2.5. ELEMENTARY SOLUTIONS TO SCHRÖDINGER’S WAVE EQUATION

The energy eigenvalue is

\[ E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left( \frac{2\pi}{L} \right)^2 (n_x^2 + n_y^2 + n_z^2) \]  

The six-fold degeneracy we mentioned earlier corresponds to the six combinations of \((\pm n_x, \pm n_y, \pm n_z)\), but the degeneracy can actually be much larger since, in some cases, there are various combinations of \(n_x, n_y, \) and \(n_z\) which can give the same \(E\). In fact, in the (realistic) limit where \(L\) is very large, there can be a large number of states \(N\) which have an energy between \(E\) and \(E + dE\). This “density of states” \(dN/dE\) is an important quantity for calculations of processes which include free particles.

To calculate the density of states, imagine a spherical shell in \(k\) space with radius \(|k| = 2\pi|x|/L\) and thickness \(d|k| = 2\pi d|x|/L\). All states within this shell have energy \(E = \hbar^2 k^2/2m\). The number of states \(dN\) within this shell is \(4\pi x^2 d|x|\). Therefore

\[
\frac{dN}{dE} = \frac{4\pi x^2 d|x|}{\hbar^2 |k| d|k| / m} = \frac{4\pi}{\hbar^2 m} \left( \frac{L}{2\pi} \right)^2 \frac{|k|}{\hbar^2} \frac{L}{2\pi} = \frac{m^{3/2} E^{1/2} L^3}{\sqrt{2\pi} \hbar^3} \]

(2.5.10)

In a typical “real” calculation, the density of states will be multiplied by some probability that involves \(u_E^*(x)u_E(x)\). In this case, the factors of \(L^3\) will cancel explicitly, so the limit \(L \to \infty\) is trivial. This “big box” normalization also yields the correct answer for the probability flux. Rewriting (2.4.21) with this normalization, we have

\[ \psi(x,t) = \frac{1}{L^{3/2}} \exp \left( i \frac{p \cdot x - iEt}{\hbar} \right) \]

(2.5.11)

in which case we find

\[ j(x,t) = \frac{\hbar}{m} \text{Im}(\psi^* \nabla \psi) = \frac{\hbar k}{m L^2} = \psi \rho \]

(2.5.12)

where \(\rho = 1/L^3\) is indeed the probability density.

**The Simple Harmonic Oscillator**

We saw an elegant solution for the case \(V(x) = m\omega^2 x^2/2\) in Section 2.3, which yielded the energy eigenvalues, eigenstates, and wave functions. Here, we demonstrate a different approach which solves the differential equation

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} u_E(x) + \frac{1}{2} m\omega^2 x^2 u_E(x) = E u_E(x) \]

(2.5.13)

Our approach will introduce the concept of generating functions, a generally useful technique which arises in many treatments of differential eigenvalue problems.

First, transform (2.5.13) using the dimensionless position \(y \equiv x/x_0\) where \(x_0 \equiv \sqrt{\hbar/m\omega}\). Also introduce a dimensionless energy variable \(\varepsilon \equiv 2E/\hbar\omega\). The differential equation we need to solve becomes therefore

\[ \frac{d^2}{dy^2} u(y) + (\varepsilon - y^2) u(y) = 0 \]

(2.5.14)

For \(y \to \pm \infty\), the solution must tend to zero, otherwise the wave function will not be normalizable and hence unphysical. The differential equation \(w''(y) - y^2 w(y) = 0\) has solutions \(w(y) \propto \exp(\pm y^2/2)\), so we would have to choose the minus sign. We then “remove” the asymptotic behavior of the wave function by writing

\[ u(y) = h(y) e^{-y^2/2} \]

(2.5.15)

where the function \(h(y)\) satisfies the differential equation

\[ \frac{d^2 h}{dy^2} - 2y \frac{dh}{dy} + (\varepsilon - 1) h(y) = 0 \]

(2.5.16)

