Contents

List of Figures

Chapter 3

Solutions to the One-Dimensional Schrödinger Equation II

3.1 The Harmonic Oscillator

The harmonic oscillator potential is one of the most important problems in physics. This is not simply because it is soluble in terms of familiar functions with simple properties, but also because it is usually the first approximation when a particle is bound to a finite region in space. In the neighborhood of a potential minimum, an analytic potential can be represented by a Taylor series:

$$V(x) = V(x_0) + \left[\frac{dV}{dx}\right]_{x_0}(x - x_0) + \frac{1}{2}\left[\frac{d^2V}{dx^2}\right]_{x_0}(x - x_0)^2 + \cdots \tag{3.1}$$

If x_0 is a point where the potential is minimum, then the second term vanishes. Since a potential is always arbitrary within a constant, we can ignore the first term. If we denote the value of the second derivative at $x = x_0$ by the symbol k:

$$V(x) = \frac{1}{2}k(x - x_0)^2 + c_2(x - x_0)^3 + \tag{3.2}$$

Unless the second derivative is 0, there is always some region in the neighborhood of x_0 in which the harmonic oscillator terms dominates the rest of the terms in the series. The infinite square well is an example of a potential that does not meet this requirement. Practically any real potential will satisfy it. In classical mechanics this feature motivates the study of *small motions*, i.e. the behavior of systems where the amplitude of motion about an equilibrium point is small enough that the higher order terms in the Taylor expansion can be ignored.

The separated S.E. that accompanies this potential is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}kx^2\psi(x) = E\psi(x) \tag{3.3}$$

Since the potential rises to infinity for both positive and negative values of x, all the states of a particle will be bound states. Moreover, since $V_{min} = 0$, the energies $E > 0$.

Just as for the classical oscillator it is convenient to define a constant ω such that $k = m\omega^2$. In classical mechanics ω is the angular frequency of the oscillator:

$$\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - \frac{m\omega^2}{2}x^2\psi(x) + E\psi(x) = 0 \tag{3.4}$$

We then divide through by $\hbar\omega/2$ to obtain:

$$\frac{\hbar}{m\omega}\frac{d^2\psi(x)}{dx^2} - \frac{m\omega}{\hbar}x^2\psi(x) + \frac{2E}{\hbar\omega}\psi(x) = 0 \tag{3.5}$$

Expressing E in units of $\hbar\omega$ by defining $K = \frac{E}{\hbar\omega}$:

$$\frac{\hbar}{m\omega}\frac{d^2\psi(x)}{dx^2} + (2K - \frac{m\omega}{\hbar}x^2)\psi(x) = 0 \tag{3.6}$$

Solution by conversion to a dimensionless equation

The standard solution to the harmonic oscillator is obtained in terms of a dimensionless variable:

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x \tag{3.7}$$

$$\frac{d\psi}{dx} = \frac{d\psi}{d\xi}\sqrt{\frac{m\omega}{\hbar}}$$

$$\frac{d^2\psi}{dx^2} = \frac{m\omega}{\hbar}\frac{d^2\psi}{d\xi^2}$$

By substitution:

$$\frac{d^2\psi}{d\xi^2} + (2K - \xi^2)\psi(\xi) = 0 \tag{3.8}$$

To solve this we first examine the behavior for $\xi^2 >> K$:

$$\frac{d^2\psi(\xi)}{d\xi^2} = \xi^2\psi(u) \tag{3.9}$$

The solutions of this equation are:

$$e^{\pm\xi^2/2} \tag{3.10}$$

Only the solution with the negative sign is physically possible. This choice is a Gaussian function. Let us try to find the solution with this asymptotic behavior by defining a new function, $f(\xi)$:

$$\psi(\xi) = f(\xi)e^{-\xi^2/2} \tag{3.11}$$

where $f(\xi)$ does not need to vanish as $\xi^2 \to \infty$. All we require is that $f(\xi)e^{-\xi^2/2} \to 0$ as $\xi^2 \to \infty$. In terms of f, the derivatives of $\psi(\xi)$ are:

$$\frac{d\psi}{d\xi} = (f' - \xi f)e^{-\xi^2/2} \tag{3.12}$$

$$\frac{d^2\psi}{d\xi^2} = -(f' - \xi f)\xi e^{-\xi^2/2} + (f'' - \xi f' - 1)f)e^{-\xi^2/2} \tag{3.13}$$

$$= \left(f'' - 2\xi f' + (\xi^2 - 1)f\right) e^{-\xi^2/2} \tag{3.14}$$

Substituting this expression for $\frac{d^2\psi}{d\xi^2}$ into the D.E. we obtain a differential equation for $f(\xi)$:

$$\left(f'' - 2\xi f' + (\xi^2 - 1)f + (2K - \xi^2)f\right) e^{-\xi^2/2} = 0 \tag{3.15}$$

so that:

$$f'' - 2\xi f' + (2K - 1)f = 0 \tag{3.16}$$

We will try to solve this equation in the form of an infinite series:

$$f = \sum_{j=0}^{\infty} c_j\xi^j \tag{3.17}$$

$$f' = \sum_{j=1}^{\infty} jc_j\xi^{j-1} \tag{3.18}$$

$$\xi f' = \sum_{j=1} jc_j\xi^j = \sum_{j=0} jc_j\xi^j \tag{3.19}$$

$$f'' = \sum_{j=2} j(j-1)c_j\xi^{j-2} = \sum_{j=0}(j+1)(j+2)c_{j+2}\xi^j \tag{3.20}$$

By substitution into the D.E.:

$$\sum_{j=0}[c_{j+2}(j+1)(j+2)\xi^j - 2jc_j\xi^j + (2K-1)c_j\xi^j] = 0 \tag{3.21}$$

For this solution to be valid for all ξ, the coefficient of every power of ξ must vanish. This means that:

$$c_{j+2} = c_j\frac{1-2K+2j}{(j+1)(j+2)} \tag{3.22}$$

Provided we specify two constants, c_0 and c_1, all the remaining coefficients in the series are determined by this recursion relation. These two arbitrary constants are what we expect for the solution of a second order differential equation. One of them multiplies a function represented as an infinite series of odd powers of ξ and the other an infinite series of even powers of ξ. These two series provide two linearly independent solutions.

Of course, an infinite series is not useful if it doesn't converge. We can check convergence using the ratio test, comparing two successive terms, s_n and s_{n+2} in the series:

$$\frac{s_{n+2}}{s_n} = \frac{(1-2K+2n)\xi^2}{(n+1)(n+2)}$$

For $n >> K$ and $n >> 1$:

$$\frac{s_{n+2}}{s_n} \to \frac{2n\xi^2}{n^2} = \frac{2\xi^2}{n}$$

For any finite value of ξ:

$$\lim_{n\to\infty}\frac{s_{n+2}}{s_n} = 0$$

According to the ratio test both the even and odd infinite series converge for any finite value of ξ.

What is the behavior of the solutions as $\xi \to \infty$. The ratio of the coefficients of successive terms in either series for large j is:

$$\frac{c_{j+2}}{c_j} \to \frac{2j}{(j+1)(j+2)} \to \frac{2}{j} \tag{3.23}$$

But this is just the relation for the series expansion of the function, e^{ξ^2}, which diverges as $\xi \to \infty$. Asymptotically both solutions for $f(\xi)$ diverge at infinity like e^{ξ^2}. Since these solutions are multiplied by $e^{-\xi^2/2}$ to obtain $\psi(x)$, we see that both of the independent solutions for ψ diverge like $e^{\xi^2/2}$. Thus, there seem to be no normalizable solutions to the harmonic oscillator potential. But, wait a minute! Notice that if any constant c_{j+2} should vanish, all the higher order constants will also vanish, and the infinite sum will become a polynomial of order j, $P_j(\xi)$. Then:

$$\psi(\xi) = P_j(\xi)e^{-\xi^2/2}, \qquad \lim \xi^2 \to \infty \psi(\xi) = 0$$

By examining the recursion relation, we see that $c_{n+2} = 0$ if $K = n+1/2$, reducing the infinite series to a polynomial of order n. If n is even, the even solution is:

$$f_e = c_0 + c_2\xi^2 + c_4\xi^4 + \cdots + c_n\xi^n$$

but the odd series that starts with $c_1\xi$ does not terminate. For this case we must set $c_1 = 0$. Similarly, if we choose an odd value for n:

$$f_o = c_1\xi + c_3\xi^3 + c_5\xi^5 + \cdots + c_n\xi^n$$

but the even solution does not terminate so we must set $c_0 = 0$. Other choices for K will not permit a normalizable solution.

