One-Dimensional Quantum Systems

The Schrodinger equation in 1-dimension is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2}+V(x)\psi_E(x)=E\psi_E(x)$$

The solutions $\psi_E(x)$ are the energy eigenstates (eigenfunctions). As we have seen, their time dependence is given by

$$\psi_E(x,t)=e^{-i\frac{E}{\hbar}t}\psi_E(x,0) \quad \text{where} \quad \psi_E(x,0)=\langle x|E\rangle$$

$$\text{and} \quad \hat{H}|E\rangle=E|E\rangle \quad \text{and} \quad \hat{H}=\frac{\hat{p}^2}{2m}+V(\hat{x})$$

We are thus faced with solving an ordinary differential equation with boundary conditions.

Since $\psi_E(x)$ is physically related to a probability amplitude and hence to a measurable probability, we **assume** that $\psi_E(x)$ is continuous.

Using this fact, we can determine the general continuity properties of $\frac{d\psi_E(x)}{dx}$. The continuity property at a particular point, say $x=x_0$, is derived as follows:

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon}\frac{d^2\psi_E(x)}{dx^2}dx=\int_{x_0-\varepsilon}^{x_0+\varepsilon}d\left(\frac{d\psi_E(x)}{dx}\right)$$

$$=-\frac{2m}{\hbar^2}\left[E\int_{x_0-\varepsilon}^{x_0+\varepsilon}\psi_E(x)dx-\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\psi_E(x)dx\right]$$

Taking the limit as $\varepsilon\to 0$

$$\lim_{\varepsilon\to 0}\left(\left.\frac{d\psi_E(x)}{dx}\right|_{x=x_0+\varepsilon}-\left.\frac{d\psi_E(x)}{dx}\right|_{x=x_0-\varepsilon}\right)$$

$$=-\frac{2m}{\hbar^2}\left[E\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}\psi_E(x)dx-\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\psi_E(x)dx\right]$$

or

$$\Delta\left(\frac{d\psi_E(x)}{dx}\right)=\frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\psi_E(x)dx$$

where we have used the continuity of $\psi_E(x)$ to set $\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}\psi_E(x)dx=0$. This makes it clear that whether or not $\frac{d\psi_E(x)}{dx}$ has a discontinuity depends directly on the potential energy function.

If $V(x)$ is continuous at $x=x_0$, i.e.,

$$\lim_{\varepsilon\to 0}\left[V(x_0+\varepsilon)-V(x_0-\varepsilon)\right]=0$$

then

$$\Delta\left(\frac{d\psi_E(x)}{dx}\right)=\frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\psi_E(x)dx=0$$

and $\frac{d\psi_E(x)}{dx}$ is continuous.

If $V(x)$ has a finite discontinuity (jump) at $x=x_0$, i.e.,

$$\lim_{\varepsilon\to 0}\left[V(x_0+\varepsilon)-V(x_0-\varepsilon)\right]=\mathit{finite}$$

then

$$\Delta\left(\frac{d\psi_E(x)}{dx}\right)=\frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\psi_E(x)dx=0$$

and $\frac{d\psi_E(x)}{dx}$ is continuous.

Finally, if $V(x)$ has an infinite jump at $x=x_0$, then we have two choices

(1) if the potential is infinite over an extended range of x, then we must force $\psi_E(x)=0$ in that region and use only the continuity of $\psi_E(x)$ as a boundary condition at the edge of the region

(2) if the potential is infinite at a single point, i.e., $V(x)=\delta(x-x_0)$, then we would have

$$\Delta\left(\frac{d\psi_E(x)}{dx}\right)=\frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}V(x)\psi_E(x)dx=\frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{x_0-\varepsilon}^{x_0+\varepsilon}\delta(x-x_0)\psi_E(x)dx$$
$$=\frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\psi_E(x_0)=\frac{2m}{\hbar^2}\psi_E(x_0)$$

and, thus, $\frac{d\psi_E(x)}{dx}$ is discontinuous.

The last thing we must worry about is the validity of our probability interpretation of $\psi_E(x)$, i.e.,

$\psi_E(x)=\langle x|\psi_E\rangle$ = probability amplitude for the particle in the state $|\psi_E\rangle$ to be found at x

which says that we must also have

$$\langle\psi_E|\psi_E\rangle=\int_{-\infty}^{\infty}|\psi_E(x)|^2dx<\infty$$

This means that we must be able to normalize the wave functions and make the total probability that the particle is somewhere on the x-axis equal to one.

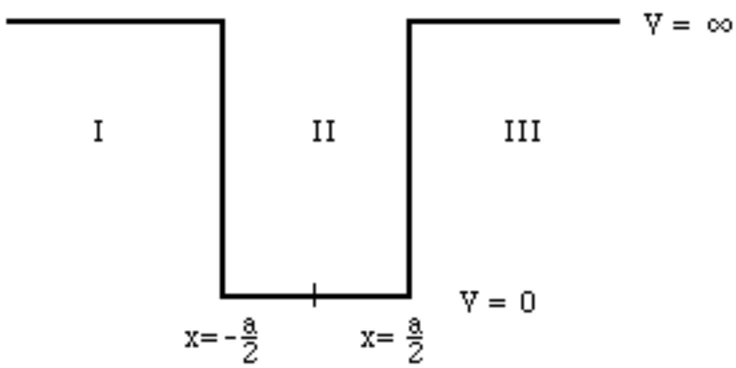
A wide range of interesting physical systems can be studied using 1-dimensional potential energy functions.

