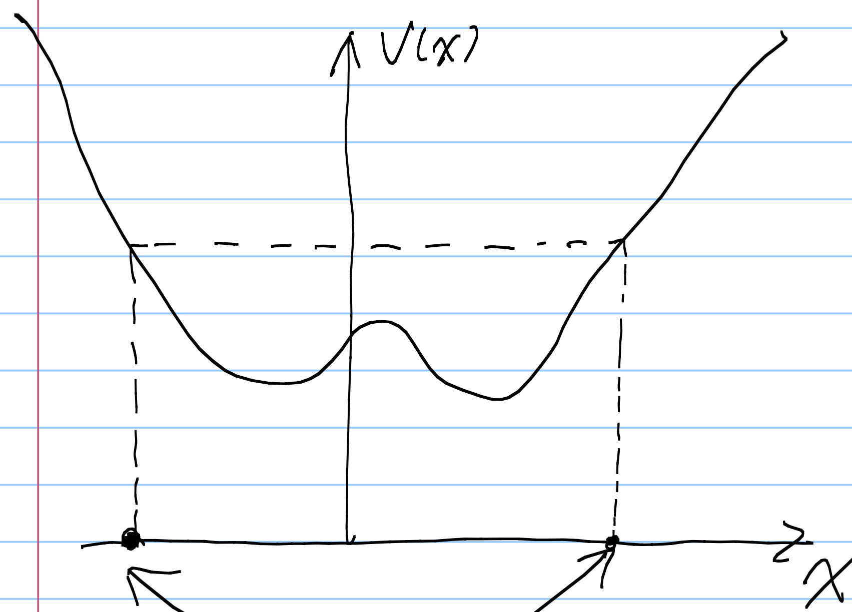
Delta function Potential

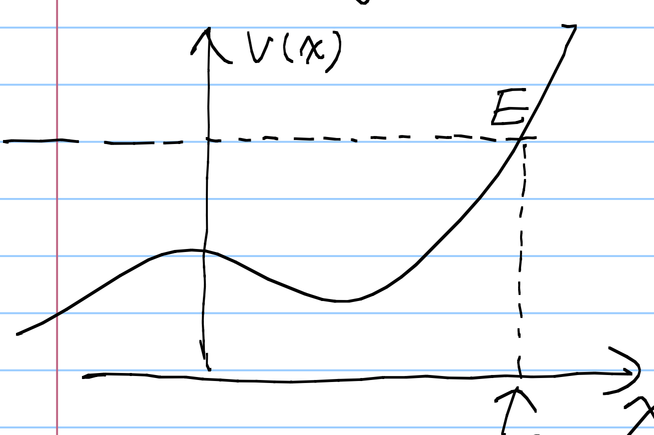
Note Title

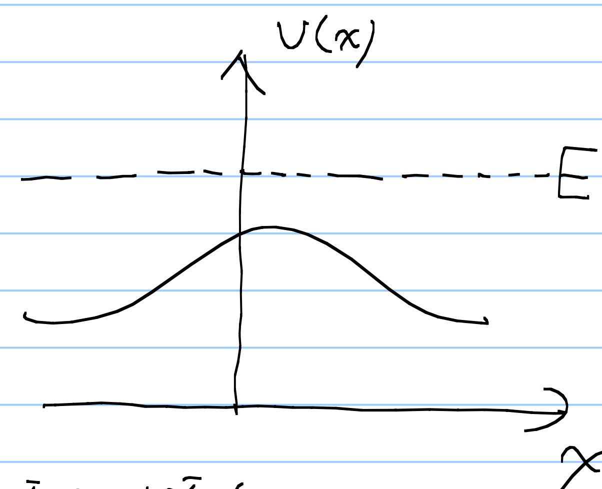
* Bound states



classical turning points

* Scattering states



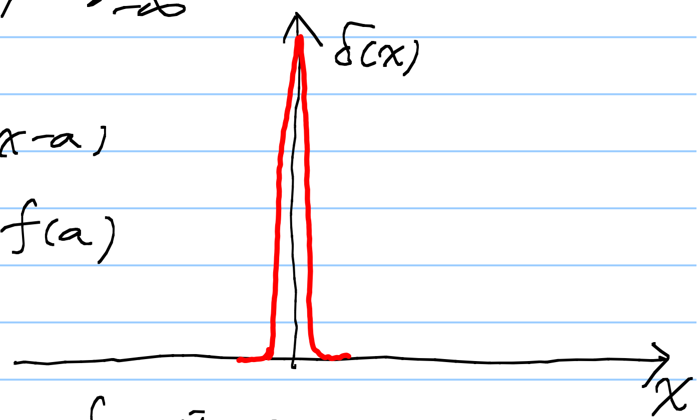


classical turning points

Bound states	vs Scattering states
Normalizable	non-normalizable
discrete energies	continuous energies
discrete summation for index "n"	integral for continuous variable "k"