The parameter K was defined as $E/(\hbar\omega)$, so the allowed values of energy are:

$$E = (n + 1/2)\hbar\omega, \qquad n = 0, 1, 2, \cdots \tag{3.24}$$

These are the allowed energies for the quantum mechanical solution to the harmonic oscillator potential. Unlike the n^2 behavior of the energy levels for the square well, the energy levels for the harmonic oscillator are evenly spaced, separated by steps of $\Delta E = \hbar\omega$. For even values of n the solutions are even functions of ξ and for odd values they are odd functions of ξ. The polynomials for different values of n are orthogonal. The lowest possible energy is $E_0 = \frac{1}{2}\hbar\omega$, which is therefore the ground state energy of the harmonic oscillator. Consistent with the uncertainty principle, the oscillator cannot be in a state of 0 energy, for which the expectation values of both the momentum and position would be identically 0.

Solutions for f:

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x \tag{3.25}$$

$$\psi = f(\xi)e^{-\frac{m\omega}{2\hbar}x^2} \tag{3.26}$$

Setting $K = n + 1/2$

$$c_{j+2} = -2c_j\frac{n-j}{(j+1)(j+2)}, \qquad j \leq n \tag{3.27}$$

$$\frac{c_{j+2}}{c_j} = -2\frac{n-j}{(j+1)(j+2)} \tag{3.28}$$

- n=0: $f = c_0$, $\quad \psi = c_0 e^{-\frac{m\omega x^2}{2\hbar}}$
- n=1: $f = c_1\xi$, $\quad \psi = c_1 x e^{-\frac{m\omega x^2}{2\hbar}}$
- n=2; $f = c_0(1-2\xi^2)$, $\quad \psi = c_0(1-\frac{2m\omega}{\hbar}x^2)e^{-\frac{m\omega x^2}{2\hbar}}$
- n=3: $f = c_1\xi(1-\frac{2}{3}\xi^2)$, $\quad \psi = c_1 x(1-\frac{2m\omega}{3\hbar}x^2)e^{-\frac{m\omega x^2}{2\hbar}}$

The ground-state wave function is:

$$\psi_0 = c_0 e^{-\frac{m\omega x^2}{2\hbar}} \tag{3.29}$$

The probability distribution is:

$$P(x) = \psi^*\psi = |c_0|^2 e^{-\frac{m\omega x^2}{\hbar}} \tag{3.30}$$

This is a Gaussian with a standard deviation for the probability distribution of x given by:

$$\sigma_x^2 = \frac{\hbar}{2m\omega} \tag{3.31}$$

To normalize the distribution:

$$|c_0|^2 = \frac{1}{\sqrt{2\pi\sigma_x^2}} = \sqrt{\frac{m\omega}{\pi\hbar}} \tag{3.32}$$

For this state, both $\langle x\rangle$ and $\langle p\rangle$ are zero. After calculating $\langle x^2\rangle$ and $\langle p^2\rangle$ one can show that:

$$\sigma_x\sigma_p = \hbar/2 \tag{3.33}$$

The higher the oscillator frequency (the greater the oscillator strength), the less the uncertainty in position for the ground state and the greater the uncertainty in momentum.

As polynomials in ξ, the solutions are known as the Hermite polynomials. The advantage of writing the solution in terms of $H_n(\xi)$ is that the functions have been thoroughly studied and there are many useful formulas relating them. Traditionally, the Hermite polynomials are normalized so that the coefficient of the highest power is 2^n. This convention, of course, precedes the invention of quantum mechanics. The stationary states are:

$$\psi_n(x) = A_n H_n(\xi)e^{-\frac{m\omega}{2\hbar}x^2} \tag{3.34}$$

At this point we have solved the harmonic oscillator problem in terms of a complete set of orthogonal states. Any physical state can be represented as linear combination of these states. Using the usual procedures one can calculate the expectation value of any physical observable.

3.1.1 Solution of the H.O. using ladder operators

In operator form the Schrödinger Equation is:

$$\left(\frac{p_x^2}{2m}+\frac{m\omega^2}{2}x^2\right)\psi=E\psi \tag{3.35}$$

where I use p_x to indicate explicitly that the momentum operator is a derivative with respect to x. The equation can be shortened to:

$$H\psi=E\psi \tag{3.36}$$

where:

$$H\equiv\left(\frac{p_x}{\sqrt{2m}}\right)^2+\left(\sqrt{\frac{m}{2}}\omega x\right)^2 \tag{3.37}$$

If we treat this operator equation like ordinary Algieba we can factor the lhs into:

$$H=\left(\frac{p_x}{\sqrt{2m}}-i\sqrt{\frac{m}{2}}\omega x\right)\left(\frac{p_x}{\sqrt{2m}}+i\sqrt{\frac{m}{2}}\omega x\right) \tag{3.38}$$

However, since $p_x=\frac{\hbar}{i}\frac{\partial}{\partial x}$ is a derivative operator that acts on x as well as on any function to the right, this algebra isn't right. Nevertheless, something very interesting happens if we push ahead with this idea. Define the two operators, a_+ and a_-, by:

$$a_\pm=\frac{p_x}{\sqrt{2m}}\pm i\sqrt{\frac{m}{2}}\,\omega x \tag{3.39}$$

The products of the two operators are:

$$a_-a_+=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2-i\frac{\omega}{2}(xp_x-p_xx)=H-i\frac{\omega}{2}(xp_x-p_xx)=H-\frac{i\omega}{2}[x,p_x]$$

and:

$$a_+a_-=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2+i\frac{\omega}{2}(xp_x-p_xx)=H+\frac{i\omega}{2}[x,p_x]$$

where the symbol $[x,p] \equiv xp - px$ is called the *commutator* of the two operators. For ordinary algebraic quantities the commutator is 0, but it need not be for operators. For any function $f(x)$:

$$[x,p_x]f(x) = (xp_x - p_x x)f(x) = \frac{\hbar}{i}\left(x\frac{df}{dx} - \frac{d(xf)}{dx}\right) = \frac{\hbar}{i}\left(x\frac{df}{dx} - x\frac{df}{dx} - f\right)$$
$$= i\hbar f \tag{3.40}$$

Since the function $f(x)$ is arbitrary, we can write:

$$[x,p_x] = i\hbar \tag{3.41}$$

The commutator of x and p_x is fundamental to the algebra of quantum mechanics. It is easy to extend the result to three dimensions:

$$\begin{cases} [x,p_x] = [y,p_y] = [z,p_z] = i\hbar; \\ [x,p_y] = [x,p_z] = [y,p_x] = [y,p_z] = [z,p_x] = [z,p_y] = 0. \end{cases} \tag{3.42}$$

Using the commutation relation:

$$a_-a_+ = H + \frac{\hbar\omega}{2} \tag{3.43}$$

Similarly, we can show that:

$$a_+a_- = H - \frac{\hbar\omega}{2} \tag{3.44}$$

so that:

$$[a_-,a_+] = \hbar\omega \tag{3.45}$$

Now suppose there is some energy E for which there is a stationary state ψ_E such that $H\psi_E = E\psi_E$. Operating on this state with a_-a_+:

$$a_-a_+\psi_E = E\psi_E + \frac{1}{2}\hbar\omega\psi_E = (E + \frac{1}{2}\hbar\omega)\psi_E \tag{3.46}$$

Applying a_+ to both sides of this equation:

$$a_+a_-a_+\psi_E = (E + \frac{1}{2}\hbar\omega)a_+\psi_E \tag{3.47}$$

Now, $a_+\psi_E$ is itself some function of x, call it $f(x)$:.

$$a_+a_-f(x) = (E + \frac{1}{2}\hbar\omega)f(x) \tag{3.48}$$

or:

$$(H - \frac{\hbar\omega}{2})f(x) = (E + \frac{1}{2}\hbar\omega)f(x) \tag{3.49}$$

so that:

$$Hf(x) = (E + \hbar\omega)f(x) \tag{3.50}$$

We see that $f(x)$ is a stationary state solution to the Schrödinger Equation for the energy $E' = E + \hbar\omega$:

$$f(x) = a_+\psi_E = \alpha\psi_{E+\hbar\omega} \tag{3.51}$$

where α is some constant that may depend on E, and $\psi_{E+\hbar\omega}$ is the solution of the Schrödinger Equation for $E' = E + \hbar\omega$.

