Phys. 2b 2025, Lecture Notes (Lectures 5 & 6) (1/21-23/2025)

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

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

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

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:

$\psi_k = Ae^{ikx} + Be^{-ikx}$ 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 $e^{-iEt/\hbar}$:

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

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:

$$\psi(x,t) \text{``}\equiv\text{''} \sum_{k=0}^{\infty} A_k e^{i(kx-\frac{\hbar k^2 t}{2m})} + B_k e^{i(-kx-\frac{\hbar k^2 t}{2m})} \Rightarrow \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{i(kx-\frac{\hbar k^2 t}{2m})}dk$$

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 momentum space wave function $\phi(p)$. Then since $p = \hbar k$ we have $\phi(p) = \frac{1}{\sqrt{\hbar}}\phi(k)$.

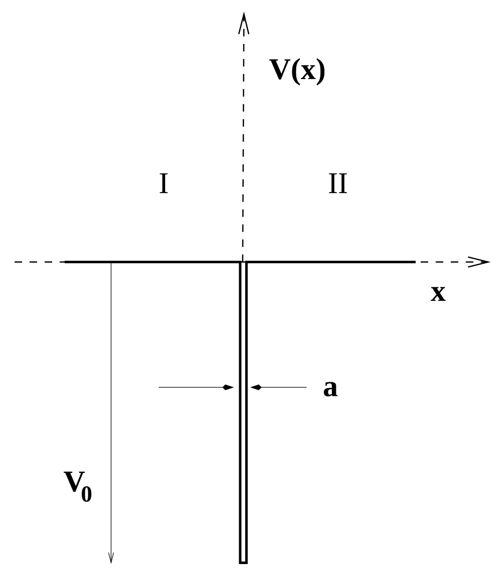
2. "Delta-function" - $\delta(x)$, and the $\delta(x)$-Potential

The properties of the Dirac Delta function $\delta(x)$ (Mathematicians call this a distribution) - are defined by an integral:
$\delta(x) = 0$ if $x \neq 0$ and $\displaystyle\int_{-\infty}^{\infty} \delta(x) f(x) dx = f(0)$

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

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

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

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 δ-function. However, due to the properties of $\delta(x)$ we can constrain $\frac{d\psi}{dx}$ by noting that

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

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

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

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

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

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

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

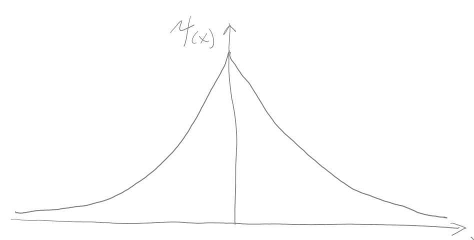
giving:

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

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 δ-well. See figure showing $\psi(x) \rightarrow$

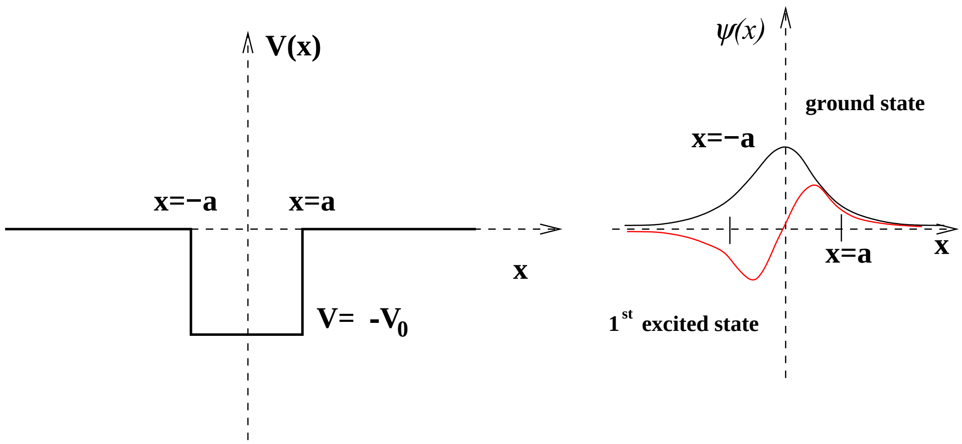


Key Concepts

1. **Finite Well Solution**
2. **Introduction to Scattering States**

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 $\hat{H}\psi_n = E_n\psi_n$.:

