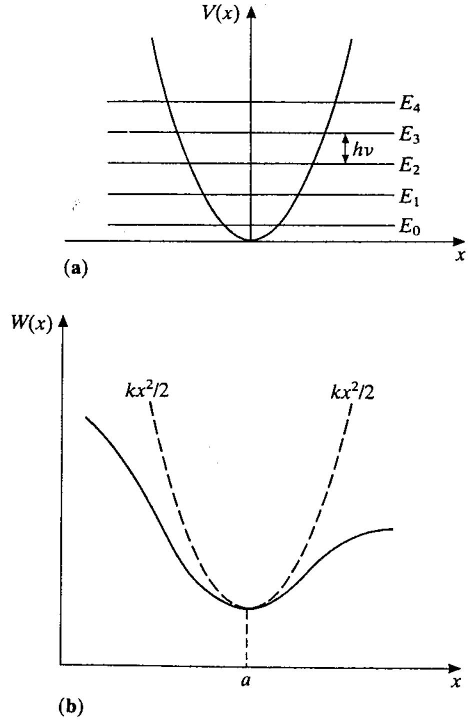
Ur Bransden & Joachain, "Introduction to quantum mechanics", Longman Scientific 1989

4.7 THE LINEAR HARMONIC OSCILLATOR

We shall now study the one-dimensional motion of a particle of mass m which is attracted to a fixed centre by a force proportional to the displacement from that centre. Thus, choosing the origin as the centre of force, the restoring force is given by $F = -kx$ (Hooke's law), where k is the force constant. This force can thus be represented by the potential energy

$$V(x) = \tfrac{1}{2}kx^2 \qquad [4.119]$$

which is shown in Fig. 4.16(a). Such a parabolic potential is of great importance in quantum physics as well as in classical physics, since it can be used to approximate an arbitrary continuous potential $W(x)$ in the vicinity of a stable equilibrium position at $x = a$ (see Fig. 4.16(b)). Indeed, if we expand $W(x)$ in



4.16 (a) The parabolic potential well $V(x) = \frac{1}{2}kx^2$. This is the potential of the linear harmonic oscillator. Also shown are the first few energy eigenvalues [4.143]. (b) A continuous potential well $W(x)$ can be approximated in the vicinity of a stable equilibrium position at $x = a$ by a linear harmonic oscillator potential.

a Taylor series about $x = a$, we have

$$W(x) = W(a) + (x-a)W'(a) + \tfrac{1}{2}(x-a)^2 W''(a) + \dots \qquad [4.120a]$$

with

$$W'(a) = \left(\frac{dW(x)}{dx}\right)_{x=a}, \qquad W''(a) = \left(\frac{d^2W(x)}{dx^2}\right)_{x=a}. \qquad [4.120b]$$

Because $W(x)$ has a minimum at $x = a$ we have $W'(a) = 0$ and $W''(a) > 0$. Choosing a as the origin of coordinates and $W(a)$ as the origin of the energy scale, we see that the harmonic oscillator potential [4.119] (with $k = W''(a)$) is the first approximation to $W(x)$. The linear harmonic oscillator is therefore the prototype for systems in which there exist small vibrations about a point of stable equilibrium. This will be illustrated in Chapter 10 for the case of the vibrational motion of nuclei in molecules.

As the potential energy for a linear harmonic oscillator is given by [4.119], the corresponding Hamiltonian operator is

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2 \qquad [4.121]$$

and the Schrödinger eigenvalue equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}kx^2\psi(x) = E\psi(x). \qquad [4.122]$$

Clearly, all eigenfunctions correspond to bound states of positive energy. It is convenient to rewrite [4.122] in terms of dimensionless quantities. To this end we first introduce the dimensionless eigenvalues

$$\lambda = \frac{2E}{\hbar\omega} \qquad [4.123]$$

where

$$\omega = \left(\frac{k}{m}\right)^{1/2} \qquad [4.124]$$

is the angular frequency of the corresponding classical oscillator. We shall also use the dimensionless variable

$$\xi = \alpha x \qquad [4.125]$$

where

$$\alpha = \left(\frac{mk}{\hbar^2}\right)^{1/4} = \left(\frac{m\omega}{\hbar}\right)^{1/2}. \qquad [4.126]$$

