series. As before, you will get a particular polynomial solution of Hermite's differential equation by putting $a_0 = 0$ and choosing a_1 as

$$a_1 = 2\frac{(-1)^\ell (2\ell+1)!}{\ell!}$$

This leads to **Hermite's polynomial of degree $2\ell+1$:**

$$H_{2\ell+1}(x) = \frac{(-1)^\ell (2\ell+1)!}{\ell!}2x + \frac{(-1)^{\ell-1}(2\ell+1)!}{3!(\ell-1)!}(2x)^3 + \frac{(-1)(2\ell+1)!}{(2\ell-1)!}(2x)^{2\ell-1}$$

$$+ (2x)^{2\ell+1} \qquad (16.4)$$

We would like to point out here that Eq. (16.4) contains only odd powers of x; the term containing the highest power of x is $(2x)^{2\ell+1}$.

We can now combine Eqs. (16.3) and (16.4) by taking $v = n$, where n is any positive integer including zero, and define the Hermite polynomial of degree n as

$$H_n(x) = (2x)^n - \frac{n(n-1)}{1!}(2x)^{n-2} + \frac{n(n-1)(n-2)(n-3)}{2!}(2x)^{n-4} + \ldots$$

$$+ \frac{(-1)^{n/2} n!}{(n/2)!} \quad \text{(if } n \text{ is even)} \qquad (16.5a)$$

$$H_n(x) = (2x)^n - \frac{n(n-1)}{1!}(2x)^{n-2} + \frac{n(n-1)(n-2)(n-3)}{2!}(2x)^{n-4} + \ldots$$

$$+ \frac{(-1)^{\frac{n-1}{2}} n!}{\left(\frac{n-1}{2}\right)!}2x \quad \text{(if } n \text{ is odd)} \qquad (16.5b)$$

where we have written the terms in decreasing powers of x.

From Eq. (16.5) we can write the first few Hermite polynomials:

$$\begin{aligned} H_0(x) &= 1 \\ H_1(x) &= 2x \\ H_2(x) &= 4x^2 - 2 \\ H_3(x) &= 8x^3 - 12x \\ H_4(x) &= 16x^4 - 48x^2 + 12 \end{aligned} \qquad (16.6)$$

A plot of some of these polynomials is shown in Fig. 16.1. For ease in scaling, $H_n(x)$ $(n \neq 0)$'s are divided by n^3.

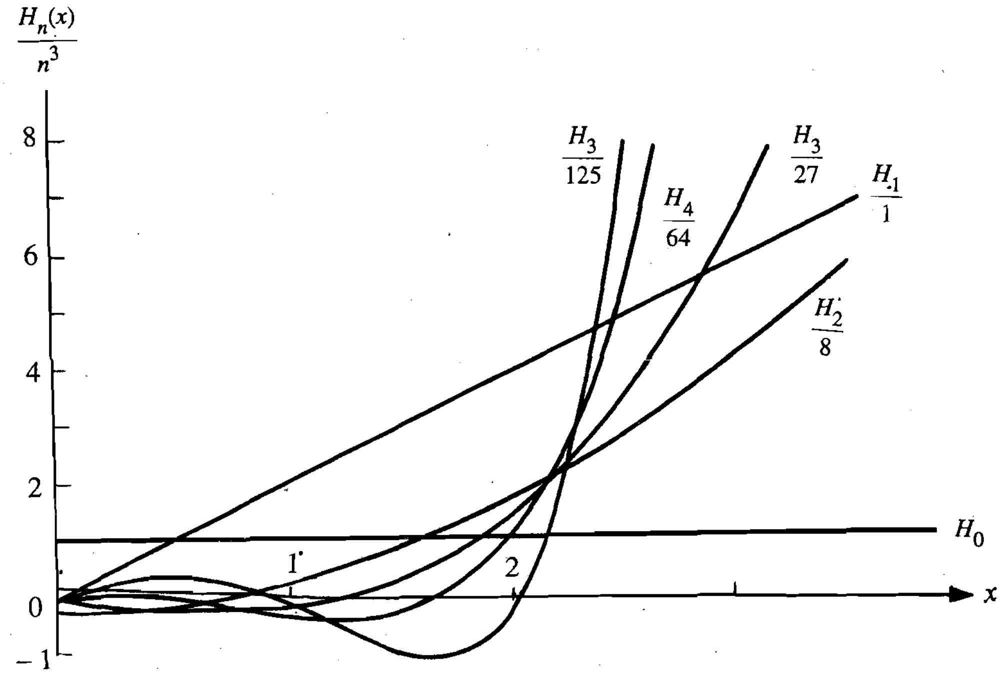

Fig.16.1: Plots of Hermite polynomials $H_0(x), \frac{H_n(x)}{n^3} (n = 1 \text{ to } 5)$

The series representation of Hermite polynomials becomes somewhat unwieldy, particularly when we have to evaluate integrals involving Hermite polynomials. In such situations and for the derivation of many other properties of Hermite polynomials, it is convenient to employ the generating function for Hermite polynomials. In the next section we introduce the generating function for the Hermite polynomials. We shall also use the generating function to derive the recurrence relations connecting Hermite polynomials of different orders and their derivatives.

16.3 GENERATING FUNCTION AND RECURRENCE RELATIONS FOR HERMITE POLYNOMIALS

The generating function for Hermite polynomials is

$$g(x,t) = e^{2xt-t^2} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} \tag{16.7}$$

As in the case of Legendre and Bessel polynomials, the generating function for Hermite polynomials is expanded in powers of t and the x-dependent coefficients are related to the special function. Therefore, we rewrite $g(x,t)$ as

$$g(x,t) = e^{2xt} \times e^{-t^2}$$

and express the exponential functions in their respective power series to get

$$g(x,t) = \sum_{j=0}^{\infty} \frac{(2xt)^j}{j!} \sum_{m=0}^{\infty} \frac{(-t^2)^m}{m!}$$

$$= \sum_{j=0}^{\infty} \sum_{m=0}^{\infty} (-1)^m \frac{(2x)^j}{j!\,m!} t^{2m+j}$$

To obtain the coefficient of t^n, we put $j + 2m = n$. You will agree that this equality can be satisfied for various combinations of the values of j and m, namely $j = n$, $m = 0$; $j = n - 2$,

$m = 1$; $j = n-4$, $m = 2$ and so on. If n is even we will have $j = 0$, $m = \frac{n}{2}$ and if n is odd, we will have $j = 1$, $m = \frac{n-1}{2}$. Thus the coefficient of t^n is

$$\frac{(2x)^n}{n!0!} - \frac{(2x)^{n-2}}{(n-2)!1!} + \frac{(2x)^{n-4}}{(n-4)!2!} - \ldots$$

The last term in this series is $\frac{(-1)^{\frac{n}{2}}}{0!\left(\frac{n}{2}\right)!}$ for even n and $\frac{(-1)^{\frac{n-1}{2}}}{1!\left(\frac{n-1}{2}\right)!}2x$ for odd n. Thus the coefficient of $\frac{t^n}{n!}$, i.e. $H_n(x)$ will be obtained by multiplying the above expression by $n!$ You will easily recognise that the resultant expression is identical to that given in Eq. (16.5).

