

Key Concepts

1. Free Particle Schrödinger Solution
2. Delta-Function Potential $\delta(x)$

II. Free Particle in One Dimension

Free particle has $\hat{H} = \frac{\hat{p}^2}{2m}$ thus the time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_k}{dx^2} = E \psi_k$$

$$\text{or rewriting } \frac{d^2 \psi_k}{dx^2} = -\frac{2mE}{\hbar^2} \psi_k \equiv -k^2 \psi_k$$

where $\psi_k(x)$ are the eigenstates. This is easy to solve via:

$\psi_k = A \cos(kx) + B \sin(kx)$ is a general soln, but these look like standing waves.

To describe moving particles we want travelling waves, so a better general soln is:

$\psi_k = A e^{ikx} + B e^{-ikx}$ where

$k = \sqrt{\frac{2mE}{\hbar^2}}$ is any real number, and $E = \frac{\hbar^2 k^2}{2m}$.

To see the travelling wave nature of these solns we include the time dependence term $e^{-iEt/\hbar}$:

$$\begin{aligned} \psi_k(x, t) &= A e^{ikx} e^{-\frac{itE}{\hbar}} + B e^{-ikx} e^{-\frac{itE}{\hbar}} \\ &= \underbrace{A e^{i(kx - \frac{\hbar k^2 t}{2m})}}_{\text{free particle moving in positive } x \text{ direction}} + \underbrace{B e^{-i(kx + \frac{\hbar k^2 t}{2m})}}_{\text{moving in negative } x \text{ direction}} \end{aligned}$$

where we have used $E = \frac{\hbar^2 k^2}{2m}$. These seem to be reasonable solns ...

But!!

\hookrightarrow We can't normalize these ψ_k since $\int_{-\infty}^{\infty} \psi_k^* \psi_k dx$ includes terms like $A^* A \int_{-\infty}^{\infty} dx = \infty$. This occurs because the exponential terms times their complex conjugate is $= 1$.

Thus ψ_k **can't** be real physical states (since they don't have finite total probability)

But we know that real particles can be localized: in your hand or in the Solar System.

Thus, even though ψ_k are not physical wavefunctions, superpositions of ψ_k can produce physical states and localized particles \Rightarrow called wave packets.

Since energies and k values are continuous we should take the discrete sums from earlier and convert them to integrals. Thus arbitrary free particle solutions should look like:

$$\psi(x, t) \equiv \sum_{k=0}^{\infty} A_k e^{i(kx - \frac{\hbar k^2 t}{2m})} + B_k e^{i(-kx - \frac{\hbar k^2 t}{2m})} \Rightarrow \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2 t}{2m})} dk$$

where the integral from $-\infty$ to ∞ allows the $\phi(k)$ to automatically include both the “ A_k ” and the “ B_k ” terms, and the $\sqrt{2\pi}$ is inserted for ”convenience” ...
 \hookrightarrow since it allows us a connection to Fourier transforms.

But how do we calculate $\phi(k)$ from a given initial state $\psi(x, 0) = \psi(x)$?

To do so we set $t = 0$ in above equation and given $\psi(x, 0) = \psi(x)$

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} dk$$

we can then solve for $\phi(k)$ via a Fourier transform

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x, 0) e^{-ikx} dx$$

Note: $\phi(k)$ is sometimes called the k-space wave function such that $\phi^*(k)\phi(k)dk$ is the probability of observing a state with wave number (k) between k and $k + dk$.

And since $p = \hbar k$ and $E = \hbar^2 k^2 / 2m = p^2 / 2m$, we can also define the momentum space wave function $\phi(p)$. Then since $p = \hbar k$ we have $\phi(p) = \frac{1}{\sqrt{\hbar}} \phi(k)$.

2. “Delta-function” - $\delta(x)$, and the $\delta(x)$ -Potential

The properties of the Dirac Delta function $\delta(x)$

(Mathematicians call this a distribution) -

are defined by an integral:

$$\delta(x) = 0 \text{ if } x \neq 0 \text{ and } \int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0)$$

Consider now a finite well with $V_0 \rightarrow -\infty, a \rightarrow 0$
 but with $V_0 a = \text{constant} \rightarrow V(x) = -V_0 a \delta(x)$.

