1. Hermite Equation

In the study of the eigenvalue problem of the Hamiltonian for the quantum harmonic oscillator we have encountered the Hermite equation which reads

\[ \frac{d^2 H}{d\xi^2} - 2\xi \frac{dH}{d\xi} + \left( \frac{2E}{\hbar \omega} - 1 \right) H = 0, \tag{1} \]

which is a well-known homogeneous second-order linear differential equation. Note that this equation has \textit{nonconstant} coefficients – otherwise we could readily solve the equation with elementary methods and it is amenable to methods encountered e.g. in the module MATH2370, using series expansions. We will show here that the physically important solutions are the polynomial ones leading to the well-known Hermite polynomials. In the next section we will study the latter polynomials in their own right.

The emergence of polynomial solutions from the equation (1) is seen as follows. Let us try first a power series expansion for the solution, given by

\[ H(\xi) = \sum_{m=0}^{\infty} a_m \xi^m, \]

where the coefficients \( a_m \) need to be determined. Inserting this expansion in the equation (1) we obtain:

\[ \sum_{m=2}^{\infty} m(m-1)a_m \xi^{m-2} - \sum_{m=1}^{\infty} 2ma_m \xi^m + \beta \sum_{m=0}^{\infty} a_m \xi^m = 0, \]

where we have abbreviated \( \beta = \frac{2E}{\hbar \omega} - 1 \). Changing the summation variable (by a shift over 2 units) in the first term we obtain:

\[ \sum_{m=0}^{\infty} (m+2)(m+1)a_{m+2} \xi^{m+2} - \sum_{m=0}^{\infty} 2ma_m \xi^m + \beta \sum_{m=0}^{\infty} a_m \xi^m = 0, \]

so that all powers of \( \xi \) within the sums are of the same form, and we can immediately read off a \textit{recursion relation} for the coefficients (since all powers of \( \xi \) are independent):

\[ (m+2)(m+1)a_{m+2} = (2m - \beta)a_m, \quad m = 0, 1, 2, \ldots. \]

Since the recursion relation increases in steps of 2 units, the implementation of it will lead to two independent solutions (as one expects!). In fact, the two independent solutions of the Hermite equation can be obtained by the following choices of initial conditions on the
recursion relation: given $\beta$ we will have one solution starting with $a_0 = 0, a_1 \neq 0,$ for which the solution series will only have odd powers of $\xi$, and another solution starting with $a_1 = 0, a_0 \neq 0$ for which the series will have only even powers of $\xi$. Clearly, the resulting two solutions are independent. Thus, upon iteration we obtain from the recursion relation the following explicit expressions for the even coefficients:

$$a_{2k} = \frac{[(4(k-1) - \beta)[4(k-2) - \beta] \ldots [-\beta]}{(2k)!} a_0$$

while for the odd coefficients we have

$$a_{2k+1} = \frac{[(2(2k - 1) - \beta)[2(2k-3) - \beta] \ldots [2-\beta]}{(2k+1)!} a_1 .$$

From these expansions one thing is immediately clear: if $\beta = 2n$ for some positive integer $n$, then either one of the sequences of coefficients will terminate:

- if $\beta = 2n = 4\nu - 2 \Rightarrow a_{2\nu + 1} = 0$ odd sequence terminates
- if $\beta = 2n = 4\nu - 4 \Rightarrow a_{2\nu} = 0$ even sequence terminates

and when these sequences terminate, the corresponding series for $H(\xi)$ will truncate (resulting in only a finite number of terms in the sum) and, hence, we have a polynomial solution.

If $\beta \neq 2n$ for any $n \in \mathbb{Z}$, then the series for $H(\xi)$ does not truncate and we will have an infinite series. We will now show that these solutions have to be rejected on the ground that an infinite series will lead to solutions that do not obey the integrability assumption associated with the normalisation of the quantum eigenfunctions. In fact, for large enough $m$ the recursion relation gives

$$\frac{a_m}{a_{m-2}} \sim \frac{2}{m} , \quad \text{as } m \to \infty ,$$

implying that for large $m$

$$a_m \sim \frac{1}{(m/2)!} a_0 \quad (m \text{ even}) \quad \text{and} \quad a_m \sim \frac{1}{((m-1)/2)!} a_1 \quad (m \text{ odd}) \quad \text{as } m \to \infty .$$

