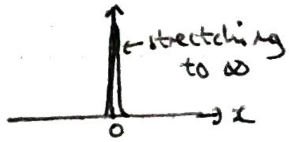
The Delta Function Potential

The dirac delta function $\delta(x)$ is defined as

$$\delta(x) = \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases}$$

so it looks like



A further property is that the function is normalised.

i.e $\int_{-\infty}^{\infty} \delta(x)\,dx = 1$

The delta function is commonly used in physics, for example to describe the charge distribution for a particle at $x=0$. The charge is 0 everywhere except at $x=0$

We can also move the peak of the delta function anywhere by using the common transform, i.e to move the peak to a, we can use $\delta(x-a)$.

This can be used to great effect, for example:

$$\int_{-\infty}^{\infty} f(x)\,\delta(x-a)\,dx = f(a)$$

we have vanished the function everywhere except at a. i.e, we have picked a value out of the fn.

So what happens if we use the δ function as a potential in our SE? Let's consider a potential that vanishes everywhere except for the point x, where we choose it to be negative:

$V(x) = -\alpha\,\delta(x)$ where α is real and positive scaling coefficient

Plugging into the TISE: $$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\,\psi(x) = E\,\psi(x)$$

writing in the convenient form: $$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}\left(E + \alpha\,\delta(x)\right)\psi(x)$$

Now let's consider solutions with $E<0$ and $E>0$

E < 0 bound state solutions:

To the left and right of the delta-function peak, the potential vanishes, so we have $V(x) = 0$. Here, the TISE is:

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = k^2\psi \qquad \text{where } k^2 = -\frac{2mE}{\hbar^2}$$

So we have ansatz $\psi(x) = Ae^{-kx} + Be^{kx}$

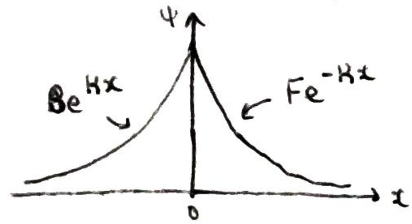
As $x \to -\infty$, this is only normaliseable if $A = 0$

so for $x < 0$: $\underline{\psi(x) = Be^{kx}}$

As $x \to \infty$, our ansatz $\psi(x) = Fe^{-kx} + Ge^{kx}$ is only normaliseable if $G = 0$

so for $x > 0$: $\underline{\psi(x) = Fe^{-kx}}$

So what about at $x = 0$? We require $\psi(x)$ to be continuous so $\psi(0)$ should be the same regardless of whether we approach from the left or right:



So at $\psi(0)$: $Be^{k \times 0} = Fe^{-k \times 0}$

$\therefore \underline{\underline{B = F}}$

This type of analysis called using continuity conditions

We can thus write $\psi(x) = \begin{cases} Be^{kx} & x \leq 0 \\ Be^{-kx} & x \geq 0 \end{cases}$

What else can we do? Let's try integrating both sides of the TISE around the origin from a tiny $-\varepsilon$ to $+\varepsilon$ and then take the limit $\varepsilon \to 0$:

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{+\varepsilon}\frac{\partial^2\psi}{\partial x^2}\,dx + \int_{-\varepsilon}^{+\varepsilon}V(x)\psi(x)\,dx = E\int_{-\varepsilon}^{+\varepsilon}\psi(x)\,dx$$

Since $\int_{-\varepsilon}^{\varepsilon}\psi(x)\,dx$ is the area under the curve between $-\varepsilon$ and ε, as $\varepsilon \to 0$, the area also $\to 0$. So the RHS $= 0$

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{+\varepsilon}\frac{d^2\psi}{dx^2}\,dx + \int_{-\varepsilon}^{+\varepsilon}V(x)\psi(x)\,dx = 0$$

$$\int_{-\varepsilon}^{\varepsilon}\frac{d^2\psi}{dx^2}\,dx = \frac{2m}{\hbar^2}\int_{-\varepsilon}^{\varepsilon}V(x)\psi(x)\,dx$$

$$\lim_{\varepsilon\to 0}\left[\frac{d\psi}{dx}\right]_{-\varepsilon}^{\varepsilon} = \lim_{\varepsilon\to 0}\frac{2m}{\hbar^2}\int_{-\varepsilon}^{\varepsilon}V(x)\psi(x)\,dx$$

$$\lim_{\varepsilon\to 0}\left[\frac{d\psi}{dx}\right]_{-\varepsilon}^{\varepsilon} = \lim_{\varepsilon\to 0}\frac{-2m}{\hbar^2}\int_{-\varepsilon}^{\varepsilon}\alpha\,\delta(x)\psi(x)\,dx$$

