2.5.4 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:

$$A + B = C, \qquad A - B = C(1 - \frac{2ma}{i\hbar^2 k}) \tag{2.226}$$

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.

2.6 The Finite Square Well

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

$$V(r) = \begin{cases} -V_0, & r \leq a; \\ 0, & r > a. \end{cases} \tag{2.227}$$

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

$$V(x) = -V_0, \qquad -a < x < a, \qquad V = 0 \ \text{ elsewhere} \tag{2.228}$$

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.

2.6.1 Bound States

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

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = \kappa^2\psi \tag{2.229}$$

where:

$$\kappa^2 = -\frac{2mE}{\hbar^2} \tag{2.230}$$

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

$$\psi(x) = Ae^{\kappa x}, \qquad x < -a \tag{2.231}$$

$$\psi(x) = Be^{-\kappa x}, \qquad x > a \tag{2.232}$$

Inside the well, where $E > V_0$:

$$\frac{d^2\psi}{dx^2} = -\frac{2m(E+V_0)}{\hbar^2}\psi = -k^2\psi \tag{2.233}$$

where:

$$k^2 = \frac{2m(V_0+E)}{\hbar^2} = \frac{2mV_0}{\hbar^2} - \kappa^2 \tag{2.234}$$

and the solutions are sines and cosines:

$$\psi(x) = C\sin(kx) + D\cos(kx). \qquad -a < x < a \tag{2.235}$$

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:

$$Be^{-\kappa a} = D\cos ka \tag{2.236}$$

$$-\kappa Be^{-\kappa a} = -kD\sin(ka) \tag{2.237}$$

while the odd functions give:

$$Be^{-\kappa a} = C\sin ka \tag{2.238}$$

$$-\kappa Be^{-\kappa a} = kC\cos(ka) \tag{2.239}$$

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:

$$k\tan(ka) = \kappa, \qquad \text{even solutions} \tag{2.240}$$

and:

$$k\cot(ka) = -\kappa, \qquad \text{odd solutions} \tag{2.241}$$

From Eqn. 2.234 :

$$\frac{\kappa^2}{k^2} = \frac{2mV_0}{\hbar^2 k^2} - 1 \tag{2.242}$$

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

$$\tan(ka) = \sqrt{\frac{2mV_0}{\hbar^2 k^2} - 1} = \sqrt{\frac{V_0}{V_0 + E} - 1} \tag{2.243}$$

and:

$$\cot(ka) = -\frac{k}{\kappa} = -\sqrt{\frac{V_0}{V_0 + E} - 1} \tag{2.244}$$

Note that:

$$\frac{V_0}{V_0 + E} > 1, \quad \text{since } E < 0 \tag{2.245}$$

These two conditions can be written more compactly by defining:

$$z^2 \equiv k^2 a^2 = \frac{2ma^2(V_0 + E)}{\hbar^2}, \qquad z_0^2 \equiv (2ma^2 V_0)/(\hbar^2) \tag{2.246}$$

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

By substitution:

$$\tan(z) = \sqrt{(z_0/z)^2 - 1}, \qquad \text{even solutions} \tag{2.247}$$

$$\cot(z) = -\sqrt{(z_0/z)^2 - 1} \qquad \text{odd solutions} \tag{2.248}$$

Eqns. 2.247 and 2.248 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:

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

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

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

We can summarize these solutions in one equation,

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

Inserting the definition of z:

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

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

$$E \approx -V_0 + \frac{n^2\pi^2\hbar^2}{2m(2a)^2}, \quad n = 1, 2, 3, \cdots \tag{2.249}$$

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 $E_n \to 0$.

2.6.2 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.

$$\Psi = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)} = (Ae^{ikx} + Be^{-ikx})e^{-i\omega t}, \quad x < -a \tag{2.250}$$

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:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \qquad x < -a \tag{2.251}$$

$$\psi(x) = C\sin(lx) + D\cos(lx), \qquad -a < x < a \tag{2.252}$$

$$\psi(x) = Fe^{ikx}, \qquad x > a \tag{2.253}$$

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

$$Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la) \tag{2.254}$$

$$Fe^{ika} = C\sin(la) + D\cos(la) \tag{2.255}$$

$$ikAe^{-ika} - ikBe^{ika} = l[C\cos(la) + D\sin(la)] \tag{2.256}$$

$$ikFe^{ika} = l[C\cos(la) - D\sin(la)] \tag{2.257}$$

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

$$\alpha = \sin(la), \qquad \beta = \cos(la), \qquad \gamma = e^{ika}, \qquad r = \frac{l}{ik} \tag{2.258}$$

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

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

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

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

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

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:

$$M^{-1} =$$

$$
\begin{pmatrix}
\frac{r\cos(2la)-r^2\sin(2la)}{2\gamma^2 X_1} & r\frac{1}{2\gamma X_1} & -\frac{\sin(2la)+r\cos(2la)}{2\gamma^2 X_1} & -\frac{r}{2\gamma X_1} \\
-\frac{1}{2\gamma X_3} & \frac{1}{2X_3} & -\frac{1}{2\gamma X_3} & \frac{1}{2X_3} \\
-\frac{1}{2\gamma X_2} & -\frac{1}{2X_2} & -\frac{1}{2\gamma X_2} & -\frac{1}{2X_2} \\
\frac{r}{2\gamma^2 X_1} & \frac{r^2\sin(1la)-r\cos(2la)}{2\gamma X_1} & \frac{r}{2g^2 X_1} & \frac{r\cos(2la)+\sin(2la)}{2\gamma X_1}
\end{pmatrix}
\tag{2.259}
$$

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. 2.258:

$$B/A = -e^{-2ika}\frac{(l^2-k^2)\sin(2la)}{(l^2+k^2)\sin(2la) + 2ilk\cos(2la)} \tag{2.260}$$

The reflection coefficient is:

$$R = |B/A|^2 = \frac{(l^2-k^2)^2\sin^2(2la)}{(l^2+k^2)^2\sin^2(2la) + 4l^2k^2\cos^2(2la)} \tag{2.261}$$

For the transmitted wave:

$$F/A = M^{-1}_{41} + M^{-1}_{43}$$

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

$$= -e^{-2ika}\frac{2lk}{2lk\cos(2la) + i(k^2+l^2)\sin(2la)} \tag{2.262}$$

The transmission coefficient is:

$$T = |F/A|^2$$

$$T^{-1} = \cos^2(2la) + \frac{(k^2+l^2)^2}{4l^2k^2}\sin^2(2la)$$

$$= 1 + \frac{(k^2 + l^2)^2 - 4l^2k^2}{4l^2k^2} \sin^2(2la)$$

$$= 1 + \frac{(k^2 - l^2)^2}{4l^2k^2} \sin^2(2la) \geq 1 \tag{2.263}$$

If:

$$2la = \frac{2a}{\hbar}\sqrt{2m(E_n + V_0)} = n\pi \tag{2.264}$$

$T = 1$, 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:

$$E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2} \tag{2.265}$$

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*.