Example 1: Relating Hermite polynomials

Establish the relation between $H_n(x)$ and $H_n(-x)$ using the generating function.

Solution

In Eq. (16.7) for the generating function, we change x to $-x$ and t to $-t$. This will leave the exponential function unchanged so that

$$e^{2xt-t^2} = \sum_n H_n(-x)\frac{(-t)^n}{n!} = \sum_n (-1)^n H_n(-x)\frac{t^n}{n!}$$

On comparing this expression with that given in Eq. (16.7), you will get

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

or

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

From this we note that if we change the sign of x, the Hermite polynomials for even positive integral values of n do not change whereas those with odd positive integral values of n just change sign. This result is, of course, obvious from the fact that Hermite polynomials contain only even (odd) powers of x when n is even (odd).

Now we will use the generating function to obtain the recurrence relations connecting the Hermite polynomials of different degrees and their differential coefficients with respect to the argument.

Recurrence Relations

If you differentiate both sides of Eq. (16.7) partially with respect to t, you will get

$$(2x-2t)e^{2xt-t^2} = \sum_{n=1}^{\infty} H_n(x)\frac{t^{n-1}}{(n-1)!}$$

Replacing e^{2xt-t^2} on the left hand side by the right hand side of Eq. (16.7), we obtain

$$(2x-2t)\sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!} = \sum_{n=1}^{\infty} H_n(x)\frac{t^{n-1}}{(n-1)!}$$

Equating coefficients of t^{n+1} from the two sides, you will obtain

$$2x\frac{H_{n+1}(x)}{(n+1)!} - 2\frac{H_n(x)}{n!} = \frac{H_{n+2}(x)}{(n+1)!}$$

On multiplying throughout by $(n+1)!$ we can write

$$H_{n+2}(x) = 2x\, H_{n+1}(x) - 2(n+1) H_n(x) \tag{16.8}$$

You should note that this recurrence relation connects Hermite polynomials of three successive orders.

We will now illustrate how the generating function and this recurrence relation can be used to obtain expressions of some lower order Hermite polynomials. You should go through the following example carefully.

Example 2: Expressions for Hermite polynomials

Starting from the generating function for the Hermite polynomials, obtain expressions for $H_0(x)$ and $H_1(x)$ and then use the recurrence relation given in Eq. (16.8) to obtain expressions for $H_2(x)$, $H_3(x)$ and $H_4(x)$.

Solution

We first write the exponential in the generating function given in Eq. (16.7) as a power series in $2xt - t^2$:

$$e^{2xt-t^2} = 1 + (2xt - t^2) + \frac{(2xt-t^2)^2}{2!} + \ldots = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}$$

You should note that $H_0(x)$ correspond to a term independent of t. On the left side, the term independent of t is 1. Hence we can write

$$H_0(x) = 1$$

Further, $H_1(x)$ occurs as coefficient of t. On the left hand side, the coefficient of t is $2x$. Therefore,

$$H_1(x) = 2x$$

From the recurrence relation in Eq. (16.8) with $n = 0$, we get

$$H_2(x) = 2xH_1(x) - 2H_0(x)$$

On substituting for $H_1(x)$ and $H_0(x)$, we obtain

$$H_2(x) = 4x^2 - 2$$

If you repeat this procedure for $n = 1$ and $n = 2$, you will get

$$H_3(x) = 2x\, H_2(x) - 4H_1(x) = 2x(4x^2 - 2) - 4(2x) = 8x^3 - 12x$$

and

$$H_4(x) = 2x\, H_3(x) - 6H_2(x) = 16x^4 - 48x^2 + 12$$

Note that these expressions for Hermite polynomials are the same as given in Eq. (16.6) and obtained from the series given by Eq. (16.5). Proceeding in this way, you can calculate higher order Hermite polynomials. You are advised to obtain expressions for a couple of these.

You can obtain another recurrence relation by partially differentiating both sides of Eq. (16.7) with respect to x:

$$H'_{n+1}(x) = 2(n+1)H_n(x) \tag{16.9}$$

where the prime denotes differentiation with respect to the argument x. The derivation of this result is left as an SAQ.

SAQ 1

Spend 3 min

Differentiate the generating function for Hermite polynomials partially with respect to x and obtain the recurrence relation given in Eq. (16.9).

If you now combine the recurrence relations given in Eqs. (16.8) and (16.9), you will get

$$\boxed{H_{n+2}(x) = 2x\, H_{n+1}(x) - H'_{n+1}(x)} \qquad (16.10)$$

By changing $(n + 1)$ to n in Eq. (16.10), we can write

$$\boxed{H_{n+1}(x) = 2x\, H_n(x) - H'_n(x)} \qquad (16.11)$$

Again differentiate both sides of this equation with respect to x. This leads to

$$H'_{n+1}(x) = 2\, H_n(x) + 2x\, H'_n(x) - H''_n(x)$$

On combining this with Eq. (16.9), we get

$$2(n+1)H_n(x) = 2\, H_n(x) + 2x\, H'_n(x) - H''_n(x)$$

You may rearrange this equation and write

$$\boxed{H''_n(x) - 2x\, H'_n(x) + 2n\, H_n(x) = 0} \qquad (16.12)$$

Do you recognise this equation? It signifies Hermite's differential equation (for positive integral or zero values of n) for $H_n(x)$. It means that if the polynomials $H_n(x)$ satisfy the recurrence relations in Eqs. (16.8) and (16.9), they must satisfy Hermite's differential equation. You may recall that a similar result was obtained for the Bessel polynomials (TQ 15.1).

The generating function has many other uses. You can utilize it to obtain Rodrigues' formula, which gives a compact expression for Hermite polynomials.