To this point, we have followed the traditional solution of the simple harmonic oscillator as found in many textbooks. Typically, one would now look for a series solution for \(h(y)\) and discover that a normalizable solution
is only possible if the series terminates. (In fact, we use this approach for the three dimensional isotropic harmonic oscillator in this book. See Section 3.7.) One forces this termination by imposing the condition that \( \varepsilon - 1 \) be an even, non-negative integer \( 2n, n = 0, 1, 2, \ldots \). The solutions are then written using the resulting polynomials \( h_n(y) \). Of course, \( \varepsilon - 1 = 2n \) is equivalent to \( E = (n + \frac{1}{2})\hbar \omega \), the quantization relation (2.3.22).

Let us take a different approach. Consider the “Hermite polynomials” \( H_n(x) \) defined by the “generating function” \( g(x, t) \) through

\[
g(x, t) = e^{-t^2 + 2xt} = \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!}
\]

Some properties of the \( H_n(x) \) are immediately obvious. For example, \( H_0(x) = 1 \). Also, since

\[
g(0, t) = e^{-t^2} = \sum_{n=0}^{\infty} (-1)^n \frac{n!}{(n/2)!} t^n \]

it is clear that \( H_n(0) = 0 \) if \( n \) is odd, since this series only involves even powers of \( t \). On the other hand, if we restrict ourselves to even values of \( n \), we have

\[
g(0, t) = e^{-t^2} = \sum_{n=0}^{\infty} (-1)^{n/2} \frac{n!}{(n/2)!} t^n
\]

and so \( H_n(0) = (-1)^{n/2} n! / (n/2)! \). Also, since \( g(-x, t) \) reverses the sign only on terms with odd powers of \( t \), \( H_n(-x) = (-1)^n H_n(x) \).

We can take derivatives of \( g(x, t) \) to build the Hermite polynomials using recursion relations between them and their derivatives. For example

\[
\frac{\partial g}{\partial x} = 2xg(x, t) = \sum_{n=0}^{\infty} 2H_n(x) \frac{t^n}{n!} = \sum_{n=0}^{\infty} 2(n+1)H_n(x) \frac{t^{n+1}}{(n+1)!}
\]

or

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

Comparing (2.5.20) and (2.5.21) shows that

\[
H_n'(x) = 2nH_{n-1}(x)
\]

This is enough information for us build the Hermite polynomials:

\[
H_0(x) = 1
\]

so \( H_1'(x) = 2 \), therefore \( H_1(x) = 2x \)

so \( H_2'(x) = 8x \), therefore \( H_2(x) = 4x^2 - 2 \)

so \( H_3'(x) = 24x^2 - 12 \), therefore \( H_3(x) = 8x^3 - 12x \)

\[
\ldots
\]

So far, this is just a curious mathematical exercise. To see why it is relevant to the simple harmonic oscillator, consider the derivative of the generating function with respect to \( t \):

\[
\frac{\partial g}{\partial t} = -2tg(x, t) + 2xg(x, t)
\]

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

\[
= -\sum_{n=0}^{\infty} 2nH_{n-1}(x) \frac{t^n}{n!} + \sum_{n=0}^{\infty} 2xH_n(x) \frac{t^n}{n!}
\]

or

\[
\sum_{n=0}^{\infty} nH_n(x) \frac{t^{n-1}}{n!} = \sum_{n=0}^{\infty} H_{n+1}(x) \frac{t^n}{n!}
\]

Comparing (2.5.23) and (2.5.24) give us the recursion relation

\[
H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)
\]
which we combine with (2.5.22) to find
\[
H_n^\prime\prime(x) = 2n \cdot 2(n - 1)H_{n-2}(x) \\
= 2n[2xH_{n-1}(x) - H_n(x)] \\
= 2xH_n^\prime(x) - 2nH_n(x)
\] (2.5.26)