Quantized Energy Levels in the Infinite Square Well Potential

We now consider the potential energy function

$$V(x) = \begin{cases} 0 & -\frac{a}{2} \leq x \leq \frac{a}{2} \\ \infty & |x| \geq \frac{a}{2} \end{cases}$$

This is the so-called **infinite square well** shown in the figure below.



We consider the three regions labeled I, II, III. This is an example of a potential that is infinite in an extended region. Therefore, we must require that the wave function $\psi(x) = 0$ in these regions or the Schrodinger equation makes no sense mathematically. In this case we have

$$\psi_I(x) = 0 \quad \text{and} \quad \psi_{III}(x) = 0$$

Digression: Second-Order diffEQs

The solution technique we will use in most cases is called **exponential substitution.**

Exponential Substitution

This method is applicable to all differential equations of the form

$$A\frac{d^2y}{dt^2} + B\frac{dy}{dt} + Cy = 0$$

where $A, B, and\ C$ are constants.

Definitions:

2nd-order = order of highest derivative
linear = no squares or worse
homogeneous = right-hand side = 0
constant coefficients = A, B, C

Therefore this equation is a 2nd-order, homogeneous, linear differential equation with constant coefficients.

The SHM equation(spring) has this form,

$$M\frac{dv}{dt} = -kx \rightarrow M\frac{d}{dt}\left(\frac{dx}{dt}\right) = -kx \rightarrow M\frac{d^2x}{dt^2} + kx = 0$$

so that $A = M$, $C = k$ and $B = 0$.

The 1-dimensional Schrodinger equation will also take this form in different regions as we shall see.

The Method: consider a typical equation of the form

$$\frac{d^2y}{dt^2} + 3\frac{dy}{dt} + 2y = 0$$

We make the exponential substitution

$$y = e^{\alpha t}$$

into the diffEQ. This will convert the diffEQ into an **algebraic** equation for α. We have

$$\frac{d^2y}{dt^2} = \frac{d^2e^{\alpha t}}{dt^2} = \alpha\frac{de^{\alpha t}}{dt} = \alpha^2 e^{\alpha t}$$
$$\frac{dy}{dt} = \frac{de^{\alpha t}}{dt} = \alpha e^{\alpha t}$$
$$y = e^{\alpha t}$$

which gives the result

$$(\alpha^2 + 3\alpha + 2)e^{\alpha t} = 0 \rightarrow \alpha^2 + 3\alpha + 2 = 0$$

since $e^{\alpha t} \neq 0$.

The solutions of this algebraic equation tell us the **allowed** values of α that give **valid** solutions to the diffEQ. In particular in this case we get

$$\alpha = -1, -2$$

as solutions to the quadratic equation. This result means that $y = e^{-t}$ and $y = e^{-2t}$ satisfy the original diffEQ as can be seen by direct substitution.

If there is more than one allowed value of α(as in this case), then the most general solution will be a linear combination of all possible solutions(because this is a linear diffEQ). Since, in this case, the allowed values of α are

$$\alpha = -1, -2$$

the most general solution of the diffEQ is

$$y(t) = ae^{-t} + be^{-2t}$$

where a and b are constants to be determined by the **initial conditions.**

The number of arbitrary constants that need to be determined by the initial conditions is equal to the order(highest derivative $\rightarrow$ 2 in this case) of the diffEQ.

Suppose the initial conditions are $y = 0$ and $dy/dt = 1$ at $t = 0$. Then we have

$$y(t) = ae^{-t} + be^{-2t}$$
$$y(0) = 0 = a + b$$
$$\frac{dy}{dt} = -ae^{-t} - 2be^{-2t}$$
$$\frac{dy}{dt}(0) = -a - 2b = 1$$

which gives $a = -b = 1$ and thus

$$y(t) = e^{-t} - e^{-2t}$$

Substitute this solution into the original equation and see that it works and has the correct initial conditions!!

Although this method is very powerful as described, we can make it even more powerful by defining a new mathematical quantity called the **complex exponential.** This will allow us to use the method for the SHM case.

Complex Exponentials - Alternative Very Powerful Method

Remember the exponential function has the power series expansions:

$$e^{\alpha x} = 1 + \alpha x + \frac{\alpha^2}{2!}x^2 + \frac{\alpha^3}{3!}x^3 + \frac{\alpha^4}{4!}x^4 + ... = \sum_{n=0}^{\infty} \frac{\alpha^n}{n!}x^n$$

Similarly the sine and cosine functions are given by:

$$\sin \alpha x = \sum_{n=0}^{\infty} (-1)^n \frac{\alpha^{2n+1}}{(2n+1)!}x^{2n+1} = \alpha x - \frac{\alpha^3}{3!}x^3 + \frac{\alpha^5}{5!}x^5 + ...$$

$$\cos \alpha x = \sum_{n=0}^{\infty} (-1)^n \frac{\alpha^{2n}}{(2n)!}x^{2n} = 1 - \frac{\alpha^2}{2!}x^{24} + \frac{\alpha^4}{4!}x^4 + ...$$

We then showed the neat result that

$$e^{\pm i\alpha t} = \cos \alpha t \pm i \sin \alpha t$$

which is very useful physics. It is called Euler's formula.