Rodrigues' Formula

We write Eq. (16.7) in expanded form

$$e^{2xt-t^2} = 1 + t\, H_1(x) + \frac{t^2}{2!} H_2(x) + \ldots + \frac{t^n}{n!} H_n(x) + \ldots$$

Successive partial differentiation of both sides with respect to t yields

$$\frac{\partial}{\partial t}\left(e^{2xt-t^2}\right) = H_1(x) + \frac{2t}{2!} H_2(x) + \ldots + \frac{nt^{n-1}}{n!} H_n(x) + \ldots$$

$$\frac{\partial^2}{\partial t^2}\left(e^{2xt-t^2}\right) = H_2(x) + \frac{3\times 2}{3!} H_3(x) + \ldots + \frac{n(n-1)}{n!} t^{n-2} H_n(x) + \ldots$$

$$\vdots$$

$$\frac{\partial^n}{\partial t^n}\left(e^{2xt-t^2}\right) = H_n(x) + \frac{(n+1)\, n(n-1)\ldots 2}{(n+1)!}\, t\, H_{n+1}(x) + \ldots$$

At $t = 0$, this expression simplifies to

$$H_n(x) = \left[\frac{\partial^n}{\partial t^n}\left(e^{2xt-t^2}\right)\right]_{t=0}$$

Since $e^{2xt-t^2} = e^{x^2} e^{-(x-t)^2}$, we can rewrite this expression as

$$H_n(x) = e^{x^2}\left[\frac{\partial^n}{\partial t^n} e^{-(x-t)^2}\right]_{t=0}$$

You should recognise that $e^{-(x-t)^2}$ is a function of $x - t$, and for such a function the partial derivative with respect to t can be obtained from the partial derivative with respect to x by just changing the sign. So for the nth order partial derivative, the sign will change n times. Hence, we can write

$$H_n(x) = e^{x^2}(-1)^n\left[\frac{\partial^n}{\partial x^n} e^{-(x-t)^2}\right]_{t=0}$$

$$= (-1)^n e^{x^2} \frac{d^n}{dx^n}(e^{-x^2}) \qquad (16.13)$$

This is **Rodrigues' formula** for the Hermite polynomials.

We will now like you to apply Rodrigues' formula for a simple case.

Spend 5 min

SAQ 2

Use Rodrigues' formula to evaluate $H_4(x)$.

Yet another interesting application of the generating function for the Hermite polynomials is in evaluation of integrals involving their product with suitable polynomials. Of particular importance is the result that the integral over x from $-\infty$ to $+\infty$ of the product of two Hermite polynomials of different degrees with e^{-x^2} is zero. (The function e^{-x^2} is called the weight function.) These are termed the orthogonality relations of Hermite polynomials. You will now learn to obtain as well as apply these relations, along with the values of similar integrals for Hermite polynomials of the same degree, to calculate the expansion coefficients when a function is expanded in terms of Hermite polynomials.

16.4 ORTHOGONALITY RELATIONS FOR HERMITE POLYNOMIALS

To obtain orthogonality relations for Hermite polynomial, we can start with Hermite differential equation as in the case of Legendre and Bessel polynomials, or the generating relation for the Hermite polynomials. For the sake of variety here we consider the latter option:

$$e^{2xt-t^2} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}$$

Next we change t to u and express the expansion as a power series in u:

$$e^{2xu-u^2} = \sum_{m=0}^{\infty} H_m(x)\frac{u^m}{m!}$$

Now we multiply these equations and the resultant expression by e^{-x^2}. This gives

$$e^{-x^2+2xt-t^2+2xu-u^2} = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} e^{-x^2} H_n(x) H_m(x)\frac{t^n u^m}{n!\,m!}$$

You can rewrite the left hand side as

$$e^{2tu}e^{-(x^2+t^2+u^2-2xt-2xu+2tu)} = e^{2tu}e^{-(x-t-u)^2}$$

Proceeding further, we integrate both sides with respect to x from $-\infty$ to $+\infty$ and, on the right hand side, interchange the order of the summations and integration. This leads to

$$e^{2tu}\int_{-\infty}^{+\infty} e^{-(x-t-u)^2}\,dx = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\int_{-\infty}^{+\infty} e^{-x^2} H_n(x)H_m(x)\,dx\,\frac{t^n u^m}{n!m!} \qquad (16.14)$$

Do you recognise the integral on the left side? By changing the variable of integration from x to z through the substitution $x - t - u = z$, so that $dx = dz$, you can rewrite it as $\int_{-\infty}^{+\infty} e^{-z^2}\,dz$ which is just $\Gamma(1/2)$ and is equal to $\sqrt{\pi}$. The left hand side of the above equation therefore reduces to $\pi^{1/2} e^{2tu}$. On expanding the exponential in a power series, we can write

Consider the integral

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

$$= 2\int_0^{\infty} e^{-z^2}\,dz$$

Put $z^2 = p$ so that

$2z\,dz = dp$

or

$$2dz = \frac{dp}{z}$$

$$= p^{-1/2}dp$$

Hence

$$I = \int_0^{\infty} p^{-1/2}e^{-p}\,dp$$

$$= \Gamma(1/2)$$

$$\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\int_{-\infty}^{+\infty} e^{-x^2} H_n(x)H_m(x)\,dx\,\frac{t^n u^m}{n!m!} = \sqrt{\pi}\sum_{n=0}^{\infty}\frac{(2tu)^n}{n!} = \sqrt{\pi}\left[1+\frac{2tu}{1!}+\frac{(2tu)^2}{2!}+\ldots\frac{(2tu)^n}{n!}+\ldots\right]$$

On equating the coefficients of $t^n u^m$, we get

$$\int_{-\infty}^{+\infty} e^{-x^2} H_n(x)H_m(x)\,dx = 0 \qquad \text{if } n \neq m$$

and

$$\int_{-\infty}^{+\infty} e^{-x^2} H_n(x)H_m(x)\,dx = 2^n n!\pi^{1/2} \qquad \text{if } n = m$$

On combining these results, we can write

$$\int_{-\infty}^{+\infty} e^{-x^2} H_n(x)H_m(x)\,dx = 2^n n!\pi^{1/2}\delta_{mn} \qquad (16.15)$$

where δ_{mn} is the Kronecker delta.

In words, the Hermite polynomials of different degrees are orthogonal to each other on the interval $(-\infty, +\infty)$ with weight function e^{-x^2}. You may recall that for Legendre polynomials, the weight function is unity and the range of integration varies from -1 to $+1$.

You may now like to solve an SAQ on evaluation of integrals involving Hermite polynomials.

SAQ 3

Spend 10 min

Use the generating function for Hermite polynomials to evaluate the integral

$$\int_{-\infty}^{+\infty} x e^{-x^2} H_n(x)H_m(x)\,dx$$

We hope that now you have understood the properties of Hermite polynomials. We will apply this knowledge to solve the one dimensional harmonic oscillator problem in quantum mechanics. This will enable you to understand the nature of small vibrations of atoms in molecules and quantization of the electromagnetic field where energy of the field may be written as a sum of harmonic oscillator type energy terms.

