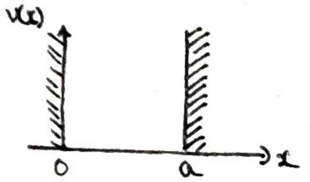
Infinite Square Well

The infinite square well is a potential of the form

$$V(x) = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}$$

which looks like:



A particle within the well ($0 \leq x \leq a$) cannot escape as an infinite amount of energy would be needed. So for $x < 0$, $x > a$, the wave function vanishes, $\psi(x) = 0$

The TISE is $-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi = E\psi$ so inside the well, it is:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = E\psi \Rightarrow \frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi$$

which we can write as: $\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi$ where $k^2 = \frac{2mE}{\hbar^2}$

We know this kind of diff. eqn. from classical mechanics so we can make the ansatz: $\psi(x) = A\sin(kx) + B\cos(kx)$ [we get this by constructing the auxiliary eqn and solving it to find which trial soln we should use]

We know that $\psi(0) = \psi(a) = 0$, so we can sub this in to find A and B:

$\psi(0) = 0 + B \Rightarrow \psi(0) = B \Rightarrow \underline{B = 0}$ so $\psi(x) = A\sin(kx)$

$\psi(a) = A\sin(ka)$ which we require to $= 0$

$\therefore ka = n\pi \Rightarrow k_n = \frac{n\pi}{a}$ where $n = 1, 2, 3 \ldots$

$\hookrightarrow$ This gives us $k_n^2 = \frac{n^2\pi^2}{a^2} = \frac{2mE_n}{\hbar^2}$

$$\underline{\underline{\psi_n(x) = A\sin\left(\frac{n\pi x}{a}\right)}}$$

$$\Rightarrow \underline{\underline{E_n = \frac{\hbar^2 \pi^2 n^2}{2a^2 m}}}$$

So now we have an equation for the energy E_n of each stationary state and an equation for the stationary states ψ_n. But we still don't know A. This is just the normalisation constant and we can normalise it the usual way

We require $\int_0^a |\Psi(x)|^2 \, dx = 1$

$$\int_0^a |\Psi(x)|^2 \, dx = |A|^2 \int_0^a \sin^2(kx) \, dx$$

$$= \frac{|A|^2}{2} \int_0^a 1 - \cos(2kx) \, dx$$

$$= \frac{|A|^2}{2} \left\{ x - \frac{1}{2k} \sin(2kx) \right|_0^a$$

$$= \frac{|A|^2}{2} \left\{ (a - 0) - (0 - 0) \right\} = \frac{|A|^2}{2} a$$

$\therefore \quad A = \pm \sqrt{\frac{2}{a}}$ and we pick positive for convenience

$\therefore \quad \psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ for $n = 1, 2, 3 \ldots$

Giving the time dependent solution:

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{-iE_n t/\hbar} \quad \text{where} \quad E_n = \frac{\hbar^2 \pi^2 n^2}{2a^2 m}$$

Notice here that the solutions are either odd (ψ_2, ψ_4, ψ_6) or even (ψ_1, ψ_3, ψ_5). By this we mean that the solutions are symmetric or antisymmetric about the centre of the well $\frac{a}{2}$.

The number of nodes of the solution increases with n.

Finally, the solutions are mutually orthognal, i.e for solutions $n = p$, $n = q$:

$$\int \psi_p^*(x) \, \psi_q(x) \, dx = 0 \quad \text{for} \quad p \neq q$$

So now we have completed the first step in the recipe. If we want to take this further and find $\Psi(x,t)$, we need to find the coefficients c_n. But how do we do that?

Working out Correlation Coefficients C_n

we saw that stationary state solutions are mutually orthogonal

↳ $\int \psi_m^* \psi_n \, dx = 0$ for $m \neq n$

we can show this for the infinite square well stationary state:

$$\int_0^a \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \sqrt{\frac{2}{a}} \sin\left(\frac{m\pi x}{a}\right) dx = \frac{2}{a} \int_0^a \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx$$

but $2\sin\alpha \sin\beta = \cos(\alpha - \beta) - \cos(\alpha + \beta)$:

$$= \frac{1}{a} \int_0^a \cos\left(\frac{m-n}{a}\pi x\right) - \cos\left(\frac{m+n}{a}\pi x\right) dx$$

$$= \frac{1}{a} \left\{ \frac{a}{(m-n)\pi} \sin\left(\frac{m-n}{a}\pi x\right) - \frac{a}{(m+n)\pi} \sin\left(\frac{m+n}{a}\pi x\right) \right\}_0^a$$

$$= \left[\frac{1}{(m-n)\pi} \sin\left(\frac{m-n}{a}\pi x\right) - \frac{1}{(m+n)\pi} \sin\left(\frac{m+n}{a}\pi x\right) \right]_0^a$$

$= 0$ if $m \neq n$

if $m = n$:

$$\int |\psi_m|^2 dx = 1$$

we can thus summarise as $\int \psi_m^* \psi_n \, dx = \delta_{mn}$

where δ_{mn} is the Kronecker delta $\delta_{mn} = \begin{cases} 0 & m \neq n \\ 1 & m = n \end{cases}$

This is called the orthonormality of stationary states.