From these results we can also derived the relations

$$\frac{e^{i\alpha t}-e^{-i\alpha t}}{2i}=\frac{\cos\alpha t+i\sin\alpha t-\cos\alpha t+i\sin\alpha t}{2i}=\sin\alpha t$$

$$\frac{e^{i\alpha t}+e^{-i\alpha t}}{2}=\frac{\cos\alpha t+i\sin\alpha t+\cos\alpha t-i\sin\alpha t}{2}=\cos\alpha t$$

Finally, we can use these results to solve the SHM equation

$$M\frac{d^2y}{dt^2}+ky=0\rightarrow\frac{d^2y}{dt^2}+\omega^2y=0 \quad , \quad \omega^2=\frac{k}{M}$$

using the exponential substitution method.

$$\frac{d^2y}{dt^2}+\omega^2y=0$$

Substituting $y=e^{\alpha t}$ we get the algebraic equation

$$\alpha^2+\omega^2=0$$

which has solutions (allowed values of α) of $\alpha=\pm i\omega$ so that the most general solution takes the form

$$y(t)=Ae^{i\omega t}+Be^{-i\omega t}$$

Suppose now that the initial conditions are $y=y_0$ and $dy/dt=0$ at $t=0$. Then we have

$$y(t)=Ae^{i\omega t}+Be^{-i\omega t}$$
$$y(0)=y_0=A+B$$
$$\frac{dy}{dt}=i\omega Ae^{i\omega t}-i\omega Be^{-i\omega t}$$
$$\frac{dy}{dt}(0)=i\omega A-i\omega B=0\rightarrow A-B=0$$

or

$$A=B=\frac{y_0}{2}$$

and

$$y(t)=y_0\frac{e^{i\omega t}+e^{-i\omega t}}{2}=y_0\cos\omega t$$

Alternatively, if the initial conditions are $y=0$ and $dy/dt=v_0$ at $t=0$, then we have

$$y(t)=Ae^{i\omega t}+Be^{-i\omega t}$$
$$y(0)=0=A+B$$
$$\frac{dy}{dt}=i\omega Ae^{i\omega t}-i\omega Be^{-i\omega t}$$
$$\frac{dy}{dt}(0)=i\omega A-i\omega B=v_0\rightarrow A-B=\frac{v_0}{i\omega}$$

or

$$A = -B = \frac{v_0}{2i\omega}$$

and

$$y(t) = \frac{v_0}{\omega}\frac{e^{i\omega t} - e^{-i\omega t}}{2i} = \frac{v_0}{\omega}\sin\omega t$$

and in general we have for the initial conditions $y = y_0$ and $dy/dt = v_0$ at $t = 0$,

$$y(t) = Ae^{i\omega t} + Be^{-i\omega t}$$
$$y(0) = y_0 = A + B$$
$$\frac{dy}{dt} = i\omega Ae^{i\omega t} - i\omega Be^{-i\omega t}$$
$$\frac{dy}{dt}(0) = i\omega A - i\omega B = v_0 \to A - B = \frac{v_0}{i\omega}$$

or

$$A = \frac{1}{2}(y_0 + \frac{v_0}{i\omega}) \quad , \quad B = \frac{1}{2}(y_0 - \frac{v_0}{i\omega})$$

and

$$\begin{aligned} y(t) = Ae^{i\omega t} + Be^{-i\omega t} &= \frac{1}{2}(y_0 + \frac{v_0}{i\omega})e^{i\omega t} + \frac{1}{2}(y_0 - \frac{v_0}{i\omega})e^{-i\omega t} \\ &= y_0\frac{e^{i\omega t} + e^{-i\omega t}}{2} + \frac{v_0}{\omega}\frac{e^{i\omega t} - e^{-i\omega t}}{2i} \\ &= y_0\cos\omega t + \frac{v_0}{\omega}\sin\omega t \end{aligned}$$

Returning to the Schrodinger equation:

Now in region II, the Schrodinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} = E\psi_{II} \quad , \quad \mathrm{E} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

which has a general solution(using the above method) given by

$$\psi_{II}(x) = Ae^{ikx} + Be^{-ikx}$$

where k is some parameter to be determined.

The continuity of the wavefunction at $x = \pm\frac{a}{2}$ says that we must have

$$\psi_{II}(-\frac{a}{2}) = Ae^{-i\frac{ka}{2}} + Be^{i\frac{ka}{2}} = 0$$
$$\psi_{II}(\frac{a}{2}) = Ae^{i\frac{ka}{2}} + Be^{-i\frac{ka}{2}} = 0$$

which imply that

$$\frac{B}{A} = -e^{-ika} = -e^{ika}$$

This is an equation for the allowed values (values corresponding to a valid solution) of the parameter k.

The equation is $e^{2ika}=1$. The allowed values of k form a discrete spectrum of energy eigenvalues (quantized energies) given by

$$2k_n a = 2n\pi \rightarrow k_n = \frac{n\pi}{a} \rightarrow E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad , \quad n = 1,2,3,4,........$$

The corresponding wave functions are

$$\psi_{II}^{(n)}(x) = A_n(e^{ik_n x} - e^{-ik_n a}e^{-ik_n x}) = A_n e^{-i\frac{k_n a}{2}}(e^{ik_n(x+\frac{a}{2})} - e^{-ik_n(x+\frac{a}{2})})$$
$$= \tilde{A}_n \sin k_n\left(x+\frac{a}{2}\right)$$

where $\tilde{A}_n$ is determined by the normalization condition

$$\int_{-\frac{a}{2}}^{\frac{a}{2}} |\psi_n(x)|^2\, dx = 1$$

Substituting the value of k_n we get

$$\psi_{II}^{(n)}(x) = \tilde{A}_n \sin\frac{n\pi}{a}(x+\frac{a}{2})$$

or

$$\psi_{II}^{(1)}(x) = \tilde{A}_1 \sin\frac{\pi}{a}(x+\frac{a}{2}) = \tilde{A}_1 \sin(\frac{\pi x}{a}+\frac{\pi}{2}) = \tilde{A}_1\cos(\frac{\pi x}{a})$$
$$\psi_{II}^{(2)}(x) = \tilde{A}_2 \sin\frac{2\pi}{a}(x+\frac{a}{2}) = \tilde{A}_1 \sin(\frac{2\pi x}{a}+\pi) = \tilde{A}_1\sin(\frac{2\pi x}{a})$$
$$\psi_{II}^{(3)}(x) = \tilde{A}_3 \sin\frac{3\pi}{a}(x+\frac{a}{2}) = \tilde{A}_3 \sin(\frac{3\pi x}{a}+\frac{3\pi}{2}) = \tilde{A}_3\cos(\frac{3\pi x}{a})$$

or

$$\psi_{II}(x) = \begin{cases} \sin(\frac{n\pi x}{a}) & \text{n even} \\ cox(\frac{n\pi x}{a}) & \text{n odd} \end{cases}$$

We have mathematically solved the ordinary differential equation problem, now what is the physical meaning of these results?