By the same process we can show that:

$$a_-\psi_E = \beta\psi_{E-\hbar\omega} \tag{3.52}$$

where β is another constant that may depend on E. The operators a_+ and a_- allow us to start from the stationary state solution for any energy, E, and work our way up and down from there obtaining solutions for higher and lower energies ad infinitum. For this reason, they are called *ladder operators.* After each ladder operation we would need to normalize the result by adjusting the proportionality constants.

But it looks like we can start from a valid stationary state and continue the lowering process to negative energies. Since the potential is everywhere positive, a negative energy implies imaginary momentum, which is non-physical. To prevent this, there must be a lowest energy, $E_0 \geq 0$, for which:

$$a_-\psi_0 = 0 \tag{3.53}$$

But:

$$H\psi_0 = (a_+a_- + \frac{1}{2}\hbar\omega)\psi_0 = E_0\psi_0 \tag{3.54}$$

Using the condition that $a_-\psi_0 = 0$:

$$\frac{1}{2}\hbar\omega\psi_0 = E_0\psi_0 \tag{3.55}$$

so:

$$E_0 = \frac{1}{2}\hbar\omega \tag{3.56}$$

Using only an algebraic argument we have deduced the ground state energy of the harmonic oscillator. Once we find the ground state wave function we can apply the raising operator to obtain successively higher energy states, separated by $\Delta E = \hbar\omega$. No other energies are possible. If there were a state at some energy not in this sequence we could apply the lowering operator indefinitely to reach negative energies.

To get the ground state, we need only solve the first order differential equation:

$$a_{-}\psi_0 = 0 \tag{3.57}$$

Using the definition of a_{-} from Eq. 3.39:

$$\left(\frac{p_x}{\sqrt{2m}} - i\sqrt{\frac{m}{2}}\omega x\right)\psi_0 = 0 \tag{3.58}$$

Multiplying through by $\sqrt{2m}$ and setting $p_x = -i\hbar\frac{d}{dx}$, this reduces to:

$$\frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar}x\psi_0 \tag{3.59}$$

After dividing by ψ_0, we get:

$$\frac{d\ln(\psi_0)}{dx} = -\frac{m\omega}{\hbar}x \tag{3.60}$$

Integrating this first order differential equation:

$$\ln(\psi_0) = \frac{m\omega}{2\hbar}x^2 \tag{3.61}$$

so that:

$$\psi_0 = Ae^{-\frac{m\omega x^2}{2\hbar}} \tag{3.62}$$

Example

The ground state wave function is $\psi_0 = Ae^{-\alpha x^2}$, where $\alpha = m\omega/(2\hbar)$. Applying the raising operator:

$$\psi_1 = C\left(\frac{p_x}{\sqrt{2m}} + i\sqrt{\frac{m\omega^2}{2}}x\right)\psi_0 \tag{3.63}$$

$$\psi_1 = C\frac{\hbar}{i\sqrt{2m}}\frac{d\psi_0}{dx} + iC\sqrt{\frac{m\omega^2}{2}}x\psi_0 \tag{3.64}$$

$$\psi_1 = C\frac{\hbar}{i\sqrt{2m}}(-2\alpha x)\psi_0 + iC\sqrt{\frac{m\omega^2}{2}}x\psi_0 = iC\left(\frac{2\hbar\alpha}{\sqrt{2m}} + \sqrt{\frac{m\omega^2}{2}}\right)x\psi_0 \tag{3.65}$$

$$\psi_1 = c_1xe^{-\alpha x^2} \tag{3.66}$$

We can get the normalization constant c_1 from a general formula (see the problems) or by setting $\int_{-\infty}^{\infty}|\psi_1(x)|^2\,dx = 1$.

3.2 Free Particle

A solution to the Schrödinger Equation for a free particle is more difficult than one might at first expect. The separated equation is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \tag{3.67}$$

Since $V = 0$, we know that $E > 0$, we can define a positive constant k^2 as:

$$2mE/\hbar^2 = \frac{p^2}{\hbar^2} = k^2, \qquad p = \hbar k, \qquad E = \frac{\hbar^2 k^2}{2m}$$

The Schrödinger Equation becomes:

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \tag{3.68}$$

For a single choice of E, the solutions are $\sin(kx)$ and $\cos(kx)$. which are not normalizable. A free particle with a unique energy is not a possibility.

Let us imagine that the particle is in a square well, and consider the limit as the walls get so far apart that we can ignore them. For the square well, we used the boundary condition that the wave function should vanish at the walls. However, if the walls are going to recede to infinity, this boundary condition is no longer relevant. Therefore we will keep both the sine and cosine functions associated with a particular energy and expand a free particle wave function as a linear sum of solutions with different energies. The solutions are limited to sines and cosines with discrete values of $k_n = n\pi x/a$.

From Fourier analysis any periodic function defined in the range, $-a \leq x \leq a$, can be represented by the series:

$$f(x) = \bar{f} + \sum_{n=1}^{\infty}\left[a_n \sin(n\pi x/a) + b_n \cos(n\pi x/a)\right] \tag{3.69}$$

where $\bar{f}$ is the average value of $f(x)$, and:

$$a_n = \frac{1}{a}\int_{-a}^{a} f(x)\ \sin(n\pi x/a)\, dx$$

$$b_n = \frac{1}{a}\int_{-a}^{a} f(x)\ \cos(n\pi x/a)\, dx$$

Using the exponential representation for the sine and cosine functions:

$$\sin(n\pi x/a) = \frac{e^{i\frac{n\pi}{a}x} - e^{-i\frac{n\pi}{a}x}}{2i} \tag{3.70}$$

and:

$$\cos(n\pi x/a) = \frac{e^{i\frac{n\pi}{a}x} + e^{-i\frac{n\pi}{a}x}}{2} \tag{3.71}$$

$$f(x) = \bar{f} + \sum_{n=1}^{\infty} \frac{1}{2}\left[(b_n - ia_n)e^{i\frac{n\pi}{a}x} + (b_n + ia_n)e^{-i\frac{n\pi}{a}x}\right]$$

$$f(x) = \bar{f} + \frac{1}{2}\sum_{m=1}^{\infty}(b_m - ia_m)e^{i\frac{n\pi}{a}x}\frac{1}{2} + \sum_{m=-\infty}^{-1}(b_{-m} + ia_{-m})e^{i\frac{m\pi}{a}x}$$

$$= \sum_{m=-\infty}^{\infty} c_m e^{i\frac{m\pi}{a}x} \tag{3.72}$$

where for $m > 0$:

$$c_m = \frac{b_m - ia_m}{2} = \frac{1}{2a}\int_{-a}^{a}\left[\cos(\frac{m\pi x}{a}) - i\sin(m\pi xa)\right] f(x)\,dx$$

$$= \frac{1}{2a}\int_{-a}^{a} e^{-i\frac{m\pi}{a}x} f(x)\,dx$$

and for $m < 0$,

$$c_m = \frac{b_{-m} + ia_{-m}}{2} = \frac{1}{2a}\int_{-a}^{a}\left[\cos(-\frac{m\pi x}{a}) + i\sin(-\frac{m\pi x}{a})\right] f(x)\,dx$$

$$= \frac{1}{2a}\int_{-a}^{a}\left[\cos(\frac{m\pi x}{a}) - i\sin(\frac{m\pi x}{a})\right] f(x)\,dx = \frac{1}{2a}\int_{-a}^{a} e^{-i\frac{m\pi}{a}x} f(x)\,dx$$