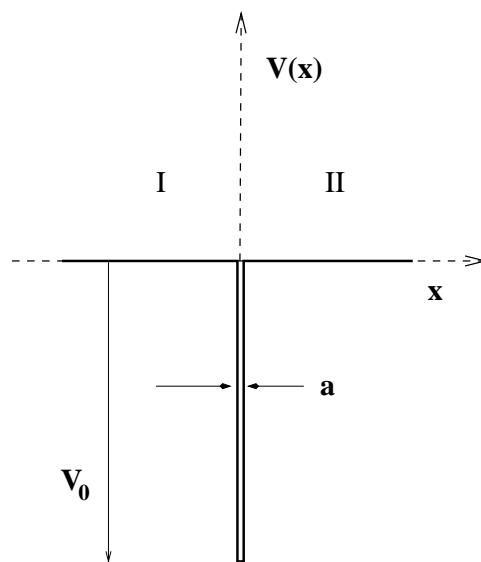
Think of $V_0 a$ as a varying strength for the potential.

And we expect the energy eigenvalues to depend on this quantity.

There are, very likely, lots of states with $E > 0$

but these will be travelling waves (see next week).

Here we ask: are there bound states for this potential?



To solve these types of problems we usually break up the space around the localized potential into regions to solve the TISE eigenvalue equation: $\hat{H}\psi = E\psi$

$$\hat{H}\psi = \frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} - V_0 a \delta(x) \psi = E\psi$$

and then use 3 steps to solve (The Recipe):

A. Guess the solution

For $x \neq 0$ note that

Diff. Eq. is $\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = \frac{2m|E|}{\hbar^2}\psi = \kappa^2\psi$ since $E < 0$:

$$\begin{aligned}\psi_I &= Ae^{+\kappa x}; \text{ for } x < 0 \text{ with } \kappa^2 = -\frac{2mE}{\hbar^2} = \frac{2m|E|}{\hbar^2}, \kappa > 0 = \text{real number} \\ \psi_{II} &= Be^{-\kappa x}; \text{ for } x > 0.\end{aligned}$$

B. Next we match the wavefunction at $x = 0$, since we need a continuous $\psi(x)$:

$$\psi_I(0) = \psi_{II}(0) \Rightarrow A = B \text{ (and from normalization } \int \psi^* \psi dx = 1, \text{ we get: } A = \sqrt{\kappa}).$$

To find allowed values of κ and thus the energy eigenvalues we need another constraint on the wave function.

What about $\frac{d\psi}{dx}$? Clearly, this can't be continuous, since there's a divergence at $x = 0$ due to the $\delta(x)$ -function. However, due to the properties of $\delta(x)$ we can constrain $\frac{d\psi}{dx}$ by noting that

$$\int_{0^-}^{0^+} dx \frac{d}{dx} \left(\frac{d\psi}{dx} \right) = \frac{d\psi_{II}}{dx} \Big|_{x=0^+} - \frac{d\psi_I}{dx} \Big|_{x=0^-} \quad \text{Eq. 1}$$

Then since the Schrodinger Eq. gives: $\frac{d^2\psi}{dx^2} = \frac{d}{dx} \left(\frac{d\psi}{dx} \right) = -\frac{2m}{\hbar^2} [V_0 a \delta(x) - |E|] \psi$, the left side is:

$$\begin{aligned}\int_{0^-}^{0^+} dx \frac{d}{dx} \left(\frac{d\psi}{dx} \right) &= - \int_{0^-}^{0^+} dx \left\{ \frac{2m}{\hbar^2} [V_0 a \delta(x) - |E|] \psi(x) \right\} \\ &= - \left(\frac{2mV_0 a}{\hbar^2} \right) \psi(0) + |E| [x\psi(x)] \Big|_{0^-}^{0^+} = - \left(\frac{2mV_0 a}{\hbar^2} \right) A.\end{aligned}$$

since $\psi(0) = A$ and $|E| [x\psi(x)] \Big|_{0^-}^{0^+} = 0$.

C. Now work out the algebra to solve for the eigenenergies

We can rewrite Eq. 1 with the new left-hand side:

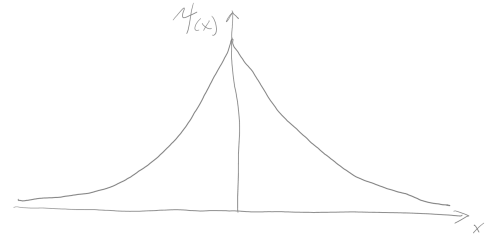
$$- \left(\frac{2mV_0 a}{\hbar^2} \right) A = \frac{d\psi_{II}}{dx} \Big|_{x=0^+} - \frac{d\psi_I}{dx} \Big|_{x=0^-} = A(-\kappa) - B\kappa = -2A\kappa$$

giving:

$$\kappa = \frac{mV_0 a}{\hbar^2}$$

and there is only a single energy eigenvalue, with energy

$$\Rightarrow E = -\frac{\hbar^2 \kappa^2}{2m} = -\frac{\hbar^2}{2m} \left(\frac{mV_0 a}{\hbar^2} \right)^2 = -\frac{mV_0^2 a^2}{2\hbar^2}$$