The Schrödinger equation [4.122] then becomes

$$\frac{d^2\psi(\xi)}{d\xi^2} + (\lambda - \xi^2)\psi(\xi) = 0. \qquad [4.127]$$

Let us first analyse the behaviour of ψ in the asymptotic region $|\xi| \to \infty$. For any finite value of the total energy E the quantity λ becomes negligible with respect to ξ^2 in the limit $|\xi| \to \infty$, so that in this limit equation [4.127] reduces to

$$\left(\frac{d^2}{d\xi^2} - \xi^2\right)\psi(\xi) = 0. \qquad [4.128]$$

For large enough $|\xi|$ it is readily verified that the functions

$$\psi(\xi) = \xi^p e^{\pm \xi^2/2} \qquad [4.129]$$

satisfy the equation [4.128] so far as the leading terms (which are of order $\xi^2\psi$) are concerned, when p has any finite value. Because the wave function ψ must be bounded everywhere, including at $\xi = \pm\infty$, the physically acceptable solution must contain only the minus sign in the exponent. The asymptotic analysis therefore suggests looking for solutions to equation [4.127] which are valid for all ξ having the form

$$\psi(\xi) = e^{-\xi^2/2} H(\xi) \qquad [4.130]$$

where $H(\xi)$ are functions which must not affect the asymptotic behaviour of ψ. Substituting [4.130] into [4.127] we obtain for $H(\xi)$ the differential equation

$$\frac{d^2 H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + (\lambda - 1)H = 0 \qquad [4.131]$$

which is called the *Hermite equation.*

In order to solve this equation, let us expand $H(\xi)$ in a power series in ξ. Since the harmonic oscillator potential [4.119] is such that $V(-x) = V(x)$, we know from our discussion of Section 4.5 that the eigenfunctions $\psi(x)$ of the Schrödinger equation [4.122] must have a definite parity. We shall therefore consider separately the even and odd states.

Even states

For these states we have $\psi(-\xi) = \psi(\xi)$ and also, therefore, $H(-\xi) = H(\xi)$, so that we can write for $H(\xi)$ the power series

$$H(\xi) = \sum_{k=0}^{\infty} c_k \xi^{2k}, \qquad c_0 \neq 0 \qquad [4.132]$$

which contains only *even* powers of ξ. Substituting [4.132] into the Hermite equation [4.131], we find that

$$\sum_{k=0}^{\infty} [2k(2k-1)c_k \xi^{2(k-1)} + (\lambda - 1 - 4k)c_k \xi^{2k}] = 0 \qquad [4.133]$$

or

$$\sum_{k=0}^{\infty} [2(k+1)(2k+1)c_{k+1} + (\lambda - 1 - 4k)c_k]\xi^{2k} = 0. \qquad [4.134]$$

This equation will be satisfied provided the coefficient of each power of ξ separately vanishes, so that we obtain the *recursion relation*

$$c_{k+1} = \frac{4k + 1 - \lambda}{2(k+1)(2k+1)} c_k. \qquad [4.135]$$

Thus, given $c_0 \neq 0$, all the coefficients c_k can be determined successively by using the above equation. We have therefore obtained a series representation of the even solution [4.132] of the Hermite equation.

If this series does not terminate, we see from [4.135] that for large k

$$\frac{c_{k+1}}{c_k} \sim \frac{1}{k}. \qquad [4.136]$$

This ratio is the same as that of the series for $\xi^{2p}\exp(\xi^2)$, where p has a finite value. Using [4.130], we then find that the wave function $\psi(\xi)$ has an asymptotic behaviour of the form

$$\psi(\xi) \underset{|\xi|\to\infty}{\sim} \xi^{2p} e^{\xi^2/2} \qquad [4.137]$$

which is obviously unacceptable. The only way to avoid this divergence of $\psi(\xi)$ at large $|\xi|$ is to require that the series [4.132] *terminates*, which means that $H(\xi)$ must be a *polynomial* in the variable ξ^2. Let the highest power of ξ^2 appearing in this polynomial be ξ^{2N}, where $N = 0, 1, 2, \ldots$, is a positive integer or zero. Thus in [4.132] we have $c_N \neq 0$, while the coefficient c_{N+1} must vanish. Using the recursion relation [4.135] we see that this will happen if and only if λ takes on the discrete values

$$\lambda = 4N + 1, \qquad N = 0, 1, 2, \ldots. \qquad [4.138]$$

To each value $N = 0, 1, 2, \ldots$, of N will then correspond an even function $H(\xi)$ which is a polynomial of order $2N$ in ξ, and an even, physically acceptable, wave function $\psi(\xi)$ which is given by [4.130].