The formulas for c_m for both the positive and negative integers can be combined into:

$$c_m = \frac{1}{2a}\int_{-a}^{a} e^{-i\frac{m\pi}{a}x}\, f(x)\,dx \tag{3.73}$$

Notice that the $m = 0$ term accounts for $\bar{f}$, since:

$$c_0 = \frac{1}{2a}\int_{-a}^{a} f(x)\,dx = \bar{f}$$

If the function $f(x)$ is complex $(f(x) = g(x) + ih(x))$ where $g(x)$ and $h(x)$ are real functions, we can write a separate Fourier series of the form of Eq. 3.69 for g and h. When we combine these into an equation for $f(x)$, we will get a result that looks just like eqn. 3.69, but the coefficients a_n and b_n will be complex numbers. The above analysis therefore works equally well for real and complex functions.

For a free particle we want the limit as $a \to \infty$. We begin by observing that successive values of $n\pi/a$ are separated by π/a, which goes to 0 as $a \to \infty$. Let us denote:

$$k_n = n\pi/a, \qquad \Delta k = \pi/a \tag{3.74}$$

If we imagine the values of k_n lying on a k axis, we see that as $a \to \infty$, the points get more and more crowded with the interval between each one diminishing to 0. Thus as we let the walls go to infinity the values of k become continuously distributed. We can write the spacing in k as:

$$\Delta k \equiv \frac{\pi}{a} \to 0 \tag{3.75}$$

We can re-express the Fourier sum by defining $c(k_n) = c_n$ and inserting $1 = a\Delta k/\pi$:

$$f(x) = \sum_{k_n=-\infty}^{\infty} c(k_n) e^{ik_n x} \left(\frac{a}{\pi}\right) \Delta k \tag{3.76}$$

Next, define $b(k) = \frac{a}{\pi} c(k)$:

$$f(x) = \sum_{k_n=-\infty}^{\infty} b(k_n) e^{ik_n x} \Delta k \tag{3.77}$$

where:

$$b(k_n) = \frac{a}{\pi} c_n = \frac{1}{2\pi} \int_{-a}^{a} f(x) e^{-ik_n x}\, dx$$

In the limit of $\Delta k \to 0$, the sum goes over into an integral:

$$f(x) \to \int_{-\infty}^{\infty} b(k) e^{ikx}\; dk \tag{3.78}$$

and:

$$b(k) \to \frac{1}{2\pi} \int_{-\infty}^{\infty} f(x) e^{-ikx}\, dx$$

We can make this symmetrical by defining:

$$F(k) = \sqrt{2\pi}\, b(k) \tag{3.79}$$

so that:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx}\; dk \tag{3.80}$$

and:

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx}\, dx$$

Equations 3.80 and 3.2 are the generalizations of the Fourier series from a finite region in x to the entire x axis. Equations 3.80 can still be thought of as a linear sum of states of different energies E_i where the energies have become continuously distributed. The function $F(k)$ plays the role of the linear expansion coefficients, and is called the *Fourier transform* of the function $f(x)$. Since the relationship between the two functions is symmetrical, they are usually called the Fourier transform of each other.

In the discrete linear sums previously used we learned that the n^{th} component is to be multiplied by $e^{-iE_n t/\hbar}$. This time dependence carries over to the integral form so that for each component $\phi(k)$ we must multiply by $e^{iE(k)t/\hbar}$ to get the solution for $t > 0$. Using:

$$E = \frac{k^2\hbar^2}{2m} > 0$$

and defining:

$$\omega = E/\hbar \tag{3.81}$$

the general time-dependent solution for the free-particle is:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} e^{-i\omega t}\, dk \tag{3.82}$$

One can show by direct substitution that $\Psi(x,t)$ defined in equation 3.82 satisfies the time-dependent Schrödinger Equation for any choice of $\phi(k)$. For a particular choice of the initial wave function:

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx}\, dx \tag{3.83}$$

We can equally well write the Fourier transforms explicitly in terms of x, p and E:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(p) e^{\frac{i}{\hbar}(px - Et)}\, dk \tag{3.84}$$

$$\phi(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-i\frac{p}{\hbar}x}\, dx \tag{3.85}$$

Example: A Gaussian wave packet

Consider the following normalized wave-function:

$$\psi(x) = \left(\frac{1}{2\pi\sigma_x^2}\right)^{1/4} e^{-\frac{x^2}{4\sigma_x^2}} = \alpha e^{-\beta^2 x^2} \tag{3.86}$$

where:

$$\alpha \equiv \left(\frac{1}{2\pi\sigma_x^2}\right)^{1/4}, \qquad \beta^2 \equiv \frac{1}{4\sigma_x^2} \tag{3.87}$$

This represents a wave packet with $\langle x \rangle = 0$ and a standard deviation of σ_x. The Fourier transform is:

$$\phi(k) = \frac{\alpha}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{(-\beta^2 x^2 - ikx)}\, dx \tag{3.88}$$

Completing the square in the exponential:

$$\phi(k) = \frac{\alpha}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e - [\beta x - ik/(2\beta)]^2 e^{-k^2/(4\beta^2)} dx \tag{3.89}$$

$$= \frac{\alpha}{\sqrt{2\pi}} e^{-k^2/(4\beta^2)} \int_{-\infty}^{\infty} e^{-[\beta x - ik/(2\beta)]^2} dx \tag{3.90}$$

Letting $u = \beta x - ik/(2\beta)$:

$$\phi(k) = \frac{\alpha}{\sqrt{2\pi}} e^{-k^2/(4\beta^2)} \int_{-\infty}^{\infty} e^{-u^2} du/\beta = \frac{\alpha}{\beta\sqrt{2\pi}} e^{-k^2/(4\beta^2)} \sqrt{\pi} \tag{3.91}$$

$$= \frac{\alpha}{\beta\sqrt{2}} e^{-\frac{k^2}{4\beta^2}} \tag{3.92}$$

Substituting in the definition of α:

$$\phi(k) = \left(\frac{1}{2\pi\sigma_x^2}\right)^{1/4} \frac{1}{\beta\sqrt{2}} e^{-\frac{k^2}{4\beta^2}} \tag{3.93}$$

Expressing σ_x in terms of β:

$$\phi(k) = \left(\frac{2\beta^2}{\pi}\right)^{1/4} \frac{1}{\beta\sqrt{2}} e^{-\frac{k^2}{4\beta^2}} = \left(\frac{1}{2\pi\beta^2}\right)^{1/4} e^{-\frac{k^2}{4\beta^2}} \tag{3.94}$$

This is exactly the same form that we started with for $\psi(x)$. The square of the distribution $|\phi(k)|^2$ is normalized over the region of k running from $-\infty$ to ∞, so it probably is not too difficult to imagine that it is the probability distribution for values of k. In fact the function plays the same role as the c_n's did in the infinite square well problem. The probability distribution is a Gaussian function with standard deviation $\sigma_k = \beta = 1/(2\sigma_x)$. Thus:

$$\sigma_k \sigma_x = \frac{1}{2} \tag{3.95}$$

If we use $p = \hbar k$, we obtain:

$$\sigma_p \sigma_x = \frac{\hbar}{2} \tag{3.96}$$

which is the minimum value allowed by the Heisenberg uncertainty principle.