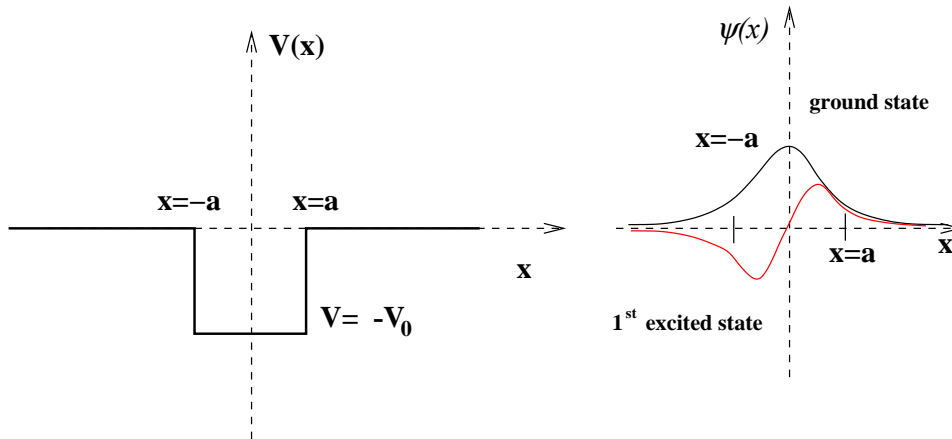
There thus exists one and only one bound state for a $\delta(x)$ -well. See figure showing $\psi(x) \uparrow$

Key Concepts

1. Bound States in a Finite Well
2. Introduction to Scattering States in 1D

1. Finite Square Well

Consider the finite square well:



For $E > 0$ we again have continuous eigenstates (“plane waves” - see later), but ...

For $E < 0$ we have a *finite* number of discrete bound states.

We can use the energy eigenstates of the infinite well as a rough guess for what the ground and first excited states look like within the well and then make them smoothly go to zero outside of well \rightarrow see Fig above for $\psi(x)$.

Thus the ground state is an “even” function where

$$\psi(x < 0) = \psi(x > 0)$$

and the 1st excited state is an odd function where

$$\psi(x < 0) = -\psi(x > 0).$$

The exact general solutions for the energy eigenstates are from $\hat{H}\psi_n = E_n\psi_n$:

$$\frac{-\hbar^2}{2m} \frac{d^2\psi_{in}}{dx^2} - V_0\psi_{in} = E\psi_{in} \quad , \quad \text{inside the well}$$

$$\frac{-\hbar^2}{2m} \frac{d^2\psi_{out}}{dx^2} = E\psi_{out} \quad , \quad \text{outside the well}$$

Use the **Recipe** for solving these types of problems:

A. First we “guess” the exact solns for these simple Diff Eqs:

$$\psi_{in} = A\cos(kx) \quad \text{for the even solns inside the well}$$

$$\psi_{in} = B\sin(kx) \quad \text{for the odd solns inside the well}$$

$$\psi_{out} = Ce^{\kappa x} + De^{-\kappa x} \quad \text{for } |x| \geq a \quad , \quad \text{outside the well}$$

with k and κ defined via:

$$E = \frac{\hbar^2 k^2}{2m} - V_0 = -\frac{\hbar^2 \kappa^2}{2m}$$

which follows from $\hat{H}\psi = E\psi$.

Note that since $E < 0$ for bound states we have k and $\kappa = \text{real number}$. This gives:

$\psi_{in} = \text{oscillatory solutions } [\cos(kx) \text{ or } \sin(kx)]$

$\psi_{out} = \text{exponentially decaying functions } (Ce^{\kappa x} \text{ for } x < -a \text{ and } De^{-\kappa x} \text{ for } x > a)$

B. Match the wave function and its first derivative at the points ($x = \pm a$) where the potential changes - we'll do it for the even solns (only need to worry about $x = +a$); thus:

$$\begin{aligned} \psi_{in}(a) &= \psi_{out}(a) \text{ which gives: } A\cos(ka) = Ce^{\kappa a} \text{ and} \\ \frac{d\psi_{in}}{dx}|_{x=a} &= \frac{d\psi_{out}}{dx}|_{x=a} \text{ giving: } -Aksin(ka) = -C\kappa e^{\kappa a} \end{aligned}$$

Then dividing the bottom equation by the top one we get:

$$k\tan(ka) = \kappa \rightarrow \text{a transcendental equation}$$

C. Solving this equation simultaneously with the energy equation from above

$$\frac{\hbar^2 k^2}{2m} - V_0 = -\frac{\hbar^2 \kappa^2}{2m}$$

gives the eigenenergies

\hookrightarrow this requires a computer or graphical soln (see text).