However, the series for $N$ large enough can then be approximated as

$$H(\xi) \sim \text{polynomial} + \sum_{m=N}^{\infty} \frac{1}{(m/2)!} \xi^{2(m/2)} \sim e^{\xi^2} .$$

Thus, if the series for $H(\xi)$ does not truncate to a finite polynomial the corresponding infinite series will roughly behave like $H(\xi) \sim e^{\xi^2}$, and inserting this into the formula for the eigenfunction $\phi(x)$ of Handout #5 we will obtain a solution that is not only not square integrable, but actually unbounded as $x$ becomes large! Clearly such solutions have to be rejected. We conclude that the only quantum mechanically acceptable solutions of the Hermite equations are the polynomial ones occurring for the values $\beta = 2n$.  

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2. Properties of the Hermite Polynomials

We will now study some of the properties of the Hermite polynomials. Most of these properties are characteristic not only of the Hermite polynomials but of other classes of so-called orthogonal polynomials as well.

The simplest way to study the Hermite polynomials is through its generating function. This is a function of $\xi$ as well as of an additional “dummy” variable $t$ (not to be confused with the time variable) of the form:

\[
S(\xi, t) = e^{2t\xi - t^2} = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} t^n.
\]

This function encodes all the Hermite polynomials in one formula. In fact, by expanding the l.h.s. in powers of $t$ and comparing the coefficients with the terms in the sum on the r.h.s. we get all Hermite polynomials in explicit form.

Let us now show how to derive the various properties from the generating function.

i) **Orthogonality:** Evaluating the integral

\[
\int_{-\infty}^{\infty} S(\xi, t)S(\xi, t')e^{-\xi^2} d\xi = \int_{-\infty}^{\infty} e^{2t\xi - t^2} e^{2t'\xi - t'^2} e^{-\xi^2} d\xi
\]

\[
= \int_{-\infty}^{\infty} e^{-[(\xi - (t+t'))^2]} e^{(t+t')^2 - t'^2 - t^2} d\xi = e^{2tt'} \sqrt{\pi} = \sum_{n=0}^{\infty} \frac{2^n \sqrt{\pi}}{n!} (tt')^n
\]

where as we see the insertion of both sides of (2) leads to a power series in $tt'$ only. Comparing both sides we are led to the orthogonality relation:

\[
\int_{-\infty}^{\infty} H_n(\xi)H_m(\xi)e^{-\xi^2} d\xi = 2^n n! \sqrt{\pi} \delta_{n,m},
\]

expressing the fact that the collection of all Hermite polynomials forms a family of orthogonal polynomials, and the function $w(x) = e^{-x^2}$, that appears in the integrand of (3) is called the weight function of the family. The weight function together with the integration region (in our case the infinite interval: $(-\infty, \infty)$) fully determine the family of orthogonal polynomials up to a common constant factor.

ii) **Recursion relation:** Taking derivatives with respect to $t$ on both sides of (2) we get:

\[
\frac{\partial S}{\partial t} = 2(\xi - t)S = \sum_{n=0}^{\infty} 2(\xi - t) \frac{H_n}{n!} t^n
\]

\[
= \sum_{n=0}^{\infty} \frac{2\xi H_n}{n!} t^n - \sum_{n=1}^{\infty} 2 \frac{H_{n-1}}{(n-1)!} t^n
\]

\[
= \sum_{n=1}^{\infty} \frac{H_n}{(n-1)!} t^{n-1} = \sum_{n=0}^{\infty} \frac{H_{n+1}}{n!} t^n
\]
which, upon comparison of both sides power by power in $t$, yields the relation:

$$H_{n+1} = 2\xi H_n - 2nH_{n-1}, \quad n = 1, 2, \ldots$$  \hspace{1cm} (4)

together with $H_1 = 2\xi H_0$ (corresponding to the term $n = 0$ in the sum). Eq. (4) is a three-point recursion relation (i.e. involving $H_{n+1}$, $H_n$ and $H_{n-1}$, which is typical for orthogonal polynomials (all families of orthogonal polynomials obey such a recursion relation, albeit with different coefficients).