For this wave-function $\langle x \rangle = 0$, and $\langle p \rangle = 0$. We can put the particle into uniform motion by modifying $\phi(k)$ to shift the centroid to a non-zero value:

$$\phi(k) = \left(\frac{2\beta^2}{\pi}\right)^{1/4} \frac{1}{\beta\sqrt{2}} e^{-\frac{(k-k_0)^2}{4\beta^2}} = \left(\frac{1}{2\pi\beta^2}\right)^{1/4} e^{-\frac{(k-k_0)^2}{4\beta^2}} \tag{3.97}$$

We can now use this as the transform of the wave-function to obtain at $t = 0$:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx}\, dk = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2\pi\beta^2}\right)^{1/4} \int_{-\infty}^{\infty} e^{-\frac{(k-k_0)^2}{4\beta^2}}\, e^{ikx}\, dk \tag{3.98}$$

Now let $\kappa = k - k_0$, so that:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx}\, dk = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2\pi\beta^2}\right)^{1/4} \int_{-\infty}^{\infty} e^{-\frac{\kappa^2}{4\beta^2}}\, e^{i(\kappa+k_0)x}\, d\kappa \tag{3.99}$$

Now let $\kappa = k - k_0$, so that:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx}\, dk = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2\pi\beta^2}\right)^{1/4} e^{ik_0x} \int_{-\infty}^{\infty} e^{-\frac{\kappa^2}{4\beta^2}}\, e^{i\kappa x}\, d\kappa \tag{3.100}$$

Again, using the trick of completing the square in the exponential:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2\pi\beta^2}\right)^{1/4} e^{ik_0x} \int_{-\infty}^{\infty} e^{-(\frac{\kappa}{2\beta} - i\beta x)^2}\, d\kappa\; e^{-\beta^2x^2} \tag{3.101}$$

Substituting $u = \frac{\kappa}{2\beta} - i\beta x$:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2\pi\beta^2}\right)^{1/4} e^{ik_0x}\; 2\beta\; e^{-\beta^2x^2} \int_{-\infty}^{\infty} e^{-u^2}\, du \tag{3.102}$$

The integral is $\sqrt{\pi}$. Collecting the terms:

$$\psi(x) = \left(\frac{2\beta^2}{\pi}\right)^{1/4} e^{ik_0 x}\ e^{-\beta^2 x^2} \tag{3.103}$$

Using the definition $2\beta^2 \equiv \frac{1}{2\sigma_x^2}$:

$$\psi(x) = \left(\frac{1}{2\pi\sigma^2}\right)^{1/4} e^{ik_0 x}\ e^{-x^2/(4\sigma^2)} \tag{3.104}$$

which is the same as before except for the additional term involving k_0.

The solution for $\Psi(x,t)$ requires still more work, using the form:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx-\omega t)}\ dk \tag{3.105}$$

where ω is a function of k:

$$\omega \equiv \frac{E}{\hbar} = \frac{p^2}{2m\hbar} = \frac{\hbar k^2}{2m} \tag{3.106}$$

3.2.1 Group Velocity

Another problem that we noticed with the single energy wave solutions of the free particle equation was that their phase velocity was half of the particle velocity. Now that we have a solution in terms of a wave packet, it is time to ask how this wave-packet moves in space. If the packet consists of waves spread over a small enough region of k or momentum space, the packet will not spread out so rapidly in time that it quickly becomes meaningless to say it represents a localized particle. We assume that the the function $\phi(k)$ peaks fairly sharply around the value k_0. We then expand $\omega(k)$ in a first order Taylor series around $k = k_0$:

$$\omega = \omega_0 + \left[\frac{d\omega}{dk}\right]_{k_0} (k - k_0) = \omega_0 + \omega'(k - k_0) \tag{3.107}$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx-\omega_O t-\omega'(k-k_0)t)}\ dk \tag{3.108}$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} e^{-i\omega_0 t} \int_{-\infty}^{\infty} \phi(k) e^{i(kx-\omega'(k-k_0)t)}\ dk \tag{3.109}$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} e^{-i\omega_0 t} \int_{-\infty}^{\infty} \phi(k) e^{ik(x-\omega' t)} e^{ik_0\omega' t}\ dk \tag{3.110}$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} e^{-i(\omega_0 - k_0\omega')t} \int_{-\infty}^{\infty} \phi(k) e^{i(k(x-\omega' t)}\ dk \tag{3.111}$$

$$= e^{-i(\omega_0 - k_0\omega')t} F(x - \omega' t) \tag{3.112}$$

The probability distribution is:

$$|\Psi(x,t)|^2 = |F(x - \omega' t)|^2 \tag{3.113}$$

To the degree of validity of our linear approximation for the dependence of frequency on k, we see that the wave packet is constant in time except that it moves with velocity, ω', along the x axis. This analysis holds for any wave-packet that maintains its shape over time. The derivative, ω' is called the group velocity:

$$v_g = \left[\frac{d\omega}{dk}\right]_{k_0} \tag{3.114}$$

For the free-particle solution to the Schrödinger Equation :

$$\omega = \frac{\hbar k^2}{2m}, \qquad v_g = \hbar k_0/m \tag{3.115}$$

Associating the value k_0 with a deBroglie wave, we see that $v_g = p_0/m$. The group velocity is the classical velocity for the central wave number in the wave-packet.

3.3 Scattering

3.3.1 Distinction between scattering and bound states

We have examined the one-dimensional S.E. for particles bound in a finite region of space, and we have developed the solution for a free particle. We now turn to a study of more general potentials, for which it may be possible to find both bound state and unbound states (resembling the free particle solutions discussed above).

An example of a one-dimensional potential that could support both types of states is shown in Fig. 3.1. In classical mechanics a particle with energy $E < 0$ is bound to a region around the orgin inside the well. For $0 \le E < V_m$ the particle is bound if it is inside the well and free but restricted to either positive or negative values of x if it is outside the well. In quantum mechanics the particle is bound only if $E < 0$ if $V \to 0$ as $x \to \pm\infty$. For $E > 0$ the solutions are called scattering states.

Real-life potentials usually go to 0 at infinity. In this case, a particle with positive energy can move from some far distance into the region where