16.5 ONE DIMENSIONAL HARMONIC OSCILLATOR

In Block 3 of your course PHE-11 on Modern Physics, the problem of a one-dimensional harmonic oscillator has been discussed as it is of significant physical interest. We begin by writing the time-independent Schrödinger equation for such a system:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi(x)=E\,\psi(x) \tag{16.16}$$

Here $\hbar = h/2\pi$; h is Planck's constant, m and ω are the mass and the classical angular frequency of the oscillating particle, E is the total energy of the oscillator, and $\psi(x)$ is the corresponding wavefunction (space dependent part). Note that $(1/2)m\omega^2x^2$ denotes the potential energy of the oscillator. In Unit 8 of PHE-11 course, only result has been quoted, without going into details. Now you will learn to solve this equation for $\psi(x)$ and calculate the possible values of E for which $\psi(x)$ is well-behaved.

First of all, we rewrite Eq.(16.16) in a dimensionless form by introducing a new independent variable through the relation

$$\xi=\left(\frac{m\omega}{\hbar}\right)^{1/2}x \tag{16.17}$$

and define a parameter λ as

$$\frac{d\psi}{dx}=\frac{d\psi}{d\xi}\cdot\frac{d\xi}{dx}=\left(\frac{m\omega}{\hbar}\right)^{1/2}\frac{d\psi}{d\xi}$$

and

$$\frac{d}{dx}\left(\frac{d\psi}{dx}\right)=\left(\frac{m\omega}{\hbar}\right)^{1/2}\frac{d}{dx}\left(\frac{d\psi}{d\xi}\right)=\left(\frac{m\omega}{\hbar}\right)^{1/2}\frac{d^2\psi}{d\xi^2}\cdot\frac{d\xi}{dx}=\left(\frac{m\omega}{\hbar}\right)\frac{d^2\psi}{d\xi^2}$$

$$E=\left(\lambda+\frac{1}{2}\right)\hbar\omega \tag{16.18}$$

Then Eq.(16.16) takes the form

$$-\frac{\hbar^2}{2m}\left(\frac{m\omega}{\hbar}\right)\frac{d^2\psi}{d\xi^2}+\frac{1}{2}m\omega^2\left(\frac{\hbar}{m\omega}\right)\xi^2\psi=\left(\lambda+\frac{1}{2}\right)\hbar\omega\psi$$

On re-arrangement, it simplifies to

$$\frac{d^2\psi}{d\xi^2}+(2\lambda+1-\xi^2)\psi=0 \tag{16.19}$$

If you now take

$$\psi(\xi)=e^{-\xi^2/2}f(\xi) \tag{16.20}$$

you can easily see that Eq.(16.19) reduces to a differential equation of the Hermite form (SAQ 4).

SAQ 4

Spend 5 min

By substituting for $\psi(\xi)$ from Eq.(16.20) in Eq.(16.19), show that

$$\frac{d^2f}{d\xi^2}-2\xi\frac{df}{d\xi}+2\lambda f(\xi)=0$$

From our earlier discussion you can easily conclude that if λ is a negative integer, both the series in the solution will be infinite. In this case, for large ξ, $f(\xi)$ will behave as e^{ξ^2}. Therefore, the wavefunction ψ defined by Eq.(16.20) approaches infinity for $x \to \pm\infty$.

Further, since $|\psi(x)|^2\,dx$ defines the probability of finding the particle between x and $x + dx$, it readily follows that the probability of finding the oscillating particle far away from the origin will be infinite. Is this physically admissible? Certainly not. So we are justified in saying that a value of λ that is neither a positive integer nor zero is not permitted. From Sec. 16.2 you will recall that for $\lambda = n$, where n is zero or a positive integer, we can get a particular polynomial solution of the Hermite's differential equation – the Hermite polynomial of degree n. In this case, we have

$$f(\xi) = N H_n(\xi)$$

so that the solution of time-independent Schrödinger equation can be written as

$$\psi = Ne^{-(1/2)\xi^2} H_n(\xi) \qquad (16.21)$$

where N is a constant. This form of the solution is well-behaved; it tends to zero as $x \to \pm\infty$. The allowed values of λ will correspond to $n = 0,1,2...$ This implies that the linear harmonic oscillator has a discrete set of equidistant energy levels:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0,1,2,... \qquad (16.22)$$

The corresponding wavefunction is

$$\psi_n(x) = N_n e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \qquad (16.23)$$

You should note that we have put a subscript n with ψ and N to signify their dependence on n, the vibrational quantum number. Since the probability of finding the oscillator somewhere between $x = -\infty$ and $x = +\infty$ is equal to one, we can write

$$\int_{-\infty}^{+\infty} |\psi_n(x)|^2 dx = 1$$

or

$$N_n^2 (\hbar / m\omega)^{1/2} \int_{-\infty}^{+\infty} e^{-\xi^2} H_n(\xi) H_n(\xi) d\xi = 1$$

The value of the integral occurring in this expression is $2^n n! \sqrt{\pi}$ from Eq. (16.15). On inserting this value of the integral, we can solve for the normalization constant N_n. The result is

$$N_n = \left[\left(\frac{m\omega}{\hbar}\right)^{1/2} \frac{1}{2^n n! \pi^{1/2}}\right]^{1/2}$$

The normalized wavefunctions are therefore given by

$$\psi_n(x) = \left[\left(\frac{m\omega}{\hbar}\right)^{1/2} \frac{1}{2^n n! \pi^{1/2}}\right]^{1/2} e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \qquad (16.24)$$

A plot of the first few wavefunctions of a linear harmonic oscillator is shown in Fig. 16.2. (For convenience in scaling, we have taken $m\omega/\hbar = 1$.) You will note that $\psi_0(-x) = \psi_0(x)$, $\psi_1(-x) = -\psi_1(x), \psi_2(-x) = \psi_2(x)$ and $\psi_3(-x) = -\psi_3(x),...$ That is, for a linear harmonic oscillator, the wavefunction $\psi_n(x)$ has even parity (i.e., on changing the sign of x, it remains unchanged) when n is an even positive integer or zero, and has odd parity (i.e., changes sign) if n is an odd positive integer. This behaviour can seen to be follow from Eq. (16.24), since $e^{-\frac{1}{2}\frac{m\omega}{\hbar}x^2}$ does not change with the sign of x and, the Hermite polynomials $H_n(x)$ show even or odd parity (Example 1). You will also note that, apart from going to zero as $x \to \pm\infty$, the wavefunctions ψ_1, ψ_2 and ψ_3 become zero (have nodes) at one, two and three points, respectively. In general, $\psi_n(x)$ will have n such nodes (corresponding to n zeros of the Hermite polynomial of nth degree). The level lines along the x-axis indicate classically permitted regions of movement of the linear harmonic oscillator. It is important to note that, although $|\psi(x)|^2 \to 0$ as $x \to \pm\infty$, it is, in general, not zero just outside the classically permitted region. It means that quantum mechanically, there is a finite (though small) probability of finding the oscillator outside the classically allowed region.