Odd states

In this case we have $\psi(-\xi) = -\psi(\xi)$, and hence $H(-\xi) = -H(\xi)$. Thus we begin by writing for $H(\xi)$ the power series

$$H(\xi) = \sum_{k=0}^{\infty} d_k \xi^{2k+1}, \qquad d_0 \neq 0 \qquad [4.139]$$

which contains only *odd* powers of ξ. Substituting [4.139] into the Hermite equation [4.131], we obtain for the coefficients d_k the recursion relation

$$d_{k+1} = \frac{4k+3-\lambda}{2(k+1)(2k+3)} d_k. \qquad [4.140]$$

For large k we have $d_{k+1}/d_k \sim k^{-1}$, so that the wave function $\psi(\xi)$, given by [4.130], will again diverge at large $|\xi|$ unless the series [4.139] for $H(\xi)$ terminates. Let the highest power of ξ in [4.139] be ξ^{2N+1}, where $N = 0, 1, 2, \ldots$. Since $d_N \neq 0$, while d_{N+1} is required to vanish, we see from the recursion relation [4.140] that λ must take one of the discrete values

$$\lambda = 4N + 3, \qquad N = 0, 1, 2, \ldots. \qquad [4.141]$$

To each value $N = 0, 1, 2, \ldots$, of N will then correspond an odd function $H(\xi)$ which is a polynomial of order $2N+1$ in ξ, and an odd, physically acceptable wave function $\psi(\xi)$ given by [4.130].

Energy levels

Putting together the results which we have obtained for the even and odd cases, we see from [4.138] and [4.141] that the eigenvalue λ must take on one of the discrete values

$$\lambda = 2n + 1, \qquad n = 0, 1, 2, \ldots \qquad [4.142]$$

where the quantum number n is a positive integer or zero. Using [4.123] we therefore find that the energy spectrum of the linear harmonic oscillator is given by

$$\begin{aligned} E_n &= (n + \tfrac{1}{2})\hbar\omega \\ &= (n + \tfrac{1}{2})h\nu, \qquad n = 0, 1, 2, \ldots \end{aligned} \qquad [4.143]$$

where $\nu = \omega/2\pi$ is the frequency of the corresponding classical oscillator.

In contrast with classical mechanics, which predicts that the energy E of a linear harmonic oscillator can have any value, we see from [4.143] that its quantum mechanical energy spectrum consists of an infinite sequence of *discrete* levels (see Fig. 4.16(a)). For any finite eigenvalue [4.143] the particle is *bound.* The energy levels [4.143] are equally spaced and are similar to those discovered in 1900 by Planck for the radiation field modes (see Section 1.1). This is due to the fact that a decomposition of the electromagnetic field into normal modes is essentially a decomposition into uncoupled harmonic oscillators. We notice, however, that according to [4.143] the linear harmonic oscillator even in its lowest state ($n = 0$), has the energy $\hbar\omega/2$. The finite value $\hbar\omega/2$ of the ground-state energy level, which is called the *zero-point energy* of the linear harmonic oscillator, is clearly also a quantum phenomenon. As in the case of the infinite square well discussed in Section 4.5, the existence of this zero-point energy is directly related to the uncertainty principle (see Problem 4.12). In classical mechanics the lowest possible energy of the oscillator would of course

be zero, corresponding to the particle being at rest at the origin, but in quantum mechanics this is forbidden by the uncertainty relation (2.70). We also remark that the eigenvalues [4.143] are *non-degnerate*, since for each value of the quantum number n there exists only one eigenfunction (apart from an arbitrary multiplicative constant); this is in agreement with the observation, already made, that one-dimensional bound states are non-degenerate.

Hermite polynomials

Let us now return to the wave functions $\psi(\xi)$. Using [4.130] and collecting our results for both even and odd cases, we see that the physically acceptable solutions of equation [4.127], corresponding to the eigenvalues [4.142], are given by

$$\psi_n(\xi) = e^{-\xi^2/2} H_n(\xi) \qquad [4.144]$$

where the functions $H_n(\xi)$ are polynomials of order n. Both $\psi_n(\xi)$ and $H_n(\xi)$ have the parity of n. Moreover, the polynomials $H_n(\xi)$ satisfy the Hermite equation [4.131] with $\lambda = 2n + 1$, namely

$$\frac{d^2 H_n}{d\xi^2} - 2\xi \frac{dH_n}{d\xi} + 2nH_n = 0. \qquad [4.145]$$

The polynomials $H_n(\xi)$ are called *Hermite polynomials*. It is clear from the foregoing discussion that they are uniquely defined, except for an arbitrary multiplicative constant. This constant is traditionally chosen so that the highest power of ξ appears with the coefficient 2^n in $H_n(\xi)$. This is consistent with the following definition of the Hermite polynomials:

$$H_n(\xi) = (-1)^n e^{\xi^2} \frac{d^n e^{-\xi^2}}{d\xi^n}. \qquad [4.146]$$

The first few Hermite polynomials, obtained from [4.146], are

$$\begin{aligned} H_0(\xi) &= 1 \\ H_1(\xi) &= 2\xi \\ H_2(\xi) &= 4\xi^2 - 2 \\ H_3(\xi) &= 8\xi^3 - 12\xi \\ H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12 \\ H_5(\xi) &= 32\xi^5 - 160\xi^3 + 120\xi. \end{aligned} \qquad [4.147]$$

Note that the definition [4.146] implies that $H_n(\xi)$ has n real zeros.