* Dirac-delta function (or just delta function)

$$\delta(x) = \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases}, \quad \int_{-\infty}^{\infty} \delta(x)\,dx = 1$$



$$f(x)\,\delta(x-a) = f(a)\,\delta(x-a)$$

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

* Examples of Dirac-delta functions

$$\delta(x) = \lim_{a\to 0} \frac{1}{\pi x} \sin\left(\frac{x}{a}\right)$$

$$\delta(x) = \lim_{a\to 0} \begin{cases} \frac{1}{a}, & \text{for } -\frac{a}{2} < x < \frac{a}{2} \\ 0, & \text{otherwise} \end{cases}$$

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx}\,dk$$

$$\delta(x) = \lim_{a\to 0} \frac{1}{a\sqrt{\pi}} e^{-x^2/a^2}$$

* Properties of delta functions

$$\delta(-x) = \delta(x), \quad \delta(cx) = \frac{1}{|c|}\,\delta(t), \ \left(c \ \begin{matrix}\text{real} \\ \neq 0\end{matrix}\right)$$

For a step function $\theta(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x < 0 \end{cases}$

$$\frac{d\,\theta(x)}{dx} = \delta(t)$$

$\boxed{\text{Ex.}}$

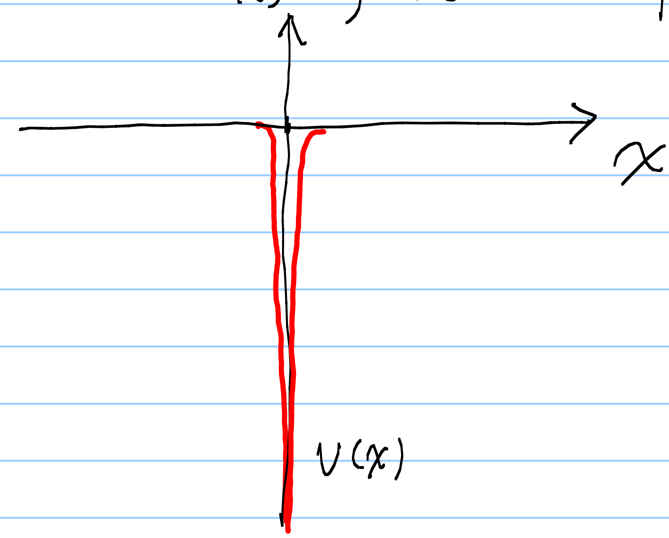
$$\int_{0}^{\infty} [\cos(3x) + 2]\,\delta(x-\pi)\,dx$$

$$= \cos(3\pi) + 2 = -1 + 2 = 1$$

$$\int_{-1}^{1} \exp(|x| + 3)\,\delta(x-2)\,dx = 0$$

* Delta-function Well

$V(x) = -\alpha\delta(x)$, α some positive constant



Time-independent Schrödinger Eq.

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

$E<0 \Rightarrow$ Bound state

$E>0 \Rightarrow$ Scattering state

* First, if $E<0$ (i.e. Bound state)

For $x<0$, $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi$

$$\Rightarrow \frac{d^2\psi}{dx^2} = \kappa^2\psi, \quad \kappa \equiv \frac{\sqrt{2m|E|}}{\hbar}$$

$\Rightarrow$ The general solution is

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}$$

Since $\psi(-\infty) = 0 \Rightarrow A = 0$, $\psi(x) = Be^{\kappa x}$

Now for $x>0$, in a similar way

$$\psi(x) = Fe^{-\kappa x} + Ge^{\kappa x}$$

with $\psi(\infty) = 0 \Rightarrow G = 0 \therefore \psi(x) = Fe^{-\kappa x}$

Now, standard boundary conditions are

1. $\psi(x)$ is always continuous.
2. $d\psi/dx$ is continuous except where the potential is infinite.