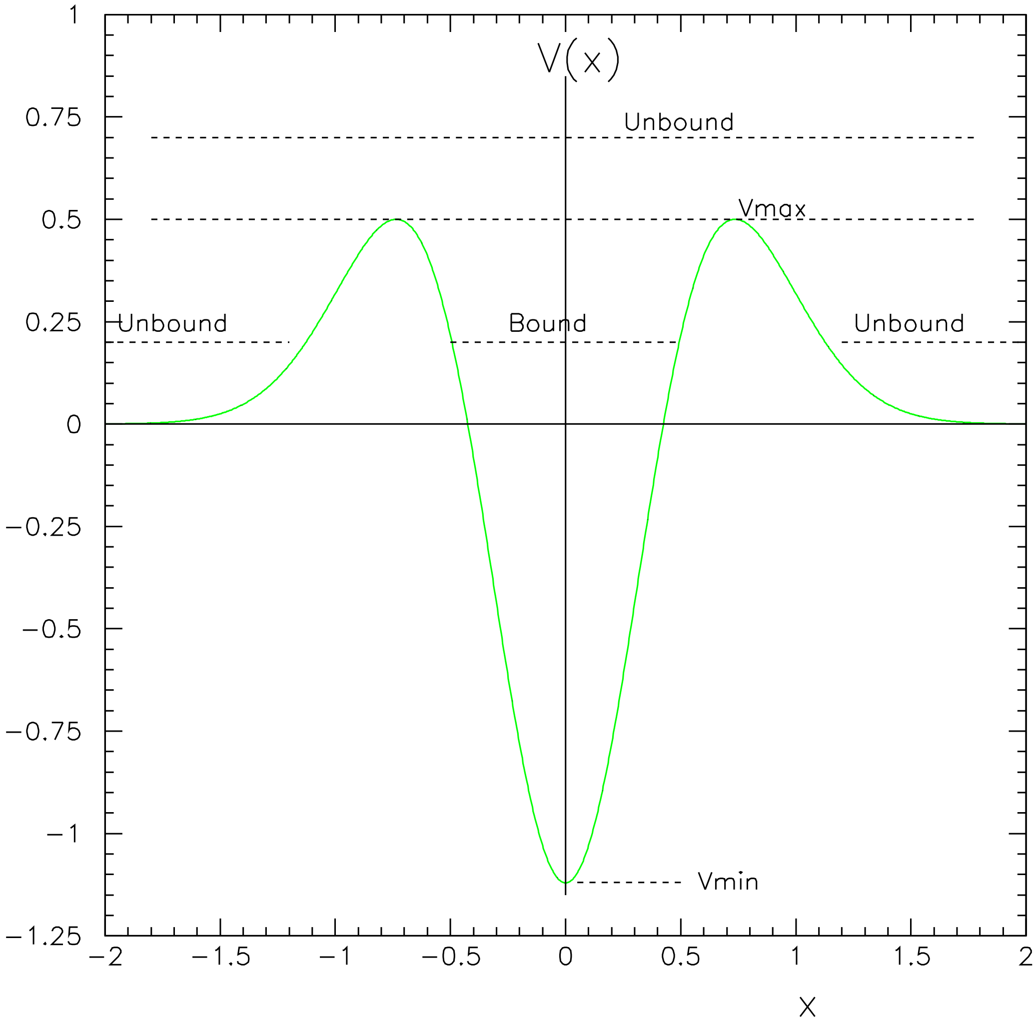

Figure 3.1: A potential that classically has both bound and unbound states. Particles with energy E, $V_{min} \leq E < 0.$ are bound to a region around the origin. If $0 \leq E < V_{max}$ the particles are bound if they are inside the well and free (but restricted to be either on the right side or the left side of the potential barrier) if they are outside the well. If $E \geq V_{max}$ the particles are free and can be anywhere. Quantum mechanically, particles with $V_{min} < E < 0.$ are bound, while particles with $E > 0$ are unbound.

the potential is noticeable, respond to it in some way, and then proceed on to infinity carrying the scars of the interaction. This process is called scattering, and the states representing it are called scattering states. In three dimensions we imagine a beam of particles impinging on a target. The interaction results in waves emerging in all directions from the target. In one dimension, the picture is like a light beam incident normally on a window. Part of the light is reflected and part is transmitted and we describe the process in terms of transmission and reflection coefficients.

For scattering problems we assume that the potential is 0 at infinity. In fact, we usually assume that it exists only in a finite region, and can be ignored everywhere outside this region. Thus, if $E > 0$ we should use free particle solutions of the S.E. outside the region of the potential. Although we know that a free particle cannot be represented by a wave of a single energy and momentum, it is convenient to represent scattering in terms of such waves. We can imagine that the waves describe a continuous stream of particles moving in the x direction. Then the probability of finding a particular particle in some finite region is 0, but the probability of finding some particle is $\rho\, dx$, where ρ is the density of particles in the beam. For a wave-function representing a beam of particles we generally normalize the wave function so that $|\Psi|^2 = \rho$.

In this regard it is interesting to note with this normalization the particle flux is equal to the probability current:

$$J = \frac{i\hbar}{2m}\left[\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right]$$

For $\Psi = \sqrt{\rho}e^{i(kx-\omega t}$:

$$J = \rho\frac{\hbar k}{m} = \rho\frac{p}{m} = \rho v$$

which is just the number of particles per second crossing any point on the x axis. Generally, a measurement would be in the form of the ratio of final amplitude to initial amplitude, so that the normalization drops out anyway.

3.3.2 The Dirac Delta function

Dirac invented a very useful function for dealing with quantum problems. The Dirac Delta function is defined by the following properties:

$$\delta(x - x_0) = 0, \qquad x \neq x_0 \tag{3.116}$$

$$\int_a^b f(x)\delta(x - x_0)\, dx = f(x_0), \qquad a < x_0 < b \tag{3.117}$$

From this integral property we see that the units of the function are the inverse of the units of its argument.

The function has an important property:

$$\delta(a(x-x_0)) = \frac{1}{|a|}\delta(x-x_0) \tag{3.118}$$

Proof: Let $a > 0$. Substitute $u = ax$, so that:

$$\int f(x)\delta(a(x-x_0))\,dx = \frac{1}{a}\int f(\frac{u}{a})\delta(u-u_0)\ du \tag{3.119}$$

$$= \frac{1}{a}f(\frac{u_0}{a}) = \frac{1}{a}f(x_0) = \frac{1}{a}\int f(x)\delta(x-x_0)\,dx \tag{3.120}$$

Let $a < 0$ and substitute $b = -a = |a|$:

$$I = \int x_1{}^{x_2} f(x)\delta(a(x-x_0))\,dx = \int_{x_1}^{x_2} f(x)\delta(-b(x-x_0))\,dx \tag{3.121}$$

Let $u = -b(x-x_0)$ so that $dx = -du/b$. The limits on u are such that $u_1 > 0$ and $u_2 < 0$. Then:

$$I = -\frac{1}{b}\int_{u_1}^{u_2} f(u)\delta(u)\ du = \frac{1}{b}\int_{u_2}^{u_1} f(u)\delta(u)\ du = \frac{1}{b}f(u)|_{u=0} \tag{3.122}$$

When $u = 0$, $x = x_0$ so:

$$I = \frac{1}{b}f(x_0) = \frac{1}{|a|}f(x_0) \tag{3.123}$$

Corollary:

$$\delta(x-x_0) = \delta(x_0-x) \tag{3.124}$$

Mathematicians have proved that the delta function is a valid concept. It is not actually a function, but is what mathematicians call a distribution.

3.3.3 Negative delta function potential

We shall try using the delta function itself as a potential in the Schrödinger Equation :

$$V(x) = -a\delta(x) \tag{3.125}$$

We can think of this as an approximation to a potential confined to a small region in space. The force will act over this entire region, but we imagine thinking of the region as shrinking to a point, and letting the potential become infinite to compensate for this approximation.

Since $\delta(x)$ has units of $1/L$, a must have units of energy times length, $E \cdot L$.

Bound state

Since the potential reaches negative, the theorem that $E > V_{min}$ does not restrict the solutions to positive energies. Let us see if we can find solutions with negative energy (bound states). We could think of these as the bound states in a potential well whose width has shrunk to 0:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - a\delta(x)\psi = E\psi \tag{3.126}$$

$$\frac{d^2\psi}{dx^2} + \frac{2ma}{\hbar^2}\delta(x)\psi = -\frac{2mE}{\hbar^2}\psi \tag{3.127}$$

With $E < 0$, we can define a positive parameter $\kappa^2 = -\frac{2mE}{\hbar^2}$ so that:

$$\frac{d^2\psi}{dx^2} + \frac{2ma}{\hbar^2}\delta(x)\psi = \kappa^2\psi \tag{3.128}$$

The δ function is 0 everywhere except at a single point, so except at $x = 0$ we have:

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi \tag{3.129}$$

The solution of this equation is:

$$\psi = Ae^{\kappa x} + Be^{-\kappa x} \tag{3.130}$$

For the wave function to vanish at $x \to \pm\infty$, we must use:

$$\psi = Ae^{\kappa x}, \qquad x < 0 \tag{3.131}$$

$$\psi = Be^{-\kappa x}, \qquad x > 0 \tag{3.132}$$

For the wave function to be continuous at $x = 0$, $A = B$. To normalize the solution:

$$1 = |A|^2\left(\int_{-\infty}^{0} e^{2\kappa x}dx + \int_0^\infty e^{-2\kappa x}dx\right) = 2|A|^2\int_0^\infty e^{-2\kappa x}dx = |A|^2/\kappa \tag{3.133}$$

so:

$$A = \sqrt{\kappa} \tag{3.134}$$

Our solution has a discontinuity in the derivative at the origin. The δ function specifies the magnitude of that discontinuity. To determine it we integrate the Schrödinger Equation over a very small interval that encloses the origin:

$$\int_{-\epsilon}^{\epsilon} \frac{d^2\psi}{dx^2}\, dx + \frac{2ma}{\hbar^2}\int_{-\epsilon}^{\epsilon} \delta(x)\psi\, dx = \kappa^2 \int_{-\epsilon}^{\epsilon} \psi\, dx \tag{3.135}$$