We find a **discrete spectrum** of allowed energies corresponding to **bound states** of the Hamiltonian. Bound states designate states which are localized in space, i.e., the probability is large only over restricted regions of space and goes to zero far from the potential region.

The **lowest** energy value or lowest energy **level** or **ground state** energy is

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2} > 0$$

with

$$y_1(x) = \begin{cases} A\cos\dfrac{px}{a} & |x| \le \dfrac{a}{2} \\ 0 & |x| \ge \dfrac{a}{2} \end{cases}$$

This minimum energy is not zero because of the Heisenberg uncertainty principle. Since the particle has a nonzero amplitude for being in the well, we say that it is localized such that $\Delta x \approx a$ and thus

$$\Delta p \ge \frac{\hbar}{\Delta x} \approx \frac{\hbar}{a}$$

This says that the kinetic energy (or energy in this case because the potential energy equals zero in region II) must have a minimum value given approximately by

$$E_{\min} = K_{\min} \approx \frac{(\Delta p)^2}{2m} \approx \frac{\hbar^2}{2ma^2}$$

The integer $n-1$ corresponds to the number of nodes (zeros) of the wave function (other than the well edges).

They solutions also have the property

$$\psi(-x) = \psi(x) \qquad \text{n odd}$$
$$\psi(-x) = -\psi(x) \qquad \text{n even}$$

The above discrete transformation of the wave function corresponds to the **parity** operator $\hat{\wp}$ where we have

$$\hat{\wp}\,\psi(x) = \psi(-x) = \psi(x) \qquad \text{means even parity}$$
$$\hat{\wp}\,\psi(x) = \psi(-x) = -\psi(x) \qquad \text{means odd parity}$$

Let us look more generally at the parity operation. Suppose that the potential energy function obeys the rule $V(\vec{x}) = V(-\vec{x})$ and let $\psi(\vec{x})$ be a solution of the Schrodinger equation with energy E

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right)\psi(\vec{x}) = E\psi(\vec{x})$$

Now let $\vec{x} \to -\vec{x}$ to get the equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(-\vec{x})\right)\psi(-\vec{x}) = E\psi(-\vec{x})$$

or

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right)\psi(-\vec{x}) = E\psi(-\vec{x})$$

This says that, if $\psi(\vec{x})$ is a solution of the Schrodinger equation with energy E, then $\psi(-\vec{x})$ is also a solution of the **same** Schrodinger equation and hence with the **same** energy E. This says that $\psi(\vec{x}) \pm \psi(-\vec{x})$

are also solutions of the same Schrodinger equation with the same energy E. Now\

$$\psi(\vec{x}) + \psi(-\vec{x}) \to \text{an even parity solution}$$
$$\psi(\vec{x}) - \psi(-\vec{x}) \to \text{an odd parity solution}$$

This says that if $V(\vec{x}) = V(-\vec{x})$, then we can always choose solutions that have a definite parity (even or odd).

We formally define the **parity operator** by the relation

$$\langle \vec{x} | \hat{\wp} | \psi \rangle = \langle -\vec{x} | \psi \rangle$$

Since $\langle \vec{x} | \hat{\wp}^2 | \psi \rangle = \langle -\vec{x} | \hat{\wp} | \psi \rangle = \langle \vec{x} | \psi \rangle$, we must have $\hat{\wp}^2 = \hat{I}$, which means the eigenvalues of $\hat{\wp}$ are ± 1 as we indicated earlier.

We can show $\left[\hat{H}, \hat{\wp}\right] = 0$ for symmetric potentials by

$$\hat{\wp}\hat{H}|E\rangle = \hat{\wp}E|E\rangle = E\hat{\wp}|E\rangle = \pm E|E\rangle$$
$$\hat{H}\hat{\wp}|E\rangle = \pm\hat{H}|E\rangle = \pm E|E\rangle$$
$$(\hat{\wp}\hat{H} - \hat{H}\hat{\wp})|E\rangle = 0$$
$$\left[\hat{H}, \hat{\wp}\right] = 0$$

since $|E\rangle$ is an arbitrary state. As we saw earlier, this commutator relationship says that

$$\hat{H}\hat{\wp} = \hat{\wp}\hat{H}$$
$$\hat{\wp}\hat{H}\hat{\wp} = \hat{\wp}^2\hat{H} = \hat{H}$$
$$\hat{\wp}^{-1}\hat{H}\hat{\wp} = \hat{H}$$

which means that $\hat{H}$ is invariant under the $\hat{\wp}$ transformation. We have used $\hat{\wp}^2 = \hat{I}$ in this derivation. It also says that

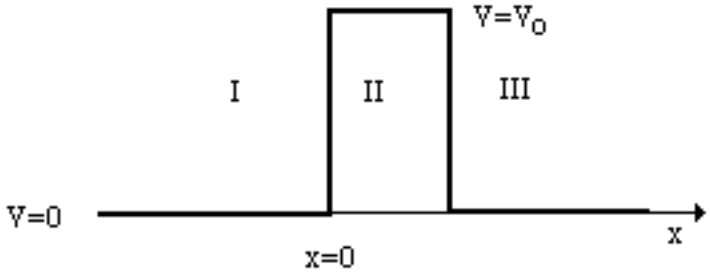
$$\hat{H}(\hat{\wp}|E\rangle) = \hat{\wp}\hat{H}|E\rangle = E(\hat{\wp}|E\rangle)$$

or $\hat{\wp}|E\rangle$ is an eigenstate of $\hat{H}$ with energy E as we stated.