Another definition of the Hermite polynomials $H_n(\xi)$, which is equivalent to [4.146] involves the use of a *generating function* $G(\xi, s)$. That is

$$G(\xi, s) = e^{-s^2+2s\xi} = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n. \qquad [4.148]$$

This relation means that if the function $\exp(-s^2 + 2s\xi)$ is expanded in a power series in s, the coefficients of successive powers of s are just $1/n!$ times the Hermite polynomials $H_n(\xi)$. Using the generating function [4.148] it is straightforward to prove (Problem 4.13) that the Hermite polynomials satisfy the recursion relations

$$H_{n+1}(\xi) - 2\xi H_n(\xi) + 2nH_{n-1}(\xi) = 0 \qquad [4.149]$$

and

$$\frac{dH_n(\xi)}{d\xi} = 2nH_{n-1}(\xi). \qquad [4.150]$$

The lowest-order differential equation for H_n which can be constructed from these two recursion relations is then readily seen to be the equation [4.145] satisfied by the Hermite polynomials. Moreover, the equivalence of the two definitions [4.146] and [4.148] of the Hermite polynomials can be proved by using both expressions for $G(\xi, s)$ given in [4.148], differentiating n times with respect to s, and then letting s tend to zero (Problem 4.14).

The wave functions for the linear harmonic oscillator

Using [4.144], we see that to each of the discrete values E_n of the energy, given by [4.143], there corresponds one, and only one, physically acceptable eigenfunction, namely

$$\psi_n(x) = N_n e^{-\alpha^2 x^2/2} H_n(\alpha x) \qquad [4.151]$$

where we have returned to our original variable x. Both $H_n(\alpha x)$ and $\psi_n(x)$ have the parity of n and have n real zeros. The quantity N_n, written on the right of [4.151] is a constant which (apart from an arbitrary phase factor) can be determined by requiring that the wave function [4.151] be normalised to unity. That is

$$\int_{-\infty}^{+\infty} |\psi_n(x)|^2 dx = \frac{|N_n|^2}{\alpha} \int_{-\infty}^{+\infty} e^{-\xi^2} H_n^2(\xi) d\xi = 1. \qquad [4.152]$$

In order to evaluate the integral on the right of [4.152], we consider the generating function $G(\xi, s)$ given by [4.148] as well as the second generating function

$$G(\xi, t) = e^{-t^2+2t\xi} = \sum_{m=0}^{\infty} \frac{H_m(\xi)}{m!} t^m. \qquad [4.153]$$

Using [4.148] and [4.153], we may then write

$$\int_{-\infty}^{+\infty} e^{-\xi^2} G(\xi, s) G(\xi, t) d\xi = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{s^n t^m}{n! m!} \int_{-\infty}^{+\infty} e^{-\xi^2} H_n(\xi) H_m(\xi) d\xi. \qquad [4.154]$$

Since

$$\int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{\pi} \qquad [4.155]$$

the integral on the left-hand side of [4.154] is simply

$$\int_{-\infty}^{+\infty} e^{-\xi^2} e^{-s^2+2s\xi} e^{-t^2+2t\xi} d\xi = e^{2st} \int_{-\infty}^{+\infty} e^{-(\xi-s-t)^2} d(\xi - s - t) = \sqrt{\pi} e^{2st} = \sqrt{\pi} \sum_{n=0}^{\infty} \frac{(2st)^n}{n!}. \qquad [4.156]$$

Equating the coefficients of equal powers of s and t on the right-hand sides of [4.154] and [4.156], we find that

$$\int_{-\infty}^{+\infty} e^{-\xi^2} H_n^2(\xi) d\xi = \sqrt{\pi} 2^n n! \qquad [4.157]$$

and

$$\int_{-\infty}^{+\infty} e^{-\xi^2} H_n(\xi) H_m(\xi) d\xi = 0, \qquad n \neq m. \qquad [4.158]$$

From [4.152] and [4.157] we see that apart from an arbitrary complex multiplicative factor of modulus one the normalisation constant N_n is given by

$$N_n = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!}\right)^{1/2} \qquad [4.159]$$

so that the normalised linear harmonic oscillator eigenfunctions are given by

$$\psi_n(x) = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!}\right)^{1/2} e^{-\alpha^2 x^2/2} H_n(\alpha x). \qquad [4.160]$$

Moreover, the result [4.158] implies that

$$\int_{-\infty}^{+\infty} \psi_n^*(x) \psi_m(x) dx = 0, \qquad n \neq m \qquad [4.161]$$

so that the (real) harmonic oscillator wave functions $\psi_n(x)$ and $\psi_m(x)$ are *orthogonal* if $n \neq m$, in agreement with the fact that they correspond to non-degenerate energy eigenvalues.