Integrating this equation:

$$\left[\frac{d\psi}{dx}\right]_{-\epsilon}^{\epsilon} + \frac{2ma}{\hbar^2}\psi(0) = 2\epsilon\kappa^2\psi(0) \tag{3.136}$$

In the limit of $\epsilon \to 0$:

$$\left[\frac{d\psi}{dx}\right]_{-\epsilon}^{\epsilon} = -\frac{2ma}{\hbar^2}\psi(0) \tag{3.137}$$

The discontinuity in the derivative at the origin is therefore:

$$\left(\frac{d\psi}{dx}\right)_{+} - \left(\frac{d\psi}{dx}\right)_{-} = -\frac{2ma}{\hbar^2}\psi(0) \tag{3.138}$$

This condition is satisfied when:

$$-\kappa - \kappa = -\frac{2ma}{\hbar^2} \tag{3.139}$$

$$\kappa = \frac{\sqrt{-2mE}}{\hbar} = \frac{ma}{\hbar^2} \tag{3.140}$$

No matter what its strength the delta function potential has one and only one bound state. The value of this single bound energy depends on the strength of the potential:

$$E = -\frac{ma^2}{2\hbar^2} \tag{3.141}$$

Scattering states

For a wave moving to the right, the solutions are:

$$\Psi = e^{i(kx-\omega t)} \tag{3.142}$$

and for a wave moving to the left, the solution is:

$$\Psi = e^{i(-kx-\omega t)} = e^{-i(kx+\omega t)} \tag{3.143}$$

If particles are incident from the left, there can be reflected waves moving to the left, but on the right side there can only be transmitted waves moving to the right:

$$\Psi = Ae^{i(kx-\omega t)} + Be^{i(-kx-\omega t)}, \qquad x < 0 \tag{3.144}$$

$$\Psi = Ce^{i(kx-\omega t)}, \qquad x > 0 \tag{3.145}$$

The matching conditions at $x = 0$ yield:

$$A + B = C, \qquad ikC - (ikA - ikB) = -\frac{2ma}{\hbar^2}C \tag{3.146}$$

Substituting from the first, $B = C - A$, into the second:

$$ikC - ikA + ik(C - A) = -\frac{2ma}{\hbar^2}C \tag{3.147}$$

$$\frac{C}{A} = \frac{1}{1 - i\frac{ma}{\hbar^2 k}} \tag{3.148}$$

and:

$$\frac{B}{A} = \frac{C}{A} - 1 = -\frac{1}{1 + i\frac{\hbar^2 k}{ma}} \tag{3.149}$$

Since the probability distribution is proportional to the square of the wave function, we can define the transmission probability as:

$$T = |C/A|^2 = \frac{1}{1 + \frac{m^2a^2}{\hbar^4k^2}} \tag{3.150}$$

For large k the transmission approaches 1, and as k goes to 0, the transmission goes to 0. The reflected probability is given by:

$$R = |B/A|^2 = \frac{\frac{m^2a^2}{\hbar^4k^2}}{1 + \frac{m^2a^2}{\hbar^4k^2}} \tag{3.151}$$

We see that $T + R = 1$.

3.3.4 Positive delta function potential

If the potential is positive, the delta function presents a barrier to the incoming wave. With the positive delta function the minimum potential energy is 0 and there are no negative energy solutions(bound states).

For positive energies, we use the same technique as above for the scattering problem. This time the matching conditions at $x = 0$ yield:

$$A + B = C, \qquad A - B = C(1 - \frac{2ma}{i\hbar^2 k}) \tag{3.152}$$

The only change is that we have changed the sign of a. Thus, T and R, which depend on a^2 are unchanged. The scattering from a negative and a positive delta function potential is identical.

3.4 The Finite Square Well

A good approximation to the force between a neutron and a nucleus is given by:

$$V(r) = \begin{cases} -V_0, & r \leq a; \\ 0, & r > a. \end{cases} \tag{3.153}$$

Because of its sharp edges and flat bottom this potential is called a *finite square well*. Its one-dimensional version is:

$$V(x) = -V_0, \qquad -a < x < a, \qquad V = 0 \ \text{ elsewhere} \tag{3.154}$$

We can solve this problem by solving the free-particle problem with separate coefficients in the three regions, $x < -a$, $-a < x < a$, and $x > a$. We match the solutions and their derivatives at the boundaries separating the three regions to get the final solution.

3.4.1 Bound States

For $-V_0 < E < 0$, we require that the wave-function vanish at infinity. Outside the well, where $V = 0$:

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = \kappa^2\psi \tag{3.155}$$

where:

$$\kappa^2 = -\frac{2mE}{\hbar^2} \tag{3.156}$$

the solutions are the same as for the delta function potential:

$$\psi(x) = Ae^{\kappa x}, \qquad x < -a \tag{3.157}$$

$$\psi(x) = Be^{-\kappa x}, \qquad x > a \tag{3.158}$$

Inside the well, where $E > |V_0|$:

$$\frac{d^2\psi}{dx^2} = -\frac{2m(E+V_0)}{\hbar^2}\psi = -k^2\psi \tag{3.159}$$

where:

$$k^2 = \frac{2m(V_0+E)}{\hbar^2} = \frac{2mV_0}{\hbar^2} - \kappa^2 \tag{3.160}$$

and the solutions are sines and cosines:

$$\psi(x) = C\sin(kx) + D\cos(kx). \qquad -a < x < a \tag{3.161}$$

Since the potential is even in x we know that we can write the solutions as even and odd functions. For the even functions, $A = B$, and $C = 0$. For the odd functions, $B = -A$ and $D = 0$. As usual the wave function must be continuous at the edge of the well, and since the well is finite the derivative must also be continuous. Imposing these conditions at $x = a$, the even functions give us:

$$Be^{-\kappa a} = D\cos ka \tag{3.162}$$

$$-\kappa Be^{-\kappa a} = -kD\sin(ka) \tag{3.163}$$

while the odd functions give:

$$Be^{-\kappa a} = C\sin ka \tag{3.164}$$

$$-\kappa Be^{-\kappa a} = kC\cos(ka) \tag{3.165}$$

Two linear homogeneous equations in two unknowns can be solved only for certain values of the coefficients of the unknowns. By taking the ratios of the two equations in each pair, we see that:

$$k\tan(ka) = \kappa, \qquad \text{even solutions} \tag{3.166}$$

and:

$$k\cot(ka) = -\kappa, \qquad \text{odd solutions} \tag{3.167}$$

From Eqn. 3.160 :

$$\frac{\kappa^2}{k^2} = \frac{2mV_0}{\hbar^2 k^2} - 1 \tag{3.168}$$

and two conditions can be written in terms of k as:

$$\tan(ka) = \sqrt{\frac{2mV_0}{\hbar^2 k^2} - 1} = \sqrt{\frac{V_0}{V_0 + E} - 1} \tag{3.169}$$

and:

$$\cot(ka) = -\frac{k}{\kappa} = -\sqrt{\frac{V_0}{V_0 + E} - 1} \tag{3.170}$$

Note that:

$$\frac{V_0}{V_0 + E} > 1, \quad \text{since } E < 0 \tag{3.171}$$

These two conditions can be written more compactly by defining:

$$z^2 \equiv k^2 a^2 = \frac{2ma^2(V_0 + E)}{\hbar^2}, \qquad z_0^2 \equiv (2ma^2 V_0)/(\hbar^2) \tag{3.172}$$

$$\frac{z_0^2}{z^2} = \frac{V_0}{V_0 + E}$$

By substitution:

$$\tan(z) = \sqrt{(z_0/z)^2 - 1}, \qquad \text{even solutions} \tag{3.173}$$

$$\cot(z) = -\sqrt{(z_0/z)^2 - 1} \qquad \text{odd solutions} \tag{3.174}$$

Eqns. 3.173 and 3.174 for z are transcendental and must be solved numerically or graphically. The solutions in z are found by plotting the left and right sides of these equations as functions of z and looking for intersections.