The concept of parity invariance and the fact that $\hat{H}$ and $\hat{\wp}$ share a common set of eigenfunctions can greatly simplify the solution of the Schrodinger equation in many cases.

Tunneling through a Potential Barrier

We now change the potential energy function so that we have a barrier. The new potential energy function is shown in the figure below.



The interesting physical case for quantum systems corresponds to when $E < V_0$.

In the classical case, there is no probability of the particle appearing on the right side of the barrier if it started out on the left side of the barrier. In order to appear on the right side of the barrier, the particle would some how have to pass through region II where $E < V_0 \to T = \frac{1}{2}mv^2 < 0$. Classically, the kinetic energy cannot be negative, which means there would have to be a violation of conservation of energy if the classical particle appeared on the right side of the barrier.

As we shall see, it turns out that a real traveling wave can appear on the other side of the barrier (even though it started on the left side and there are no sources of particles on the right side) in this case. This is called **quantum tunneling.** Let us see how it works.

We have three regions I, II and III to consider as shown in the figure. We get three equations in the three regions

$$x \le 0 \qquad -\frac{\hbar}{2m}\frac{d^2\psi_I}{dx^2} = E\psi_I$$

$$\psi_I = A_1 e^{ikx} + B_1 e^{-ikx} \quad , \qquad \mathrm{E} = \frac{\mathrm{p}^2}{2\mathrm{m}} = \frac{\hbar^2 \mathrm{k}^2}{2\mathrm{m}} \quad , \ k \text{ real}$$

$$0 \le x \le a \qquad -\frac{\hbar}{2m}\frac{d^2\psi_{II}}{dx^2} + \mathrm{V}_0\psi_{II} = E\psi_{II}$$

$$\psi_{II} = Ce^{\gamma x} + De^{-\gamma x} \quad , \qquad \mathrm{V}_0 - \mathrm{E} = \frac{\hbar^2\gamma^2}{2\mathrm{m}} \quad , \ \gamma \text{ real}$$

$$x \ge a \qquad -\frac{\hbar}{2m}\frac{d^2\psi_{III}}{dx^2} = E\psi_{III}$$

$$\psi_{III} = A_2 e^{ikx} + B_2 e^{-ikx} \quad , \qquad \mathrm{E} = \frac{\mathrm{p}^2}{2\mathrm{m}} = \frac{\hbar^2 \mathrm{k}^2}{2\mathrm{m}} \quad , \ k \text{ real}$$

A term of the form $A_1 e^{ikx}$ corresponds physically to a particle traveling towards $+x$ (to the right) and a term of the form $B_1 e^{-ikx}$ corresponds physically to a particle traveling towards $-x$ (to the left).

If we set up the experiment so that there are particles moving towards $+x$ (on the left) at the start, then later we expect particles also to be traveling to towards $-x$ (on the left). Hence, we expect both coefficients A_1 and B_1 to be nonzero. On the other hand, there are no particle sources on the right and thus, the only way particles can be on the right is if they came from the left side and therefore must be traveling towards $+x$. We therefore assume that the coefficient $B_2 = 0$

We have two sets of continuity equations (at $x=0$ and $x=a$). At $x=0$ we get

$$\psi_I(0) = \psi_{II}(0) \qquad \rightarrow A_1 + B_1 = C + D$$
$$\frac{d\psi_I(0)}{dx} = \frac{d\psi_{II}(0)}{dx} \rightarrow ik(A_1 - B_1) = \gamma(C - D)$$

and at $x=a$ we get

$$\psi_{II}(a) = \psi_{III}(a) \qquad \rightarrow Ce^{\gamma a} + De^{-\gamma a} = A_2 e^{ika}$$
$$\frac{d\psi_I(a)}{dx} = \frac{d\psi_{II}(a)}{dx} \rightarrow \gamma(Ce^{\gamma a} - De^{-\gamma a}) = ikA_2 e^{ika}$$

The reflection and transmission probabilities are given by

$$R = \frac{|B_1|^2}{|A_1|^2} \quad , \quad T = \frac{|A_2|^2}{|A_1|^2}$$

Algebra shows $R + T = 1$ as it must in order to conserve probability (or particles). Evaluating (horrible algebra that you will do in a later course) the expression for T we get is

$$T = \frac{1}{1 + \dfrac{V_0^2 \sinh^2 \gamma a}{4E(V_0 - E)}} \quad , \quad \gamma^2 = (V_0 - E)\frac{2m}{\hbar^2}$$

The fact that $T > 0$ for $E < V_0$ implies the existence of **tunneling.** The probability amplitude **leaks through the barrier.**

It is important to realize that the fact that $T > 0$ **DOES NOT** say that particles passed through the barrier.

No measurement can be done on the system that will allow us to observe a particle in the region $0 < x < a$ with $E < V_0$, since this would violate energy conservation.

It is **ONLY** probability that is leaking through.