So with the first boundary condition at $x=0$

$$\psi_-(0) = \psi_+(0) \Rightarrow B = F$$

$$\therefore \psi(x) = \begin{cases} B e^{\kappa x} & \text{for } x<0 \\ B e^{-\kappa x} & \text{for } x>0 \end{cases}$$

Now the second B.C. requires special treatment here, because $V(x) = -\alpha\delta(x)$ infinite at $x=0$.

Considering that $\int_{-\infty}^{\infty}\delta(x)f(x)dx = \int_{-\epsilon}^{\epsilon}\delta(x)f(x)dx = f(0)$, $\epsilon\to 0$

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

$$\Rightarrow -\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}dx - \alpha\int_{-\epsilon}\delta(x)\psi(x)dx = E\int_{-\epsilon}^{\epsilon}\psi dx$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left.\frac{d\psi}{dx}\right|_{-\epsilon}^{\epsilon} - \alpha\psi(0) = E\int_{-\epsilon}^{\epsilon}\psi dx$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left(\frac{d\psi_+(0)}{dx} - \frac{d\psi_-(0)}{dx}\right) - \alpha\psi(0) = 0$$

with $\epsilon\to 0$

$$\Rightarrow \boxed{\Delta\left(\frac{d\psi}{dx}\right)} = \frac{d\psi_+(0)}{dx} - \frac{d\psi_-(0)}{dx} = \boxed{-\frac{2m\alpha}{\hbar^2}\psi(0)}$$

$$\Delta\left(\frac{d\psi}{dx}\right) = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

$$\Rightarrow \frac{d\psi_+(0)}{dx} = \frac{d}{dx}\left(B e^{-\kappa x}\right)\Big|_{x=0} = -\kappa B$$

$$\frac{d\psi_-(0)}{dx} = \frac{d}{dx}\left(B e^{\kappa x}\right)\Big|_{x=0} = \kappa B$$

$$\therefore \Delta\left(\frac{d\psi}{dx}\right) = -2\kappa B = -\frac{2m\alpha}{\hbar^2}\underbrace{\psi(0)}_{=B}$$

$$\Rightarrow \kappa = \frac{m\alpha}{\hbar^2}, \quad E = -\frac{\hbar^2\kappa^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}$$

Finally "B" can be found by normalization

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 2\int_0^{\infty} |B e^{-\kappa x}|^2 dx$$

$$= 2\int_0^{\infty} B^2 e^{-2\kappa x} dx = 2B^2 \frac{1}{2\kappa} = \frac{B^2}{\kappa}$$

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

So we have only one bound state regardless of the value "α", which is

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar}\exp\left(-\frac{m\alpha}{\hbar^2}|x|\right)$$

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

Scattering from Delta-function Potential

Now from the previous problem, $E > 0$ case corresponds to scattering states because there are no turning points.

In this case,

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

for both $x>0$ and $x<0$, and we have to use boundary conditions at $x=0$

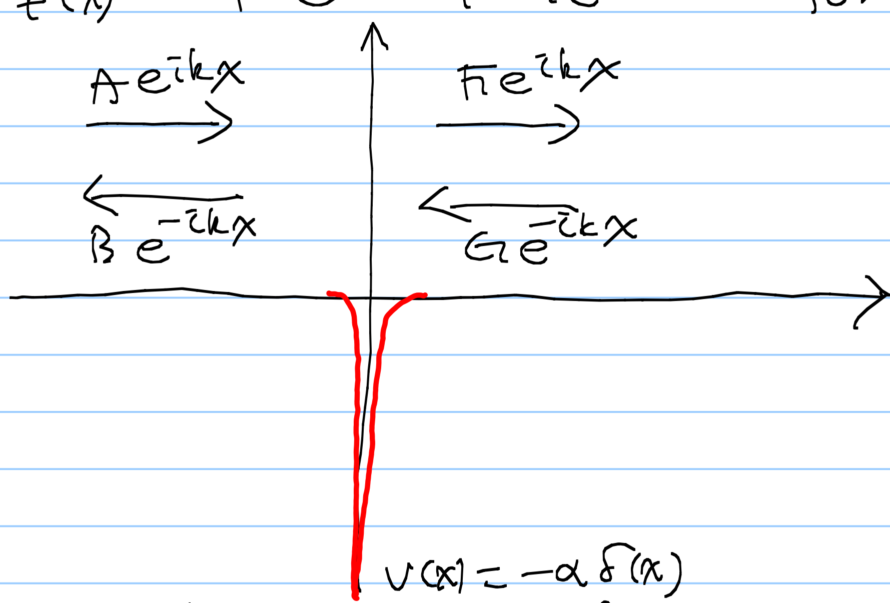
$$\rightarrow \quad \frac{d^2\psi(x)}{dx^2} = -k^2\psi(x), \quad k^2 = \frac{2mE}{\hbar^2}$$