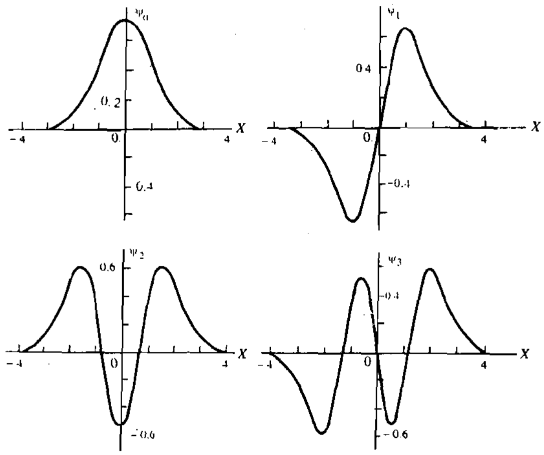

Fig.16.2: Energy eigenfunctions of a linear harmonic oscillator for n = 0,1,2,3

16.6 LAGUERRE'S DIFFERENTIAL EQUATION AND LAGUERRE POLYNOMIALS

Laguerre's differential equation is a linear second order ODE:

$$x\frac{d^2y}{dx^2} + (1-x)\frac{dy}{dx} + \nu y(x) = 0 \tag{16.25}$$

where ν is a parameter. You can easily convince yourself that $x = 0$ is a regular singular point of this equation and its solution around this point can be obtained using the power series method (Unit 3, Block 1 of PHE-05 course):

$$y(x) = \sum_{j=0}^{\infty} a_j x^{\alpha+j}, a_0 \neq 0 \tag{16.26}$$

You can easily verify that the indicial equation (Unit 3 of PHE-05 course) in this case will be $\alpha^2 = 0$, which has repeated root $\alpha = 0$. For this value of α, insert Eq. (16.26) in Eq. (16.25). This leads to the equation

$$\sum_j a_j j(j-1)x^{j-1} + \sum_j a_j x^{j-1} - \sum_j j a_j x^j + \nu \sum_j a_j x^j = 0$$

On equating the coefficient of x^j to zero, we obtain a recurrence relation between a_{j+1} and a_j:

$$a_{j+1}[j(j+1)+(j+1)] + (\nu - j)a_j = 0$$

On slight rearrangement, we get

$$a_{j+1} = -\frac{\nu - j}{(j+1)^2} a_j \tag{16.27}$$

This relation suggests that all the coefficients can be expressed in terms of a_0, and one of the solutions of Eq. (16.25) is

$$y(x) = a_0\left[1-\frac{\nu}{1^2}x+\frac{\nu(\nu-1)}{1^2\times 2^2}x^2-...+(-1)^j\frac{\nu(\nu-1)...(\nu-j+1)}{1^2\times 2^2\times...\times j^2}x^j+...\right] \tag{16.28}$$

If ν is not a positive integer or zero, this will remain an infinite series. However, for the particular case $\nu = n$, where n is a positive integer or zero, the series will terminate at the $(n+1)$ th term and reduce to an nth degree polynomial in x. If we further choose $a_0=1$, the resultant expression defines the Laguerre polynomial, $L_n(x)$:

$$L_n(x) = 1-\frac{n}{(1!)^2}x+\frac{n(n-1)}{(2!)^2}x^2-...+(-1)^n\frac{n(n-1)...1}{(n!)^2}x^n$$

$$= 1-{}^nC_1\frac{x}{1!}+{}^nC_2\frac{x^2}{2!}-...+(-1)^n\,{}^nC_n\frac{x^n}{n!} \tag{16.29}$$

The notation ${}^nC_r$ denotes the number of combinations of n things r at a time. It is given by

$${}^nC_r = \frac{n!}{(n-r)!r!}$$

From this equation it readily follows that Laguerre polynomials for the first few values of n are

$$L_0(x) = 1$$
$$L_1(x) = 1-x$$
$$L_2(x) = 1-2x+\frac{x^2}{2}$$
$$L_3(x) = 1-3x+\frac{3}{2}x^2-\frac{x^3}{6}$$

and

$$L_4(x) = 1-4x+3x^2-\frac{2}{3}x^3+\frac{x^4}{24} \tag{16.30}$$

Fig. 16.3 shows a plot of Laguerre polynomials versus x.

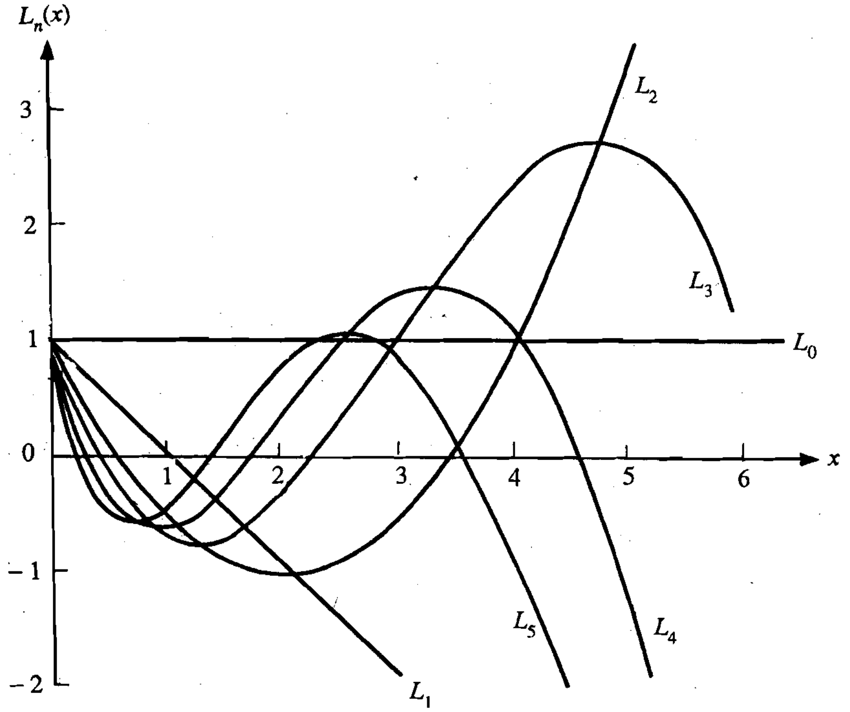

Fig.16.3: Laguerre polynomials $L_n(x)$ for $n = 0$ to $n = 5$

The Rodrigues' formula for $L_n(x)$ enables us to express it in a compact form:

$$L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}(x^n e^{-x}) \qquad (16.31)$$

You may now like to solve an SAQ.

SAQ 5

Spend 2 min

Show that the Laguerre polynomial defined in Eq. (16.31) is identical with that given in Eq. (16.29).