iii) **Differential relation:** Taking derivatives with respect to $\xi$ of the generating function, we get:

$$\frac{\partial S}{\partial \xi} = 2tS = \sum_{n=0}^{\infty} 2 \frac{H_n}{n!} t^n = \sum_{n=1}^{\infty} 2 \frac{H_{n-1}}{(n-1)!} t^n = \sum_{n=0}^{\infty} \frac{H_n'}{n!} t^n$$

leading, by comparison of the coefficients of the same power of $t$, to the relation:

$$H'_n = 2nH_{n-1}, \quad n = 1, 2, \ldots$$  \hspace{1cm} (5)

together with $H'_0 = 0$ (which implies $H_0(\xi) = \text{constant}$) for the lowest-order term. Combining the recursion relation (4) with the differential relation (5) we can actually write down a second-order differential equation in terms of one single $H_n$ (so eliminating shifts in $n$). In fact, combining (4) and (5) we get

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

which after some easy manipulation yields the Hermite equation:

$$H''_n - 2\xi H'_n + 2nH_n = 0.$$  \hspace{1cm} (6)

iv) **Rodrigues’ formula:** The $n^{th}$ order coefficient in the series on the r.h.s. of (2) is obtained by $n$ differentiations as follows:

$$H_n(\xi) = \left( \frac{\partial}{\partial t} \right)^n S(\xi, t) \bigg|_{t=0} = \left( \frac{\partial}{\partial t} \right)^n e^{2\xi t - t^2} \bigg|_{t=0} = e^{\xi^2} \left( \frac{\partial}{\partial \xi} \right)^n e^{-(t-\xi)^2} \bigg|_{t=0} = e^{\xi^2} \left( \frac{\partial}{\partial \xi} \right)^n e^{-\xi^2}$$

This is Rodrigues’ formula, which can also be cast in the form of the recursion relation:

$$H_{n+1}(\xi) = e^{\xi^2} \left( \frac{d}{d\xi} \right) e^{-\xi^2} H_n(\xi).$$  \hspace{1cm} (7)
v) **Mehler’s formula:** From the Gaussian integral formula one has immediately the following result:

\[ e^{-\xi^2} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2+2ix\xi} \, dx \]

and inserting this into Rodrigues’ formula we get:

\[ H_n(\xi) = e^{\xi^2} \left( -\frac{d}{d\xi} \right)^n \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2+2ix\xi} \, dx = \frac{1}{\sqrt{\pi}} e^{\xi^2} \int_{-\infty}^{\infty} (-2ix)^n e^{-x^2+2ix\xi} \, dx \]

which provides us with an *integral representation* for the Hermite polynomials. To obtain Mehler’s formula we use this representation as follows:

\[
\sum_{n=0}^{\infty} \frac{t^n}{2^n n!} H_n(\xi) H_n(\eta) = \sum_{n=0}^{\infty} \frac{t^n}{2^n n!} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy (-2ix)^n (-2iy)^n e^{-(x-i\xi)^2-(y-i\eta)^2} \\
= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy e^{-(x-i\xi)^2-(y-i\eta)^2} \frac{(-2txy)^n}{n!} \\
= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \exp \left[ -(x-i\xi)^2 - (y-i\eta)^2 - 2txy \right] \\
= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx e^{-(x-i\xi)^2+2itx\eta-2t^2x^2} \int_{-\infty}^{\infty} dy e^{-(y-i\eta+tx)^2} \\
= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx e^{-(1-t^2)x^2+\xi^2+2ix(\xi-t\eta)} = \frac{1}{\sqrt{1-t^2}} \exp \left[ \frac{\xi^2 - ((\xi-t\eta)^2)}{1-t^2} \right]
\]

from which Mehler’s formula follows immediately:

\[
\sum_{n=0}^{\infty} \frac{t^n}{2^n n!} H_n(\xi) H_n(\eta) = \frac{1}{\sqrt{1-t^2}} \exp \left( \frac{2t\xi\eta - t^2(\xi^2 + \eta^2)}{1-t^2} \right). \tag{8}
\]

The completeness relation for the quantum oscillator eigenfunctions of Handout #5 follows by setting \(1 - t^2 = \varepsilon\) and taking the limit \(\varepsilon \to 0\), using the representation of the Dirac \(\delta\)-function:

\[
\delta(x) = \lim_{\varepsilon \to 0} \frac{1}{\sqrt{\pi \varepsilon}} e^{-x^2/\varepsilon},
\]

(see Appendix A).