$$\Rightarrow k = \frac{\sqrt{2mE}}{\hbar}$$

The general solution looks like

$$\psi_L(x) = Ae^{ikx} + Be^{-ikx} \quad \text{for } x<0$$

$$\psi_R(x) = Fe^{ikx} + Ge^{-ikx} \quad \text{for } x>0$$



If we consider a particle injected from the left, G must be zero. Then

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad \text{for } x<0$$
$$\psi_{+}(x) = Fe^{ikx} \quad \text{for } x>0$$

We already know that the unbound scattering states are not normalizable and all "k" values are possible.

So our objectives are not finding the allowed k values or A, B and F values.

But it is still meaningful to find the relative values of A, B and F w.r.t. each other.

These values will provide reflection coefficient and transmission coefficient.

Considering that classical definition of current density is $J = nv$, with n being the density

We can expect that $|\psi(x)|^2 v$ is some kind of current density

$$v = \frac{p}{m} = \frac{\hbar k}{m} \Rightarrow J = \frac{\hbar k}{m}|\psi(x)|^2$$

[More formal definition of J is

$$J(x,t) \equiv \frac{i\hbar}{2m}\left(\Psi(x,t)\frac{\partial\Psi^*(x,t)}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right)$$

as shown in G. Prob. 1.14]

We can now define the reflection coefficient as

$$R = \frac{v_-|B|^2}{v_-|A|^2} = \frac{k_-|B|^2}{k_-|A|^2} = \frac{|B|^2}{|A|^2}$$

$$\Rightarrow \quad R = \left|\frac{B}{A}\right|^2$$

Similarly, the transmission coefficient is defined as

$$T \equiv \frac{v_+ |F|^2}{v_- |A|^2} = \frac{k_+ |F|^2}{k_- |A|^2}$$

Now let's continue solving the delta-function scattering problem from above.

$$\psi_-(x) = A e^{ikx} + B e^{-ikx}$$

$$\psi_+(x) = F e^{ikx}$$

With the 1st boundary condition

$$\psi_-(0) = \psi_+(0) \Rightarrow A + B = F \quad - \circledast$$

with the 2nd B.C.,

$$\Delta\left(\frac{d\psi}{dx}\right) = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

$$\Rightarrow (ikF) - ik(A - B) = -\frac{2m\alpha}{\hbar^2} F$$

$$\Rightarrow \quad F - A + B = -\frac{2m\alpha}{ik\hbar^2} F = 2i\beta F$$

$$, \quad \beta \equiv \frac{m\alpha}{\hbar^2 k}$$

$$\Rightarrow \quad A - B = F(1 - 2i\beta) \quad - \circledast\circledast$$

Combining $\circledast$ & $\circledast\circledast$, $2A = 2F(1 - i\beta)$

$$\Rightarrow \quad F = \frac{A}{1 - i\beta}, \quad B = \frac{i\beta}{1 - i\beta} A$$

So $R = \left|\frac{B}{A}\right|^2 = \left|\frac{i\beta}{1-i\beta}\right|^2 = \frac{\beta^2}{1+\beta^2}$

$$T = \frac{k_+ |F|^2}{k_- |A|^2} = \left|\frac{F}{A}\right|^2 = \frac{1}{1+\beta^2}$$

$k_+ = k_- = k$

Note that $R+T=1$, as it should be

So with $\beta \equiv \frac{m\alpha}{\hbar^2 k} \Rightarrow \beta^2 = \left(\frac{m\alpha}{\hbar^2}\right)^2 \cdot \frac{\hbar^2}{2mE}$

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

$$R = \frac{1}{\left(\frac{1}{\beta}\right)^2 + 1} = \frac{1}{1 + \frac{2\hbar^2 E}{m\alpha^2}}$$

$$T = \frac{1}{1+\beta^2} = \frac{1}{1+(m\alpha^2/2\hbar^2 E)}$$

Note: In this case, $k_+ = k_-$, so the transmission coefficient was trivially $T = \left|\frac{F}{A}\right|^2$. However, in the case of step potential we will study in next lecture $k_+ \neq k_1$ and so $T \neq \left|\frac{F}{A}\right|^2$.

Also see prob. 2.34.