16.7 GENERATING FUNCTION AND RECURRENCE RELATIONS FOR LAGUERRE POLYNOMIALS

The generating function for Laguerre polynomials is

$$g(x,t) = \frac{e^{-xt/(1-t)}}{1-t} = \sum_{n=0}^{\infty} L_n(x)\,t^n \qquad |t| < 1 \qquad (16.32)$$

If you differentiate both sides of Eq. (16.32) partially with respect to t, you will get

$$(1-t-x)\frac{e^{-xt/(1-t)}}{(1-t)^3} = \sum_{n=1}^{\infty} L_n(x) n t^{n-1}$$

On combining this result with Eq. (16.32), you can write

$$(1-t-x)\sum_{n=0}^{\infty} L_n(x)\,t^n = (1-t)^2 \sum_{n=1}^{\infty} L_n(x) n t^{n-1}$$

On equating the coefficients of t^{n+1} from the two sides and rearranging terms, we obtain a recurrence relation which connects Laguerre polynomials of three successive degrees:

$$(n+2)\,L_{n+2}(x) = (2n+3-x)L_{n+1}(x) - (n+1)L_n(x) \qquad (16.33)$$

The binomial series of e^x and $(1+x)^p$ (all x and p) are

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots$$

$$(1+x)^p = 1 + px + \frac{p(p-1)}{2!}x^2 + \frac{p(p-1)(p-2}{3!}x^3 + \cdots$$

We now make a direct expansion of $g(x,t)$ given in Eq. (16.32) in powers of t:

$$g(x,t) = \left[1 - \frac{xt}{1-t} + \left(\frac{xt}{1-t}\right)^2 + \ldots\right]\left(\frac{1}{1-t}\right)$$

$$= \left(1 - \frac{xt}{1-t} + \ldots\right)(1-t)^{-1}$$

$$= 1 + t - xt - 2xt^2 - \ldots$$

Using binomial expansion we can write

$$\left(1 - \frac{xt}{1-t} + \ldots\right)(1-t)^{-1}$$

$$= \left(1 - xt(1-t)^{-1} + \ldots\right)(1-t)^{-1}$$

$$= \left[1 - xt\left(1 + t + \frac{t^2}{2!} + \ldots\right) + \ldots\right]\left(1 + t + \frac{t^2}{2!} + \ldots\right)$$

$$= \left(1 - xt - xt^2 - x\frac{t^3}{2!} + \ldots\right)(1 + t + \ldots)$$

$$\doteq 1 - xt - xt^2 - \frac{xt^3}{2!} + \ldots + t - xt^2 - xt^3 - \ldots$$

From this you will note that the coefficient of t^0 and t^1 are 1 and $1-x$, respectively. So we car say that $L_0(x) = 1$ and $L_1(x) = 1-x$. If you now put $n = 0$ in Eq. (16.33) and substitute for $L_0(x$ and $L_1(x)$, you will obtain $L_2(x) = 1-2x + \frac{x^2}{2}$. Proceeding in the same way you can successively generate the Laguerre polynomials of all degrees.

In order to get another recurrence relation for the Laguerre polynomials, we differentiate bot sides of Eq.(16.32) partially with respect to x. This gives

$$-\frac{t}{(1-t)^2}e^{-xt/(1-t)} = \sum_{n=0}^{\infty}\frac{dL_n}{dx}t^n$$

This can be rewritten as

$$-t\sum_{n=0}^{\infty} L_n(x)t^n = (1-t)\sum_{n=0}^{\infty} \frac{dL_n}{dx} t^n$$

On equating the coefficients of t^{n+1} on both sides, we get

$$\frac{dL_{n+1}}{dx} = \frac{dL_n}{dx} - L_n(x) \qquad (16.34)$$

The recurrence relations given in Eqs. (16.33) and (16.34) can be combined to obtain other relations. However, we will not go into these details.

You have earlier learnt the orthogonality relations for Legendre, Bessel and Hermite functions and their importance in understanding various physical problems. In the following section, we obtain orthogonality relations of Laguerre polynomials.

16.8 ORTHOGONALITY RELATIONS FOR LAGUERRE POLYNOMIALS

There are different ways of obtaining orthogonality relations for Laguerre polynomials. We start with the differential equations satisfied by Laguerre polynomials of degrees n and k:

$$x\frac{d^2 L_n}{dx^2} + (1-x)\frac{dL_n}{dx} + nL_n(x) = 0 \qquad (16.35a)$$

$$x\frac{d^2 L_k}{dx^2} + (1-x)\frac{dL_k}{dx} + kL_k(x) = 0 \qquad (16.35b)$$

Multiply Eq.(16.35(a)) by $e^{-x} L_k(x)$ and Eq. (16.35(b)) by $e^{-x} L_n(x)$ and subtract the latter from the former. You can wr'' the resultant expression as

$$\frac{d}{dx}\left[xe^{-x}\left\{L_k(x)\frac{dL_n}{dx} - L_n(x)\frac{dL_k}{dx}\right\}\right] + (n-k)e^{-x}L_n(x)L_k(x) = 0$$

We integrate this expression over x from 0 to ∞:

$$xe^{-x}\left[L_k(x)\frac{dL_n}{dx} - L_n(x)\frac{dL_k}{dx}\right]_0^{\infty} + (n-k)\int_0^{\infty} e^{-x}L_n(x)L_k(x)\,dx = 0$$

Note that the expression within the square bracket is zero for both the limits (at ∞ because of the exponential factor and at zero because of the x factor). Consequently, we obtain

$$(n-k)\int_0^{\infty} e^{-x}L_n(x)L_k(x)\,dx = 0$$

Thus, if $n \neq k$

$$\int_0^{\infty} e^{-x}L_n(x)L_k(x)\,dx = 0 \qquad (16.36)$$

That is, the Laguerre polynomials of different degrees are orthogonal to each other on the interval $(0,\infty)$ with weight factor e^{-x}.

To obtain the orthogonality relation for $n = k$, we take the products of the two sides of Eq. (16.32) with themselves. This gives

$$\frac{e^{-2xt/(1-t)}}{(1-t)^2} = \sum_{n=0}^{\infty} L_n(x)t^n \sum_{k=0}^{\infty} L_k(x)t^k$$

As before, we multiply both sides of this equation by e^{-x} and integrate from 0 to ∞. This gives

$$\frac{1}{(1-t)^2}\int_0^{\infty} e^{-\frac{1+t}{1-t}x}\,dx = \sum_{n=0}^{\infty}\sum_{k=0}^{\infty} t^n t^k \int_0^{\infty} e^{-x} L_n(x) L_k(x)\,dx \qquad (16.37)$$

You will note that we have changed the orders of summations and integration on the right hand side. For $n = k$, the right side of above equation reduces to $\sum_{n=0}^{\infty} t^{2n}\int_0^{\infty} e^{-x} L_n^2(x)\,dx$.