The delta fn here has a peak at 0 so it selects $\psi(0)$ which is B

$$\underbrace{\lim_{\varepsilon\to 0}\left[\frac{d\psi}{dx}\right]_{-\varepsilon}^{\varepsilon}}_{\text{so how do we simplify this?}} = \frac{-2m\alpha}{\hbar^2}\psi(0) = \frac{-2m\alpha}{\hbar^2}B$$

$$\lim_{\varepsilon\to 0}\left[\frac{d\psi}{dx}\right]_{-\varepsilon}^{\varepsilon} = \left.\begin{cases}\frac{d}{dx}Be^{Kx} & x\le 0 \rightarrow BK \\ \frac{d}{dx}Be^{-Kx} & x\ge 0 \rightarrow -BK\end{cases}\right|_{-\varepsilon}^{\varepsilon} = -2BK = \frac{-2m\alpha}{\hbar^2}B$$

$$\therefore\ -2BK = \frac{-2m\alpha}{\hbar^2}B \qquad \text{but } K = \sqrt{\frac{-2mE}{\hbar^2}}$$

$$\frac{-2B}{\hbar}\sqrt{-2mE} = \frac{-2m\alpha}{\hbar^2}B \Rightarrow \sqrt{-2mE} = \frac{m\alpha}{\hbar} \Rightarrow -2mE = \frac{m^2\alpha^2}{\hbar^2}$$

$$\underline{\underline{E = -\frac{m\alpha^2}{2\hbar^2}}}$$

So now we have the energy of the bound state.

The final step is to determine the normalisation B:

$$|B|^2\int_{-\infty}^{0}e^{2Kx}\,dx + |B|^2\int_{0}^{\infty}e^{-2Kx}\,dx = 1$$

But the two integrals are symmetric

$$\Rightarrow 2|B|^2\int_0^\infty e^{-2Kx}\,dx = 2|B|^2\left(\frac{e^{-2Kx}}{-2K}\right)_0^\infty = \frac{2|B|^2}{2K} = \frac{|B|^2}{K} = 1$$

$$\therefore\ B = \pm\sqrt{K} \qquad \text{but } K = \frac{m\alpha}{\hbar^2} \qquad \text{so } \underline{\underline{B = \frac{\sqrt{m\alpha}}{\hbar}}}$$

choose +ve

So the stationary state solution for the bound state is:

$$\underline{\psi(x) = \frac{\sqrt{m\alpha}}{\hbar}e^{-m\alpha|x|/\hbar^2}} \qquad \text{with } \underline{E = \frac{-m\alpha^2}{2\hbar^2}}$$

Interestingly, there is only one single bound state, not infinite like SHO or ISW

Note, we used $|x|$ just so we wouldn't have to write out the cases $x<0$ $x>0$

$E > 0$ Scattering State Solutions

we once again have $\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -K^2\psi$

where $K^2 = \frac{2mE}{\hbar^2}$ Notice we didn't include the negative sign in the definition of K like we did for the bound state.

This gives ansatz:

$$\psi(x) = \begin{cases} Ae^{iKx} + Be^{-iKx} & \text{for } x < 0 \\ Fe^{iKx} + Ge^{-iKx} & \text{for } x > 0 \end{cases}$$

Since this is the scattering state, we don't require that $\psi(x)$ be normaliseable so we can't apply the same constraints as with the scattering state. We are stuck with 4 unknowns ABFG.

We can apply continuity conditions though:

at $x = 0$: $A + B = F + G$ ①

we can get further properties by looking at derivatives of ψ around $x = 0$:

$$\underbrace{\lim_{\varepsilon \to 0} \left.\frac{d\psi}{dx}\right|_{-\varepsilon}^{\varepsilon}} = \begin{cases} \frac{d\psi}{dx} = iK(Fe^{iKx} - Ge^{-iKx}) & x > 0 \\ \frac{d\psi}{dx} = iK(Ae^{iKx} - Be^{-iKx}) & x < 0 \end{cases}$$

we get this by:

$$\lim_{\varepsilon \to 0} \left.\frac{d\psi}{dx}\right|_{-\varepsilon}^{\varepsilon} = \frac{2m}{\hbar^2}\int_{-\varepsilon}^{\varepsilon} V(x)\psi(x)\,dx$$