Since time-independent solutions constitute a complete set, any wave function $\Psi(x,0)$ can be represented as:

$$\Psi(x,0) = \psi(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

so $\psi(x) = \sqrt{\frac{2}{a}} \sum_1^{\infty} c_n \psi_n(x)$ for our infinite square well example.

We can turn this around to get an expression for C_n

$$\psi(x) = \sum_{m=1}^{\infty} c_m \psi_m(x)$$

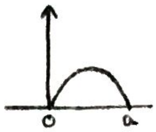
$$\Rightarrow \int \psi_n^*(x)\psi(x)\,dx = \sum_{m=1}^{\infty} c_m \underbrace{\int \psi_n^*(x)\psi_m(x)\,dx}_{\delta_{mn}}$$

$$= \sum_{m=1}^{\infty} c_m \delta_{nm} = \underline{\underline{c_n}}$$

So we can say $\boxed{c_n = \int \psi_n^*(x)\,\psi(x)\,dx}$

Let's look at an example:

$$\Psi(x,0) = \psi(x) = \begin{cases} Ax(a-x) & 0 \le x \le a \\ 0 & \text{otherwise} \end{cases}$$



we have to first find A: $\int_0^a |\psi|^2 dx = |A|^2 \int_0^a x^2(a-x)^2 dx$

$$|A|^2 \int_0^a x^2(a-x)^2 dx = |A|^2 \left[\frac{a^2}{3}x^3 - \frac{a}{2}x^4 + \frac{x^5}{5}\right]_0^a$$

$$= |A|^2 \cdot \frac{a^5}{30} \quad \Rightarrow A = \pm\sqrt{\frac{30}{a^5}}$$ we choose the +ve sign

$$\therefore \quad \underline{\psi(x) = \sqrt{\frac{30}{a^5}}\,x(a-x)}$$

For a infinite square well $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$

We can now find c_n: $c_n = \int \psi_n^*(x)\,\psi(x)\,dx$

$$c_n = \int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\sqrt{\frac{30}{a^5}}\,x(a-x)\,dx$$

$$= \frac{2\sqrt{15}}{a^3}\left\{ a\int_0^a x\sin\left(\frac{n\pi x}{a}\right)dx - \int_0^a x^2\sin\left(\frac{n\pi x}{a}\right)dx \right\}$$

$$= \frac{2\sqrt{15}}{a^3}\left\{ a\left[\left(\frac{a}{n\pi}\right)^2\sin\left(\frac{n\pi x}{a}\right) - \left(\frac{ax}{n\pi}\right)\cos\left(\frac{n\pi x}{a}\right)\right]_0^a \right.$$

$$\left. - \left[2\left(\frac{a}{n\pi}\right)^2 x\sin\left(\frac{n\pi x}{a}\right) - \frac{\left(\frac{n\pi x}{a}\right)^2}{\left(\frac{n\pi}{a}\right)^2}\cos\left(\frac{n\pi x}{a}\right)\right]_0^a \right\}$$

$$c_n = \frac{4\sqrt{15}}{(n\pi)^3}\left(\cos(0) - \cos(n\pi)\right) = \begin{cases} 0 & n \text{ even} \\ \frac{8\sqrt{15}}{(n\pi)^3} & n \text{ odd} \end{cases}$$

We have therefore found $\underline{c_n}$ and thus we can state the full time dependent solution for the infinite square well:

$$\underline{\underline{\Psi(x,t) = \sum_{n=1,3,5}^{\infty} \frac{8\sqrt{15}}{(n\pi)^3}\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)e^{-iE_n t/\hbar}}}$$

So what is this coefficient c_n? c_n measures the admixture of a given stationary state to the full solution, It is the proportional contribution of each stationary state.

A further property of c_n is:

$$1 = \int |\Psi(x,0)|^2 \, dx = \int \left(\sum_n c_n \psi_n\right)^* \left(\sum_m c_m \psi_m\right) dx$$

$$= \sum_{n,m} c_n^* c_m \int \psi_n^* \psi_m \, dx = \sum_{n,m} c_n^* c_m \, \delta_{nm}$$

$$= \sum |c_n|^2 \qquad \therefore \quad \boxed{\sum_1^\infty |c_n|^2 = 1}$$

Based on these findings, we can compute $\langle H \rangle$

$$\langle H \rangle = \int \Psi^*(x,t) \, \hat{H} \, \Psi(x,t) \, dx$$

$$= \int \sum_m c_m^* \psi_m^* e^{iE_m t/\hbar} \, \hat{H} \sum_n c_n \psi_n e^{-iE_n t/\hbar}$$

$$= \sum_{n,m} c_m^* c_n e^{-i(E_n - E_m)t/\hbar} \int \psi_m^* \hat{H} \psi_n \, dx$$

$$= \sum_{n,m} c_m^* \underbrace{c_n e^{-i(E_n - E_m)t/\hbar}}_{=1 \text{ if } m=n} E_n \underbrace{\int \psi_m^* \psi_n \, dx}_{= \delta_{mn}}$$

$$= \underline{\underline{\sum_m^\infty E_m |c_n|^2}} \qquad \text{This is the conservation of energy.}$$

We can therefore see that $|c_n|^2$ tells us the probability of finding a particular energy E_n.