In particular, note that if either the well depth or width is “too small” there will only be one bound state (= the even ground state). We can see this, since as $V_0 \rightarrow 0$, the first excited state (the odd \sin function) has only 1/2 of a wavelength inside the well such that

$$2a = \frac{\lambda}{2}; \text{ or } \lambda = 4a = \frac{2\pi}{k}; \text{ } k = \frac{\pi}{2a}$$

But to be a bound state we must also have $E < 0$ such that the first excited state (or any excited state for that matter) will not exist if

$$\frac{\hbar^2 k^2}{2m} > |V_0|; \text{ or } \sqrt{\frac{2ma^2 V_0}{\hbar^2}} < \frac{\pi}{2}, \text{ or } a^2 V_0 < \frac{\pi^2 \hbar^2}{8m}$$

since $k = \pi/2a$.

Introduction to 1-D Scattering States

Why Discuss scattering?

\hookrightarrow Essential tool in many branches of physics:

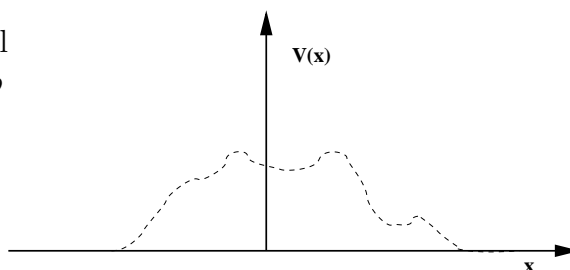
- Condensed Matter Physics \Rightarrow neutron-materials, X-ray-materials
- Nuclear Physics \Rightarrow p-Nucleus, e^- -nucleus
- Atomic Physics \Rightarrow e^- -Atom, Laser-Atom
- Particle Physics \Rightarrow $p - \bar{p}$, $e^- - e^+$
- Astrophysics \Rightarrow Cosmic Microwave Background Radiation- e^-

Scattering reveals information on elementary force laws and the structure of objects. We will consider only elastic scattering (energy and number of particles are conserved).

Consider a localized potential

$$\Rightarrow V(x) \neq 0, \quad a \leq x \leq b$$

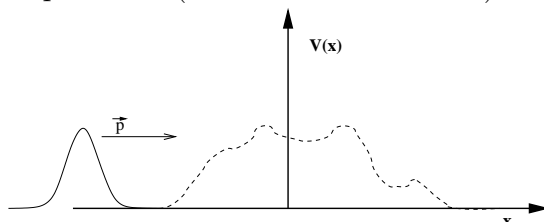
$$\rightarrow 0, \quad |x| \rightarrow \infty$$



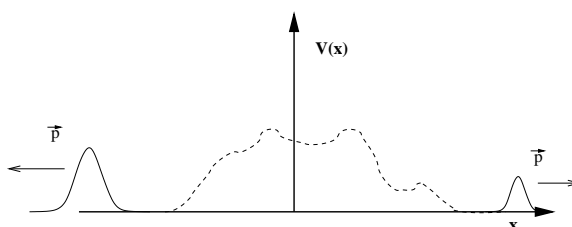
Now consider a wave packet incident on a localized $V(x)$.

The packet can “scatter” from potential (like e^- -Atom collision)

$t < t_0 \Rightarrow$
Wave packet incident
from the left



$t > t_0 \Rightarrow$
May get both a
reflected and a
transmitted wave packet.



We will solve a simpler problem: “shooting” a beam of particles at the potential and determining the form of the wave function far from the potential. By a beam of particles, we mean plane waves [a.k.a. momentum eigenstates: $\psi(x, t) = Ae^{i(k_0x - \omega t)}$].

\hookrightarrow These solutions can then be superposed to create arbitrary wave packets.

To characterize the scattering of a beam, it is useful to define a particle flux $J_x(x)$

$$J_x \equiv \left(\frac{\hbar}{2mi} \right) \left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x} \psi \right)$$

\hookrightarrow text calls this “Probability Current”.

J_x has dimensions of “particles/sec”.

Example: Consider Particle beam moving towards $+x$:

$$\psi(x, t) = \lambda^{\frac{1}{2}} e^{i(k_0 x - \omega t)}$$

where $|\lambda|^2$ is number of particles per unit length. Then:

$$J_x = \frac{\hbar}{2mi}(\lambda)[ik_0 - (-ik_0)] = \lambda \frac{\hbar k_0}{m} = \lambda v_0 \text{ . which has units of particles/sec = flux!}$$