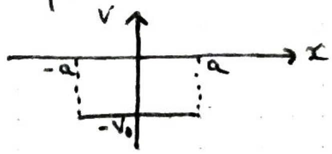
Finite Square Well

In a finite square well, we have potential $V(x)$ defined by $V(x) = \begin{cases} -V_0 & -a < x < a \\ 0 & |x| \geq a \end{cases}$



We expect both bound and scattering states here.

For bound states $-V_0 < E < 0$:

* Left of the well:

$$\frac{d^2\psi}{dx^2} = \frac{-2mE}{\hbar^2}\psi = K^2\psi \quad \text{where } K = \sqrt{\frac{-2mE}{\hbar^2}}$$

This gives us ansatz: $\psi = Ae^{-Kx} + Be^{Kx}$

Left of the well, where x is negative, for normaliseability we see $A = 0$. This gives us $\underline{\psi = Be^{Kx}}$ for $x < -a$

* inside the well:

$$\frac{d^2\psi}{dx^2} = \frac{-2m(E+V_0)}{\hbar^2}\psi = -l^2\psi \quad \text{where } l = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

This gives us ansatz $\psi = C\sin(lx) + D\cos(lx)$

For the purpose of this example, lets only consider even solutions (although odd solutions are also valid).

$\therefore \underline{\psi = D\cos(lx)}$

* Right of the well:

Similar to left of the well, we get ansatz $\psi = Fe^{-Kx} + Ge^{Kx}$

but this time for normaliseability, $G = 0$

$\therefore \underline{\psi = Fe^{-Kx}}$

So we have $\psi(x) = \begin{cases} Be^{Kx} & x < -a \\ D\cos(lx) & -a < x < a \\ Fe^{-Kx} & x > a \end{cases}$

But since we are only considering even solutions, we can say that $\psi(x)$ is symmetric about $x=0$ so anything below $x=0$ mirrors that above $x=0$ so:

$$\psi(x) = \begin{cases} Fe^{-Kx} & x > a \\ D\cos(lx) & 0 \le x \le a \\ \psi(-x) & x < 0 \end{cases}$$

To constrain the coefficients, lets apply some continuity conditions. At $x=a$, we require:

① $Fe^{-Ka} = D\cos(la)$ we also require $\frac{d\psi}{dx}$ to be continuous so:

$-KFe^{-Ka} = -lD\sin(la)$

$\Rightarrow KFe^{-Ka} = lD\sin(la)$ ②

if we do ② ÷ ① we find:

$K = l\tan(la)$ where $K = \frac{\sqrt{-2mE}}{\hbar}$ and $l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$

$K = l\tan(z)$ where $z = la$

$$K^2 + l^2 = \frac{2m}{\hbar^2}V_0 \Rightarrow K^2 = l^2\left(\frac{2mV_0}{\hbar^2 l^2} - 1\right)$$

$$K^2 = l^2\left(\frac{2mV_0a^2}{\hbar^2(la)^2} - 1\right) \Rightarrow K = l\sqrt{\frac{z_0^2}{z} - 1} \quad \text{where } z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$$

We can therefore say: $\tan(z) = \sqrt{\frac{z_0^2}{z} - 1}$

This equation will give us the allowed energy levels.

This equation cannot be solved analytically, only numerically but we can look at some special cases.

a) wide and deep well (a, V_0) are large. This means that z_0 is also very large, so the intersections of $\tan(z)$ and $\sqrt{\frac{z_0^2}{z} - 1}$ is pushed "upwards". we numerically find solutions that coincide with $z_n = \frac{n\pi}{2}$ so:

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

we have a finite number of bound state energies but the energies correspond to those from infinite square well

b) shallow and narrow well (a, V_0) small. Here, the number of intersections is smaller (there is only one) and we only find one solution in bound state for even functions. In odd functions, we don't find any.

As always, lets normalise the function:

$$2\int_a^\infty |F|^2 e^{-2Kx}\,dx + 2\int_0^a |D|^2 \underbrace{\cos^2(lx)}_{\cos^2\theta = \frac{1}{2}(1+\cos 2\theta)}\,dx$$

we have both multiplied by 2 since this is only the positive half of ψ

$$= 2\left\{ |F|^2 \frac{e^{-2Kx}}{2K} + |D|^2\left(\frac{a}{2} + \frac{\sin(2la)}{4l}\right)\right\}$$

If we use the continuity condition $Fe^{-Ka} = D\cos(la) \Rightarrow F = D\cos(la)\,e^{Ka}$:

$$= |D|^2\left(a + \frac{\sin(2la)}{2l} + \frac{\cos^2(la)}{K}\right)$$ with some playing around, we get:

$$\underline{\underline{D = \frac{1}{\sqrt{a+\frac{1}{K}}}}} \quad ; \quad \underline{\underline{F = \frac{e^{Ka}\cos(la)}{\sqrt{a+\frac{1}{K}}}}}$$

Since the potential is finite, we also expect scattering states:

Scattering states $E > 0$:

* left of the well:
  $\psi(x) = Ae^{iKx} + Be^{-iKx}$ with $K = \frac{\sqrt{2mE}}{\hbar}$

* inside the well:
  $\psi(x) = C\sin(lx) + D\cos(lx)$ with $l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$

* right of the well:
  $\psi(x) = Fe^{iKx}$ with $G=0$ since we expect no waves coming from the right

Now we can apply some continuity conditions to these.

At $x = -a$:

$$Ae^{-iKa} + Be^{iKa} = -C\sin(la) + D\cos(la) \quad \text{(1a)}$$

we require continuity for the derivatives as well:

$$iK\left[Ae^{-iKa} - Be^{iKa}\right] = l\left[C\cos(la) + D\sin(la)\right] \quad \text{(1b)}$$

At $x = a$:

$$Fe^{iKa} = C\sin(la) + D\cos(la) \quad \text{(2a)}$$

For the derivatives:

$$iK\,Fe^{iKa} = l\left[C\cos(la) - D\sin(la)\right] \quad \text{(2b)}$$

we can combine (1a), (1b), (2a), (2b) to eliminate C and D:
After some playing around, we find:

$$B = i\frac{\sin(la)}{2Kl}(l^2 + K^2)F \quad ; \quad F = \frac{e^{-2iKa}A}{\cos(2la) - i\frac{(K^2+l^2)}{2Kl}\sin(2la)}$$

Playing around some more, we arrive at an expression for the transmission coefficient. The inverse looks nicer so we will look at that:

$$T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)$$

So we see that for certain E, the sin term will vanish and there is 100% transmission, i.e if the sin argument is $n\pi$, the potential becomes transparent.

so if $\frac{2a}{\hbar}\sqrt{2m(E+V_0)} = n\pi = 2a\frac{2\pi}{\lambda}$ where λ is de Broglie wavelength

$$\Rightarrow \frac{n\lambda}{2} = 2a$$

Interestingly, the wavelengths for which the finite square well becomes transparent correspond to the ones found for the infinite square well. And indeed the energies for which the potential becomes transparent are $E + V_0 = \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2}$

i.e. the energies we found for the infinite square well.