If this causes the probability amplitude and hence the probability to be nonzero on the other side of the barrier, than it **must be possible for us to observe** the particle on the other side, i.e., we can observe the particle on the left side of the barrier with $E < V_0$ and later in time on the right side of the barrier with $E < V_0$, but we can never observer it in the region of the barrier with $E < V_0$.

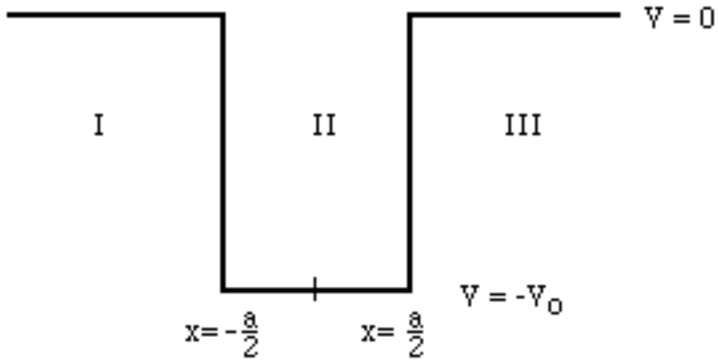
That is what is being said here.

The Finite Square Well

We now consider the potential energy function

$$V(x) = \begin{cases} -V_0 & -\frac{a}{2} \le x \le \frac{a}{2} \\ 0 & |x| \ge \frac{a}{2} \end{cases}$$

This is the so-called **finite square well** shown in the figure below.



The solutions are:

Region I : $x < -\frac{a}{2}$, $-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} = E\psi_I$, $0 \ge E \ge -V_o$, $\hbar^2 k^2 = 2m|E|$, $E = -|E|$

$$\psi_I(x) = Ae^{-kx} + Be^{kx}$$

Since $x = -\infty$ is included in this region, we must exclude the e^{-kx} term by choosing $A = 0$ (otherwise the wave function cannot be normalized), which gives

$$\psi_I(x) = Be^{kx} \qquad x < -\frac{a}{2}$$

Region II: $\frac{a}{2} \ge x \ge -\frac{a}{2}$, $-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} - V_0\psi_{II} = E\psi_{II}$

$$0 \ge E \ge -V_o \ , \ \hbar^2 k^2 = 2m|E| \ , \ E = -|E| \ , \ p^2 = 2m(V_0 - |E|)$$

$$\psi_{II}(x) = Ce^{i\frac{p}{\hbar}x} + De^{-i\frac{p}{\hbar}x}$$

Region III: $x > \frac{a}{2}$, $-\frac{\hbar^2}{2m}\frac{d^2\psi_{III}}{dx^2} = E\psi_{III}$, $0 \ge E \ge -V_o$, $\hbar^2 k^2 = 2m|E|$, $E = -|E|$

$$\psi_{III}(x) = Fe^{kx} + Ge^{-kx}$$

Since $x = \infty$ is included in this region, we must exclude the e^{kx} term by choosing $F = 0$, which gives

$$\psi_{III}(x) = Ge^{-kx} \qquad x > \frac{a}{2}$$

This represents a general solution to the problem. There seems to be 4 unknown constants, namely, B, C, D, and G. However, since $V(x) = V(-x)$, parity is conserved and we can choose even and odd solutions, or solutions of definite parity.

Even parity implies $\psi(x) = \psi(-x)$ or G = B and C = D. This solution is

$$\psi_{even}(x) = \begin{cases} C\cos\dfrac{px}{\hbar} & , \quad |x| \le \dfrac{a}{2} \\ Be^{-kx} & , \quad x > \dfrac{a}{2} \\ Be^{kx} & , \quad x < -\dfrac{a}{2} \end{cases}$$

Odd parity implies $\psi(x) = -\psi(-x)$ or G = -B and D = -C. This solution is

$$\psi_{odd}(x) = \begin{cases} C\sin\dfrac{px}{\hbar} & , \quad |x| \le \dfrac{a}{2} \\ Be^{-kx} & , \quad x > \dfrac{a}{2} \\ -Be^{kx} & , \quad x < -\dfrac{a}{2} \end{cases}$$

Thus, by using parity we reduce the number of unknowns in the problem to two for each type of solution. We now impose the continuity conditions of the wave function and its derivative only at $x = \frac{a}{2}$ for both solutions. Since these are definite parity solutions the continuity condition at $x = -\frac{a}{2}$ will give no new information and is not needed.

Even parity

$$A\cos\frac{pa}{2\hbar} = Ce^{-\frac{ka}{2}} \quad \text{and} \quad -\frac{p}{\hbar}A\sin\frac{pa}{2\hbar} = -kCe^{-\frac{ka}{2}}$$

$$\frac{C}{A} = e^{\frac{ka}{2}}\cos\frac{pa}{2\hbar} = \frac{p}{\hbar k}e^{\frac{ka}{2}}\sin\frac{pa}{2\hbar}$$

$$p\tan\frac{pa}{2\hbar} = \hbar k$$

This last equation is a **transcendental** equation for the E and its solutions determine the allowed E values for the even parity states for this potential energy function. These E values are the even parity energies or energy levels of a particle in the finite square well potential.

Odd Parity

$$A\sin\frac{pa}{2\hbar} = Ce^{-\frac{ka}{2}} \quad \text{and} \quad \frac{p}{\hbar}A\cos\frac{pa}{2\hbar} = -kCe^{-\frac{ka}{2}}$$

$$\frac{C}{A} = e^{\frac{ka}{2}}\sin\frac{pa}{2\hbar} = -\frac{p}{\hbar k}e^{\frac{ka}{2}}\cos\frac{pa}{2\hbar}$$

$$p\cot\frac{pa}{2\hbar} = -\hbar k$$

Again, this last equation is a transcendental equation for the E and its solutions determine the allowed E values for the odd parity states for this potential energy function. These E values are the odd parity energies or energy levels of a particle in the finite square well potential.