These solutions for $z = ka$ specify the allowed values of:

$$E = \frac{\hbar^2 k^2}{2m} - V_0.$$

Please see the lecture slides posted on the web for the illustrations of graphical solutions.

We obtain solutions only if $z < z_0$, No matter how small z_0 there will be at least one even solution. There is no odd solution unless $z_0 > \pi/2$. The total number of solutions is given by

$$N = \mathrm{Int}(2z_0/\pi) + 1$$

where $\mathrm{Int}(x)$ is the integer part of x.

For a **wide, deep well**, we can find many values of k for which $z_0 >> z$. For the even wave functions the solutions of the transcendental equation occur where $\tan(z)$ is very large so that:

$$z \approx (n - 1/2)\pi, \qquad n = 1, 2 \cdots \qquad \text{even wave} - \text{functions}$$

For the odd wave functions the solutions of the transcendental equation occur where $\tan(z)$ is close to 0 so that:

$$z \approx n\pi, \qquad n = 1, 2 \cdots \qquad \text{odd wave} - \text{functions}$$

We can summarize these solutions in one equation,

$$z \approx l\pi/2, \qquad l = 1, 2 \cdots$$

Inserting the definition of z:

$$z^2 = \frac{2ma^2(V_0 + E)}{\hbar^2} \approx l^2\pi^2/4$$

$$V_0 + E \approx \frac{l^2\hbar^2\pi^2}{8ma^2}$$

$$E \approx -V_0 + \frac{n^2\pi^2\hbar^2}{2m(2a)^2}, \qquad n = 1, 2, 3, \cdots \tag{3.175}$$

where odd values of n are associated with the even solutions and even values of n are associated with the odd solutions. The values of these energies relative to the bottom of the well are the energies associated with the infinite square well of width $2a$. The approximation that $z_0 >> z$ breaks down as $E_n \to 0$.

3.4.2 Scattering States

We can solve the equations for positive energies, using states outside the well corresponding to left-moving and right-moving waves, just as we did for the delta function potential. Inside the well, the wave function is a linear combination of sine and cosine functions. Matching the wave function and its derivative at $x = \pm a$, we can solve for the transmission and reflection coefficients.

$$\Psi = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)} = (Ae^{ikx} + Be^{-ikx})e^{-i\omega t}, \qquad x < -a \tag{3.176}$$

Since the wave function in all three regions will have a common factor of $e^{-i\omega t}$, we can drop that term from the matching conditions and work with:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \qquad x < -a \tag{3.177}$$

$$\psi(x) = C\sin(lx) + D\cos(lx), \qquad -a < x < a \tag{3.178}$$

$$\psi(x) = Fe^{ikx}, \qquad x > a \tag{3.179}$$

For continuity of the wave function and its derivative at $x = \pm a$:

$$Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la) \tag{3.180}$$

$$Fe^{ika} = C\sin(la) + D\cos(la) \tag{3.181}$$

$$ikAe^{-ika} - ikBe^{ika} = l[C\cos(la) + D\sin(la)] \tag{3.182}$$

$$ikFe^{ika} = l[C\cos(la) - D\sin(la)] \tag{3.183}$$

Our goal is to solve for B and F in terms of A. We can simplify the arithmetic by defining some constants:

$$\alpha = \sin(la), \qquad \beta = \cos(la), \qquad \gamma = e^{ika}, \qquad r = \frac{l}{ik} \tag{3.184}$$

$$-\gamma^2 Be - \alpha\gamma C + \beta\gamma D = A$$

$$\alpha C + \beta D + \gamma F = 0$$

$$\gamma^2 B - r\gamma[\beta C + \alpha D] = A$$

$$r\beta C - r\alpha D - \gamma F = 0$$

$$\begin{pmatrix} -\gamma^2 & -\alpha\gamma & \beta\gamma & 0 \\ 0 & \alpha & \beta & \gamma \\ \gamma^2 & -r\gamma\beta & -r\gamma\alpha & 0 \\ 0 & r\beta & -r\alpha & -\gamma \end{pmatrix} \begin{pmatrix} B \\ C \\ D \\ F \end{pmatrix} = A \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

If we denote the matrix by M, the desired solution is obtained by inverting it to obtain:

$$\begin{pmatrix} B \\ C \\ D \\ F \end{pmatrix} = AM^{-1} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

The inverse matrix is:

$$M^{-1} =$$

$$\begin{pmatrix} \frac{r\cos(2la) - r^2\sin(2la)}{2\gamma^2 X_1} & r\frac{1}{2\gamma X_1} & -\frac{\sin(2la) + r\cos(2la)}{2\gamma^2 X_1} & -\frac{r}{2\gamma X_1} \\ -\frac{1}{2\gamma X_3} & \frac{1}{2X_3} & -\frac{1}{2\gamma X_3} & \frac{1}{2X_3} \\ -\frac{1}{2\gamma X_2} & -\frac{1}{2X_2} & -\frac{1}{2\gamma X_2} & -\frac{1}{2X_2} \\ \frac{r}{2\gamma^2 X_1} & \frac{r^2\sin(1la) - r\cos(2la)}{2\gamma X_1} & \frac{r}{2g^2 X_1} & \frac{r\cos(2la) + \sin(2la)}{2\gamma X_1} \end{pmatrix} \tag{3.185}$$

where:

$$X_1 \equiv \frac{1}{2}(r^2 - 1)\sin(2la) - r\cos(2la)$$

$$X_2 = r\sin(la) - \cos(la)$$

$$X_3 = r\cos(la) + \sin(la)$$

From this we obtain:

$$B/A = M^{-1}_{11} + M^{-1}_{13}$$

$$B/A = -e^{-2ika}\frac{(r^2+1)\sin(2la)}{(r^2-1)\sin(2la) - 2r\cos(2la)}$$

Replacing r with its definition from eqns. 3.184:

$$B/A = -e^{-2ika}\frac{(l^2-k^2)\sin(2la)}{(l^2+k^2)\sin(2la) + 2ilk\cos(2la)} \tag{3.186}$$

The reflection coefficient is:

$$R = |B/A|^2 = \frac{(l^2 - k^2)^2 \sin^2(2la)}{(l^2 + k^2)^2 \sin^2(2la) + 4l^2k^2 \cos^2(2la)} \tag{3.187}$$

For the transmitted wave:

$$\begin{aligned} F/A &= M_{41}^{-1} + M_{43}^{-1} \\ &= \frac{r}{g^2 X_1} = 2g^{-2} \frac{r}{(r^2 - 1)\sin(2la) - 2r\cos(2la)} \\ &= -e^{-2ika} \frac{2lk}{2lk\cos(2la) + i(k^2 + l^2)\sin(2la)} \end{aligned} \tag{3.188}$$

The transmission coefficient is:

$$\begin{aligned} T &= |F/A|^2 \\ T^{-1} &= \cos^2(2la) + \frac{(k^2 + l^2)^2}{4l^2k^2} \sin^2(2la) \\ &= 1 + \frac{(k^2 + l^2)^2 - 4l^2k^2}{4l^2k^2} \sin^2(2la) \\ &= 1 + \frac{(k^2 - l^2)^2}{4l^2k^2} \sin^2(2la) \geq 1 \end{aligned} \tag{3.189}$$

If:

$$2la = \frac{2a}{\hbar}\sqrt{2m(E_n + V_0)} = n\pi \tag{3.190}$$

$T = 1$, and the wave passes through the interaction region as if it weren't there. This is the condition for an integer number of half-wave lengths to fit inside the potential well. It is the same condition that we obtained for the stationary states of an infinite square well. For perfect transmission:

$$E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2} \tag{3.191}$$

which are the conditions for the stationary states of the infinite square well. This effect has been observed for the scattering of low energy electrons (≈ 0.7 eV) by rare gas atoms, and is known as the *Ramsauer effect*.