To proceed further, we use the formula $\int e^{-ax}dx = -\frac{e^{-x}}{a}$. Then left hand side of Eq. (16.37) can be written as

$$\frac{1}{(1-t)^2}\times(-)\left(\frac{1-t}{1+t}\right) e^{-\frac{1+t}{1-t}x}\Bigg|_0^{\infty} = \frac{1}{(1-t)(1+t)} = \frac{1}{1-t^2}$$

For $t \ll 1$, we have

$$\frac{1}{1-t^2} = 1 + t^2 + t^4 + \ldots = \sum_{n=0}^{\infty} t^{2n}$$

so that

$$\sum_{n=0}^{\infty} t^{2n} = \sum_{n=0}^{\infty} t^{2n}\int_0^{\infty} e^{-x} L_n^2(x)\,dx$$

On comparing the coefficients of t^{2n} for all n, we obtain

$$\int_0^{\infty} e^{-x} L_n^2(x)\,dx = 1 \qquad (16.38)$$

Eqs. (16.36) and (16.38) may now be combined to write the orthonormality relation for Laguerre polynomials as

$$\int_0^{\infty} e^{-x} L_n(x) L_k(x)\,dx = \delta_{nk} \qquad (16.39)$$

We will now summarise what you have learnt in this unit.

16.9 SUMMARY

- The **Hermite polynomial**

$$H_n(x) = (2x)^n - \frac{n(n-1)}{1!}(2x)^{n-2} + \frac{n(n-1)(n-2)(n-3)}{2!}(2x)^{n-4} + \ldots + \frac{(-1)^{n/2} n!}{(n/2)!} \quad n \text{ even}$$

$$= (2x)^n - \frac{n(n-1)}{1!}(2x)^{n-2} + \ldots + \frac{(-1)^{\frac{n-1}{2}} n!}{\left(\frac{n-1}{2}\right)!} \quad n \text{ odd}$$

is a polynomial solution of **Hermite's differential equation**

$$\frac{d^2 H_n}{dx^2} - 2x\frac{dH_n}{dx} + 2n H_n(x) = 0$$

where n is any positive integer or zero.

- The **generating function** for Hermite polynomials is

$$e^{2xt-t^2} = \sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!}$$

- The **Rodrigues' representation** for the Hermite polynomials is

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

- The Hermite polynomials are **orthonormal functions** such that

$$\int_{-\infty}^{+\infty} e^{-x^2} H_n(x) H_m(x)\, dx = 2^n n! \pi^{1/2} \delta_{nm}$$

- The **Laguerre polynomials** are polynomial solutions of Laguerre's differential equation

$$x\frac{d^2 L_n}{dx^2} + (1-x)\frac{dL_n}{dx} + n\, L_n(x) = 0$$

where n is a positive integer or zero, with $L_n(0)=1$.

- The **Rodrigues' formula** for Laguerre polynomials is

$$L_n(x) = \frac{e^x}{n!}\frac{d^n}{dx^n}(x^n e^{-x})$$

- The **generating function** for Laguerre polynomials is

$$\frac{e^{-xt/(1-t)}}{(1-t)} = \sum_{n=0}^{\infty} L_n(x) t^n \qquad |t| < 1$$

- The **orthonormality relations** for the Laguerre polynomials are given by

$$\int_0^{\infty} e^{-x} L_n(x) L_k(x)\, dx = \delta_{nk}$$

16.10 TERMINAL QUESTIONS

Spend 20 *min*

1. Two operators

$$a = \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right)$$

and

$$a^+ = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)$$

where $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$ operate on the harmonic oscillator wavefunction

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

where

$$N_n = \left[\left(\frac{m\omega}{\hbar}\right)^{1/2} \frac{1}{2^n n! \pi^{1/2}}\right]^{1/2}$$

Show that

$$a\psi_n = \sqrt{n}\,\psi_{n-1}$$

$$a^+ \psi_n = \sqrt{n+1}\,\psi_{n+1}$$

and

$$(aa^+ - a^+a)\psi_n = \psi_n$$

2. The 'zero' line in the fundamental band of the near infrared absorption spectrum of HCl^{35} gas occurs at 3.46×10^{-6}m. This corresponds to a transition from a state with vibrational quantum number zero to a state with quantum number one. Calculate the force constant for HCl bond assuming harmonic oscillator potential.

16.11 SOLUTIONS AND ANSWERS

Self-assessment Questions

1. Differentiate both sides of Eq. (16.7) partially with respect to x. This gives

$$2t\,e^{2xt-t^2} = \sum_{n=0}^{\infty} H_n'(x)\frac{t^n}{n!}$$

We can rewrite it as

$$2t\sum_{n=0}^{\infty} H_n(x)\frac{t^n}{n!} = \sum_{n=0}^{\infty} H_n'(x)\frac{t^n}{n!}$$

Equate coefficients of t^{n+1} from both sides to get

$$2\frac{H_n(x)}{n!} = \frac{H_{n+1}'(x)}{(n+1)!}$$

or

$$H_{n+1}'(x) = 2(n+1)H_n(x)$$

2. According to Rodrigues' formula

$$H_4(x) = (-1)^4 e^{x^2} \frac{d^4}{dx^4}\left(e^{-x^2}\right)$$

Since

$$\frac{d}{dx}\left(e^{-x^2}\right) = -2xe^{-x^2}$$

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

$$\frac{d^3}{dx^3}\left(e^{-x^2}\right) = -(2x)^3 e^{-x^2} + 8x\, e^{-x^2} + 4x\, e^{-x^2}$$

$$= -(2x)^3 e^{-x^2} + 12x\, e^{-x^2}$$

$$\frac{d^4}{dx^4}\left(e^{-x^2}\right) = (2x)^4 e^{-x^2} - 24x^2 e^{-x^2} - 24x^2 e^{-x^2} + 12 e^{-x^2}$$

$$\therefore\ H_4(x) = 16x^4 - 48x^2 + 12$$

3. From the expression for the generating function of Hermite polynomials, we can write

$$\int_{-\infty}^{+\infty} x\, e^{-x^2} e^{2xt - t^2 + 2xu - u^2} dx = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\int_{-\infty}^{+\infty} x\, e^{-x^2} H_n(x) H_m(x)\, dx \frac{t^n u^m}{n!\, m!} \qquad \text{(i)}$$