In general, at this stage of the solution, we must either devise a clever numerical or graphical trick to find the solutions of the transcendental equations or resort to a computer.

The first thing one should always do is change variables to get rid of as many extraneous constants as possible. In this case we let

$$\beta = ka = \frac{a}{\hbar}\sqrt{2m|E|} \quad , \quad \alpha = \gamma a = \frac{p}{\hbar}a = \frac{a}{\hbar}\sqrt{2m(V_0 - |E|)}$$

The first useful equation we can derive is

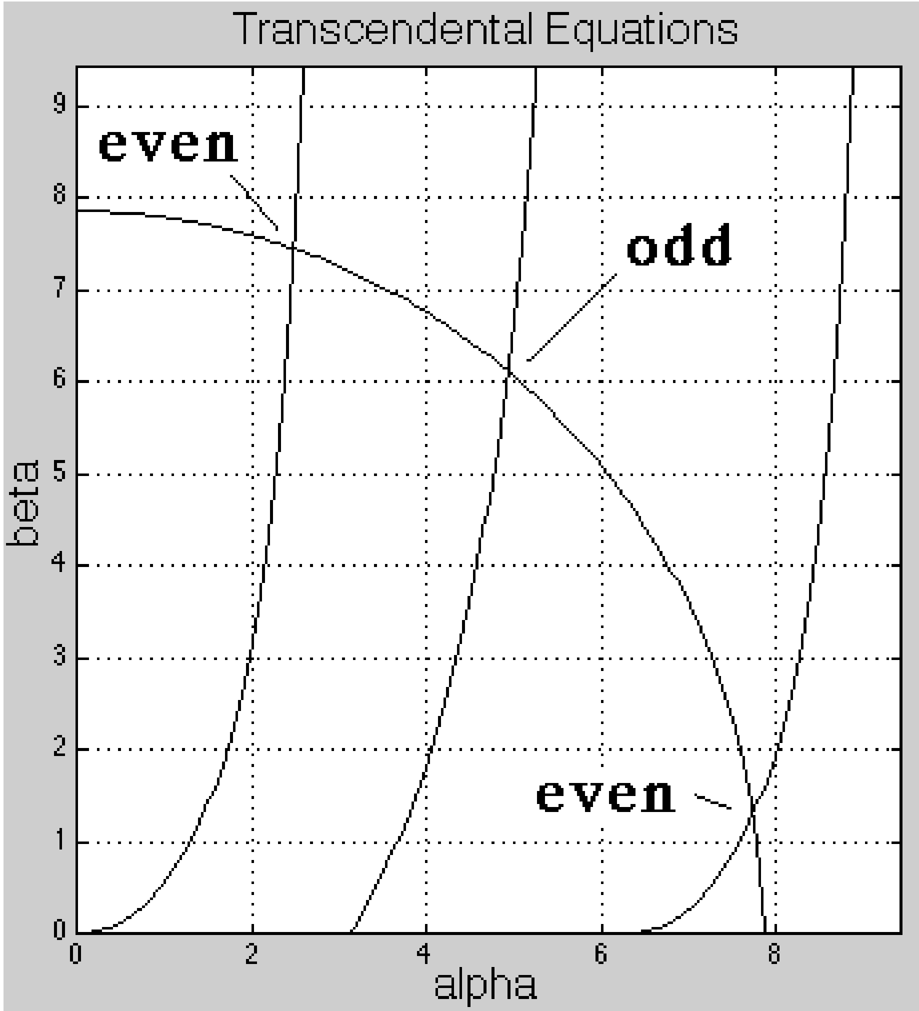
$$\alpha^2 + \beta^2 = \frac{2mV_0a^2}{\hbar^2} = \text{constant for a given well}$$

This is the equation of a circle or radius $\sqrt{\frac{2mV_0a^2}{\hbar^2}}$. With these new variables the two transcendental equations are

$$\beta = \alpha\tan\frac{\alpha}{2} \quad \text{even parity} \quad \text{and} \quad \beta = -\alpha\cot\frac{\alpha}{2} \quad \text{odd parity}$$

We can find solutions graphically by plotting as shown below for the case (effectively a choice of the quantity V_0a^2)

$$\text{circle radius} = \sqrt{\frac{2mV_0a^2}{\hbar^2}} = \frac{5\pi}{2}$$



The solutions correspond to the intersections of the circle (fixed for a given well) and the curves represented by the two transcendental equations. It is shown in the figure.

For the choice of potential well shown in the figure we have 2 even parity solutions and 1 odd parity solution. These correspond to the allowed energy levels for this particular well and the corresponding wave functions and energies represent bound states of the well.

We can also do a straight numerical solution for even parity by rearranging the equations as follows:

$$\alpha^2 + \beta^2 = \frac{2mV_0a^2}{\hbar^2} \quad \text{and} \quad \beta = \alpha \tan\frac{\alpha}{2}$$

$$\alpha^2(1+\tan^2\frac{\alpha}{2}) = \frac{\alpha^2}{\cos^2\frac{\alpha}{2}} = \frac{2mV_0a^2}{\hbar^2}$$

$$\alpha^2 - \frac{2mV_0a^2}{\hbar^2}\cos^2\frac{\alpha}{2} = 0$$

For the case $\sqrt{\frac{2mV_0a^2}{\hbar^2}} = \frac{5\pi}{2}$ we have $\alpha^2 - \frac{25\pi^2}{4}\cos^2\frac{\alpha}{2} = f(\alpha) = 0$

The numerical solution of this equation can be carried out by any standard technique (Newton-Raphson method, for instance) for finding the zeros of the function $f(\alpha)$. For this case we get

$$\alpha = 2.4950 \quad \text{and} \quad 7.1416$$

which is clearly in agreement with the graphical result.