In other words, the Hermite polynomials satisfy the differential equation
\[
H_n^\prime(x) - 2xH_n^\prime(x) + 2nH_n(x) = 0
\] (2.5.27)
where \( n \) is a non-negative integer. This, however, is the same as the Schrödinger equation written as (2.5.16) since \( \varepsilon - 1 = 2n \). That is, the wave functions for the simple harmonic oscillator are given by
\[
u_n(x) = H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)e^{-m\omega^2/2\hbar}
\] (2.5.28)

Generating functions have a usefulness that far outreaches our limited use here. Among other things, many of the orthogonal polynomials which arise from solving the Schrödinger equation for different potentials, can be derived from generating functions. The interested reader is encouraged to pursue this further, probably best from any one of many excellent texts on mathematical physics.

The Linear Potential

Perhaps the first potential energy function, with bound states, to come to mind is the linear potential, namely
\[
V(x) = k|x|
\] (2.5.29)
where \( k \) is an arbitrary positive constant. Given a total energy \( E \), this potential has a classical turning point at a value \( x = a \) where \( E = ka \). This point will be important for understanding the quantum behavior of a particle of mass \( m \) bound by this potential.

The Schrödinger equation becomes
\[
\frac{\hbar^2}{2m} \frac{d^2u_E}{dx^2} + k|x|u_E(x) = Eu_E(x)
\] (2.5.30)
It is easiest to deal with the absolute value by restricting our attention to \( x \geq 0 \). We can do this because \( V(-x) = V(x) \), so there are two types of solutions, namely \( u_E(-x) = \pm u_E(x) \). In either case, we need \( u_E(x) \) to tend towards zero as \( x \to \infty \). If \( u_E(-x) = -u_E(x) \), then we need \( u_E(0) = 0 \). On the other hand, if \( u_E(-x) = +u_E(x) \), then we have \( u_E(0) = 0 \), since \( u_E(\varepsilon) - u_E(-\varepsilon) \equiv 0 \), even for \( \varepsilon \to 0 \). (As we will discuss in Chapter 4, we refer to these solutions as “odd” and “even” parity.)

Once again, we write the differential equation in terms of dimensionless variables, based on appropriate scales for length and energy. In this case, the dimensionless length scale is \( x_0 = (\hbar^2/mk)^{1/3} \) and the dimensionless energy scale is \( E_0 = kx_0 = (\hbar^2k^2/m)^{1/3} \). Defining \( y \equiv x/x_0 \) and \( \varepsilon \equiv E/E_0 \) allows us to rewrite (2.5.30) as
\[
\frac{d^2u_E}{dy^2} - 2(y-\varepsilon)u_E(y) = 0 \quad y \geq 0
\] (2.5.31)
Notice that \( y = \varepsilon \) when \( x = E/k \), i.e. the classical turning point \( x = a \). In fact, defining a translated position variable \( z \equiv 2^{1/3}(y-\varepsilon) \), (2.5.31) becomes
\[
\frac{d^2u_E}{dz^2} - zu_E(z) = 0
\] (2.5.32)
This is the Airy Equation, and the solution is the Airy Function \( Ai(z) \), plotted in Figure 2.1. The Airy Function has a peculiar behavior, oscillatory for negative values of the argument, and decreasing rapidly towards zero for positive values. Of course, we are exactly the behavior we expect for the wave function, since \( z = 0 \) is the classical turning point.

Note that the boundary conditions at \( x = 0 \) translate into zeros for either \( Ai'(z) \) or \( Ai(z) \) where \( z = -2^{1/3}\varepsilon \). In other words, the zeros of the Airy Function or its derivative determine the quantized energies. One finds that
\[
\begin{align*}
Ai'(z) &= 0 \quad \text{for } z = -1.019, -3.249, -4.820, \ldots \quad \text{(even)} \quad (2.5.33) \\
Ai(z) &= 0 \quad \text{for } z = -2.338, -4.088, -5.521, \ldots \quad \text{(odd)} \quad (2.5.34)
\end{align*}
\]