Following the steps used in arriving at Eq. (16.14), we can rewrite the left hand side as

$$I = e^{2tu}\int_{-\infty}^{+\infty} x\, e^{-(x-t-u)^2} dx$$

We now change the variable of integration and put $z = x - t - u$. Then above integral takes the form

$$I = e^{2tu}\int_{-\infty}^{+\infty} (z + t + u) e^{-z^2} dz$$

$$= e^{2tu}\left(0 + t\sqrt{\pi} + u\sqrt{\pi}\right)$$

$$= \sqrt{\pi}\sum_{n=0}^{\infty} (t + u)\frac{(2tu)^n}{n!}$$

$$= \sqrt{\pi}\sum_{n=0}^{\infty} \frac{2^n}{n!}\left(t^{n+1}u^n + t^n u^{n+1}\right) \qquad \text{(ii)}$$

On equating the coefficients of $t^n u^m$ of the series in (ii) with the corresponding coefficients from the right hand side of (i), we obtain the required result:

$$\int_{-\infty}^{+\infty} x\, e^{-x^2} H_n(x)\, H_m(x)\, dx = 2^n\sqrt{\pi}(n+1)! \text{ if } m = n+1$$

$$= 2^{n-1}\sqrt{\pi}\, n! \qquad \text{if } m = n-1$$

$$= 0 \qquad \text{otherwise}$$

4. $$\psi = e^{-\frac{1}{2}\xi^2} f(\xi)$$

The right hand side is a product of two polynomials. Differentiating it with respect to ξ, we obtain

$$\frac{d\psi}{d\xi} = e^{-\xi^2/2}\frac{df}{d\xi} - \xi\, e^{-\xi^2/2} f(\xi)$$

Differentiating it again with respect to ξ, we get

$$\frac{d^2\psi}{d\xi^2} = e^{-\frac{1}{2}\xi^2}\frac{d^2 f}{d\xi^2} - 2\xi e^{-\frac{1}{2}\xi^2}\frac{df}{d\xi} + \xi^2 e^{-\frac{1}{2}\xi^2} f(\xi) - e^{-\frac{1}{2}\xi^2} f(\xi)$$

If you substitute this in Eq. (16.19) and take out the common factor $e^{-\frac{1}{2}\xi^2}$, you will get the required result:

$$\frac{d^2 f}{d\xi^2} - 2\xi\frac{df}{d\xi} + 2\lambda f(\xi) = 0$$

5. Recall Leibnitz rule for the nth derivative of the product of two polynomials $u(x)$ and $v(x)$:

$$\frac{d^n}{dx^n}(uv) = \frac{d^n u}{dx^n}v + {}^nC_1\frac{d^{n-1}u}{dx^{n-1}}\frac{dv}{dx} + \ldots + {}^nC_n u\frac{d^n v}{dx^n}$$

Now we choose $u(x) = x^n$ and $v(x) = e^{-x}$. Then using Leibnitz rule, we can write

$$\frac{e^x}{n!}\frac{d^n}{dx^n}\left(x^n e^{-n}\right) = \frac{e^x}{n!}\left[n!e^{-x} + {}^nC_1\frac{n!}{1!}x(-)e^{-x} + {}^nC_2\frac{n!}{2!}x^2(-1)^2 e^{-x} + \ldots + {}^nC_n x^n(-1)^n e^{-x}\right]$$

$$= 1 - {}^nC_1\frac{x}{1!} + {}^nC_2\frac{x^2}{2!} - \ldots (-1)^n\, {}^nC_n\frac{x^n}{n!}$$

Terminal Questions

1.
$$\frac{d\psi_n}{d\xi} = N_n e^{-(1/2)\xi^2}\left(-\xi H_n(\xi) + \frac{dH_n}{d\xi}\right)$$

$$= N_n e^{-(1/2)\xi^2}(-\xi H_n(\xi) + 2n H_{n-1}(\xi))$$

$$\therefore \quad a\psi_n = \frac{1}{\sqrt{2}}\left(\xi + \frac{d}{d\xi}\right)\psi_n$$

$$= \frac{N_n}{\sqrt{2}}e^{-(1/2)\xi^2}2n H_{n-1}(\xi)$$

But

$$\frac{N_n}{\sqrt{2}}2n = \left[\left(\frac{m\omega}{\hbar}\right)^{1/2}\frac{1}{2^n n!\pi^{1/2}}\right]^{1/2}\sqrt{2}\,n$$

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

$$= \sqrt{n}\,N_{n-1}$$

Hence

$$a\psi_n = \sqrt{n}\,N_{n-1}e^{-(1/2)\xi^2}H_{n-1}(\xi)$$

$$= \sqrt{n}\,\psi_{n-1}$$

Further,

$$a^{+}\psi_n = \frac{1}{\sqrt{2}}\left(\xi - \frac{d}{d\xi}\right)\psi_n$$

$$= \frac{N_n}{\sqrt{2}} e^{-(1/2)\xi^2}\left[2\xi H_n(\xi) - 2n H_{n-1}(\xi)\right]$$

$$= \frac{N_n}{\sqrt{2}} e^{-(1/2)\xi^2} H_{n+1}(\xi)$$

$$= \sqrt{n+1}\frac{1}{\sqrt{2}\sqrt{n+1}}\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} \frac{1}{2^n n!\pi^{1/2}}\right] e^{-(1/2)\xi^2} H_{n+1}(\xi)$$

$$= \sqrt{n+1}\, N_{n+1} e^{-(1/2)\xi^2} H_{n+1}(\xi) = \sqrt{n+1}\, \psi_{n+1}$$

The operators a^{+} and a are called raising and lowering operators (step up and step down operators) or (in the context of quantum field theory) creation and annihilation operators. Again,

$$\left(a a^{+} - a^{+} a\right)\psi_n = a\sqrt{n+1}\ \psi_{n+1} - a^{+}\sqrt{n}\ \psi_{n-1}$$

$$= \sqrt{n+1}\sqrt{n+1}\,\psi_n - \sqrt{n}\sqrt{n}\,\psi_n = (n+1-n)\,\psi_n$$

$$= \psi_n$$

2. Let ν be the frequency of the 'zero' line. Then

$$\nu = \frac{c}{\lambda} = \frac{3\times 10^8}{3.46\times 10^{-6}}\ \text{Hz}$$

Also,

$$h\nu = E_{n=1} - E_{n=0} = \hbar\omega = \hbar\sqrt{\frac{k}{\mu}}$$

$$\therefore\ \frac{k}{\mu} = \left(\frac{2\pi\times 3}{3.46}\times 10^{14}\right)^2$$

where k is the force constant and μ is the reduced mass of H and Cl^{35}, i.e.

$$\mu = \frac{1\times 35}{1+35}\times 1.66\times 10^{-27}\,\text{kg}$$

Then

$$k = \frac{35}{36}\times 1.66\times\left(\frac{6\pi}{3.46}\right)^2 \times 10\,\text{Nm}^{-1} = 479\,\text{Nm}^{-1}.$$