Delta-Function Potentials

We now consider the potential energy function

$$V(x) = A\delta(x-a)$$

where

$$\delta(x-a) = 0 \quad x \neq a$$

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

and solve the corresponding Schrodinger equation

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

As we discussed earlier the wave function $\psi(x)$ is assumed to be continuous for physical reasons relating to the probability interpretation. The derivative of the wave function, however, is not continuous at $x = a$ for this potential. We can see this as follows. We have

$$-\frac{\hbar^2}{2m}\int_{a-\varepsilon}^{a+\varepsilon}\frac{d^2\psi(x)}{dx^2}dx + A\int_{a-\varepsilon}^{a+\varepsilon}\delta(x-a)V(x)\psi(x)dx = E\int_{a-\varepsilon}^{a+\varepsilon}\psi(x)dx$$

In the limit $\varepsilon \to 0$, using the continuity of $\psi(x)$, we get

$$-\frac{\hbar^2}{2m}\left[\left.\frac{d\psi}{dx}\right|_{a+\varepsilon} - \left.\frac{d\psi}{dx}\right|_{a-\varepsilon}\right] = E\psi(a)\int_{a-\varepsilon}^{a+\varepsilon}dx - A\psi(a)$$

$$-\frac{\hbar^2}{2m}\left[\left.\frac{d\psi}{dx}\right|_{a+\varepsilon} - \left.\frac{d\psi}{dx}\right|_{a-\varepsilon}\right] = E\psi(a)\int_{a-\varepsilon}^{a+\varepsilon}dx - A\psi(a)$$

$$discontinuity\left(\frac{d\psi}{dx}\right)_{x=a} = \Delta\left(\frac{d\psi}{dx}\right) = \frac{2mA}{\hbar^2}\psi(a)$$

For simplicity we choose $a = 0$. We have two regions to consider

region I $x < 0$, region II $x > 0$

and the derivative is discontinuous at $x = 0$.

Transmission Problem

We first carry out the calculation of the transmission and reflection probabilities. We assume that $A > 0$ (we have a delta function barrier), $E > 0$ and an incident wave of unit intensity coming in form the left.

In region I we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} = E\psi_I \to \psi_I(x) = e^{ikx} + Be^{-ikx} \quad \text{with} \quad E = \frac{\hbar^2 k^2}{2m} > 0$$

We have **both** an incident and a reflected wave.

In region II we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} = E\psi_{II} \to \psi_{II}(x) = Ce^{ikx} \quad \text{with} \quad E = \frac{\hbar^2 k^2}{2m} > 0$$

There is **only** a transmitted wave.

The boundary conditions (at $x = 0$) give

$$\psi_I(0) = \psi_{II}(0) \to 1 + B = C$$
$$\frac{d\psi_{II}(0)}{dx} - \frac{d\psi_I(0)}{dx} = \frac{2m}{\hbar^2}A\psi_{II}(0) \to ikC - ik(1-B) = \frac{2m}{\hbar^2}AC$$

The solutions are

$$C = \frac{ik}{ik - \frac{mA}{\hbar^2}} \quad \text{and} \quad B = \frac{\frac{mA}{\hbar^2}}{ik - \frac{mA}{\hbar^2}}$$

We then have

$$T = \text{transmission probability} = |C|^2 = \frac{1}{1 + \frac{mA^2}{2\hbar^2 E}}$$
$$R = \text{reflection probability} = |B|^2 = \frac{1}{1 + \frac{2\hbar^2 E}{mA^2}}$$

We note that $T + R = 1$ as it must for the probability interpretation to make sense.

From our previous discussion, we suspect that the energy values of the poles of the transmission probability correspond to the bound state energies for the delta function well problem ($A < 0$). For the single delta function potential, T has a pole at

$$E = -\frac{mA^2}{2\hbar^2}$$

Bound-State Problem

We let $A \to -A, A > 0$. In region I we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} = -|E|\psi_I \to \psi_I(x) = Be^{\alpha x} \quad \text{with} \quad E = -|E| = -\frac{\hbar^2\alpha^2}{2m} < 0$$

We have excluded the negative exponential term since it would diverge in region I as $x \to -\infty$.

In region II we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} = -|E|\psi_{II} \to \psi_{II}(x) = Ce^{-\alpha x} \quad \text{with} \quad E = -|E| = \frac{\hbar^2\alpha^2}{2m} < 0$$

We have excluded the positive exponential term since it would diverge in region II as $x \to +\infty$.

The boundary conditions give

$$\psi_I(0) = \psi_{II}(0) \to B = C$$
$$\frac{d\psi_{II}(0)}{dx} - \frac{d\psi_I(0)}{dx} = -\frac{2m}{\hbar^2}A\psi_I(0) \to -\alpha C - \alpha B = -\frac{2m}{\hbar^2}AB$$

The resulting equation for α gives the allowed the bound state energies. We have

$$\alpha = \frac{mA}{\hbar^2} \to \text{only 1 solution only} \to \text{ 1 bound state}$$
$$E = -|E| = -\frac{\hbar^2\alpha^2}{2m} = -\frac{mA^2}{2\hbar^2}$$

which is the **same** value as we obtained from the pole of the transmission probability.

We also note that the solution has definite parity (even) since $\psi(x) = \psi(-x)$. This must occur since $V(x) = V(-x)$ and hence parity commutes with the Hamiltonian. As we also saw in the square well case, if only one solution exists then it is always an even parity solution.