4.1: Bound States

One of the simplest potentials to study the properties of is the so-called *square well potential* (Figure 4.1.1),

$$V(x) = \begin{cases} 0 & |x| > a \\ -V_0 & |x| < a \end{cases}$$

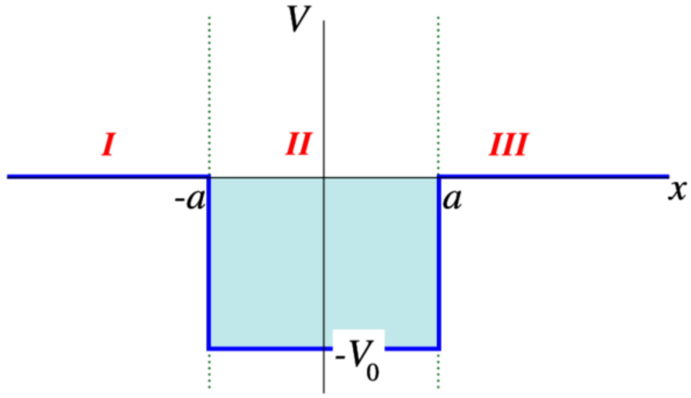

***Figure 4.1.1**: The square well potential*

We define three areas, from left to right in Figure 4.1.1: I, II and III. In areas I and III we have the Schrödinger equation for a free particle

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \tag{4.1.1}$$

whereas in area II we have the equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = (E+V_0)\psi(x) \tag{4.1.2}$$

Solution to a few Ordinary Differential Equations

In this class we shall quite often encounter the ordinary differential equations

$$\frac{d^2}{dx^2}f(x) = -\alpha^2 f(x) \tag{4.1.3}$$

which has as solution

$$f(x) = A_1\cos(\alpha x) + B_1\sin(\alpha x) \tag{4.1.4}$$

$$= C_1 e^{i\alpha x} + D_1 e^{-i\alpha x}, \tag{4.1.5}$$

and

$$\frac{d^2}{dx^2}g(x) = +\alpha^2 g(x) \tag{4.1.6}$$

which has as solution

$$g(x) = A_2\cosh(\alpha x) + B_2\sinh(\alpha x) \tag{4.1.7}$$

$$= C_2 e^{\alpha x} + D_2 e^{-\alpha x}. \tag{4.1.8}$$

Case 1: E> 0

Let us first look at $E > 0$. In that case the equation in regions I and III can be written as

$$\frac{d^2}{dx^2}\psi(x) = -\frac{2m}{\hbar^2}E\psi(x) = -k^2\psi(x), \tag{4.1.9}$$

where

$$k=\sqrt{\frac{2m}{\hbar^2}E} \tag{4.1.10}$$

The solution to this equation is a sum of sines and cosines of kx, which cannot be normalized: Write

$$\psi_{III}(x)=A\cos(kx)+B\sin(kx) \tag{4.1.11}$$

where (A and B can be complex) and calculate the part of the norm originating in region III,

$$\int_a^\infty |\psi(x)|^2 dx \ = \int_a^\infty |A|^2\cos^2 kx+|B|^2\sin^2 kx+2\Re(AB^*)\sin(kx)\cos(kx)dx \tag{4.1.12}$$

$$=\lim_{N\to\infty} N\int_a^{2\pi/k} |A|^2\cos^2(kx)+|B|^2\sin^2(kx) \tag{4.1.13}$$

$$=\lim_{N\to\infty} N\left(\frac{|A|^2}{2}+\frac{|B|^2}{2}\right)=\infty. \tag{4.1.14}$$

We also find that the energy cannot be less than $-V_0$, since we cannot construct a solution for that value of the energy. We thus restrict ourselves to $-V_0<E<0$. We write

$$E=-\frac{\hbar^2}{k^2 2m} \tag{4.1.15}$$

and

$$E+V_0=\frac{\hbar^2\kappa^2}{2m}. \tag{4.1.16}$$

The solutions in the areas I and III are of the form ($i=1,\ 3$)

$$\psi(x)=A_i e^{kx}+B_i e^{-kx}. \tag{4.1.17}$$

In region II we have the oscillatory solution

$$\psi(x)=A_2\cos(\kappa x)+B_2\sin(\kappa x). \tag{4.1.18}$$

Now we have to impose the conditions on the wave functions we have discussed before, continuity of ψ and its derivatives. Actually we also have to impose normalisability, which means that $B_1=A_3=0$ (exponentially growing functions can not be normalized). As we shall see we only have solutions at certain energies. Continuity implies that

$$A_1 e^{-ka}+B_1 e^{ka} \ = A_2\cos(\kappa a)-B_2\sin(\kappa a) \tag{4.1.19}$$

$$A_3 e^{ka}+B_3 e^{-ka} \ = A_2\cos(\kappa a)+B_2\sin(\kappa a) \tag{4.1.20}$$

$$kA_1 e^{ka}-kB_1 e^{ka} \ = \kappa A_2\sin(\kappa a)+\kappa B_2\cos(\kappa a) \tag{4.1.21}$$

$$kA_3 e^{ka}-kB_3 e^{-ka} \ = -\kappa A_2\sin(\kappa a)+\kappa B_2\cos(\kappa a) \tag{4.1.22}$$

Tactical Approach

We wish to find a relation between k and κ (why?), removing as maby of the constants A and B. The trick is to first find an equation that only contains A_2 and B_2. To this end we take the ratio of Equations 4.1.19 and 4.1.21 and then the ratio of Equations 4.1.20 and 4.1.22:

$$k=\frac{\kappa[A_2\sin(\kappa a)+B_2\cos(\kappa a)]}{A_2\cos(\kappa a)-B_2\sin(\kappa a)} \tag{4.1.23}$$

$$k=\frac{\kappa[A_2\sin(\kappa a)-B_2\cos(\kappa a)]}{A_2\cos(\kappa a)+B_2\sin(\kappa a)} \tag{4.1.24}$$

We can combine Equations 4.1.23 and \ref4.15B} to a single one by equating the right-hand sides. After deleting the common factor κ, and multiplying with the denominators we find

$$[A_2\cos(\kappa a)+B_2\sin(\kappa a)][A_2\sin(\kappa a)-B_2\cos(\kappa a)]=[A_2\sin(\kappa a)+B_2\cos(\kappa a)][A_2\cos(\kappa a)-B_2\sin(\kappa a)], \tag{4.1.25}$$

which simplifies to

$$A_2B_2=0 \tag{4.1.26}$$

We thus have two families of solutions, those characterized by $B_2=0$ and those that have $A_2=0$.