$$= -\frac{2m\alpha}{\hbar^2}\int_{-\varepsilon}^{\varepsilon} \delta(x)\psi(x)\,dx = -\frac{2m\alpha}{\hbar^2}\psi(0) \text{ as } \varepsilon \to 0$$

$$= -\frac{2m\alpha}{\hbar^2}(A + B)$$

$$\therefore \; iK(F - G - A + B) = -\frac{2m\alpha}{\hbar^2}(A + B)$$

$$F - G = A(1 + 2i\beta) - B(1 - 2i\beta) \quad ② \qquad \text{where } \beta = \frac{m\alpha}{K\hbar^2}$$

So now we have ① and ② but these are still not enough to fully determine the wavefunction, we have 4 unknowns!

So we can't really solve the SE for scattering states but we can still describe some general properties.

Let's look at the individual terms in the ansatz with the time-dependent terms put back in:

$Ae^{ikx}e^{-iEt/\hbar}$: this is for $x<0$ so starts on left, propagates right
INCOMING WAVE

$Be^{-ikx}e^{-iEt/\hbar}$: for $x<0$ so starts on left, propagates to the left
REFLECTED WAVE

$Fe^{ikx}e^{-iEt/\hbar}$: for $x>0$ so starts on right, propagates right
TRANSMITTED WAVE

$Ge^{-ikx}e^{-iEt/\hbar}$: for $x>0$ so starts on right, propagates left
This doesn't make sense in this example as nothing comes from the right so $\underline{G=0}$

So in our scenario, we imagine a wave coming from the left and meeting the delta function potential at $x=0$. Some of the wave is reflected and some is transmitted through. So B is the coefficient of the reflected wave and F is the coefficient of the transmitted wave. A is the coefficient of the incoming wave. So we can use these to find transmission and reflection probabilities.

From ① : $F = A+B$ since $G=0$

② : $F = A(1+2i\beta) - B(1-2i\beta)$

equating these: $A+B = A(1+2i\beta) - B(1-2i\beta)$

$$A-A-A2i\beta = -B-B+B2i\beta \Rightarrow -2Ai\beta = -2B+2Bi\beta$$

$$-2Ai\beta = -2B(1-i\beta) \Rightarrow \frac{B}{A} = \frac{i\beta}{1-i\beta}$$

The reflection probability $R = \frac{|B|^2}{|A|^2}$

$$\text{so } R = \frac{(i\beta)^* i\beta}{(1-i\beta)^*(1-i\beta)} \qquad \underline{\underline{R = \frac{\beta^2}{1+\beta^2}}}$$

So we have found the reflection probability for our case.

Similarly if we do ① + $\frac{1}{1-2i\beta}$ ② :

$$F + F \cdot \frac{1}{1-2i\beta} = A + A\frac{1+2i\beta}{1-2i\beta} + B - B\frac{1-2i\beta}{1-2i\beta}$$

$$F + F(1-2i\beta) = A(1-2i\beta) + A(1+2i\beta)$$

$$F + F - 2i\beta F = 2A \Rightarrow 2F - 2i\beta F = 2A$$

$$F(1-i\beta) = A \qquad \therefore \frac{F}{A} = \frac{1}{1-i\beta}$$

The transmission coefficient is given by $T = \frac{|F|^2}{|A|^2}$

$$T = \frac{1}{(1-i\beta)^*(1-i\beta)} \Rightarrow T = \frac{1}{1+\beta^2}$$

we have thus calculated the transmission coefficient.

we can sub in $\beta = \frac{m\alpha}{k\hbar^2} = \frac{m\alpha}{\sqrt{\frac{2mE}{\hbar^2}}\,\hbar^2} = \frac{\sqrt{m}\,\alpha}{\sqrt{2}\,\hbar\sqrt{E}}$

$$T = \frac{1}{1+\frac{m\alpha^2}{2\hbar^2 E}} \qquad R = \frac{1}{1+\frac{2\hbar^2 E}{m\alpha^2}}$$

So we see that the larger the energy E, the larger the transmission coefficient and the smaller the reflection coefficient

α plays the role of a coupling between the particle wave and the potential.

Here, the potential was negative but what happens if we use a negative α so the potential is positive? This makes the potential into a "barrier". We don't expect any bound states since $E > V_{min}$ and it turns out R and T remain unchanged since they only depend on α^2.

So the transmitted wave function somehow get's through this infinite potential. This is a process called tunneling.