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

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

Consider a **Recipe** for solving these types of problems:

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

$$\psi_{in} = Acos(k_1 x) \text{ for the even solns inside the well}$$

$$\psi_{in} = Bsin(k_1 x) \text{ for the even solns inside the well}$$

$$\psi_{out} = Ce^{ik_2 x} + De^{-ik_2 x} \text{ for } |x| \geq a \text{ , outside the well}$$

with k_1 and k_2 defined via:

$$E = \frac{\hbar^2 k_1^2}{2m} - V_0 = \frac{\hbar^2 k_2^2}{2m}$$

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

Note that since $E < 0$ for bound states we have k_1 a Real number while k_2 is Imaginary (since we must have $k_2^2 < 0$). Thus let $k_2 = i\kappa$ where κ is a Real number. This gives:

ψ_{in} = oscillatory solutions [$\cos(k_1 x)$ or $\sin(k_1 x)$]

ψ_{out} = exponentially decaying functions ($Ce^{\kappa x}$ for $x < -a$ and $De^{-\kappa x}$ 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 one sign of a; thus:

$$\psi_{in}(a) = \psi_{out}(a) \text{ which gives: } Acos(k_1 a) = Ce^{\kappa a} \text{ and}$$
$$\frac{d\psi_{in}}{dx}|_{x=a} = \frac{d\psi_{out}}{dx}|_{x=a} \text{ giving: } -Ak_1 sin(k_1 a) = -C\kappa^{\kappa a}$$

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

$$k_1 tan(k_1 a) = \kappa \text{ , a transcendental equation}$$

C. Solving this equation gives the eigenenergies
↪ 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 $V_0 \to 0$, the first excited state (the odd *sin* function) has only 1/2 of a wavelength inside the well such that

$$2a = \frac{\lambda}{2}; \text{ or } \lambda = 4a = \frac{2\pi}{k_1}; \; k_1 = \frac{\pi}{2a}$$

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

$$\frac{\hbar^2 k_1^2}{2m} > |V_0| \text{ ; or } \sqrt{\frac{2ma^2 V_0}{\hbar^2}} < \frac{\pi}{2} \text{ , or } a^2 V_0 < \frac{\pi^2 \hbar^2}{8m}$$

since $k_1 = \pi/2a$.

Introduction to 1-D Scattering States

Why Discuss scattering?
↪ Essential tool in many branches of physics:

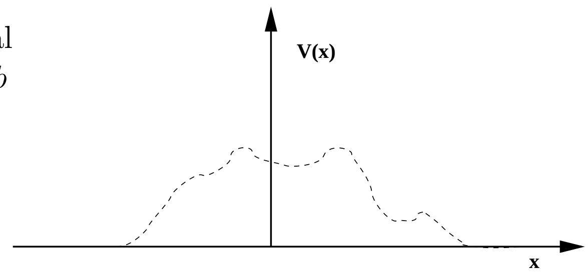
- Condensed Matter Physics ⇒ neutron-materials, X-ray-materials

- Nuclear Physics ⇒ p-Nucleus, e^--nucleus
- Atomic Physics ⇒ e^--Atom, Laser-Atom
- Particle Physics ⇒ $p - \bar{p}$, $e^- - e^+$
- Astrophysics ⇒ Cosmic Microwave Background Radiation-e^-

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

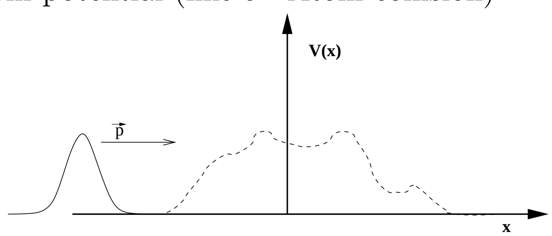
Consider a localized potential

$$\Rightarrow V(x) \neq 0,\ a \leq x \leq b$$
$$\rightarrow 0,\ |x| \rightarrow \infty$$

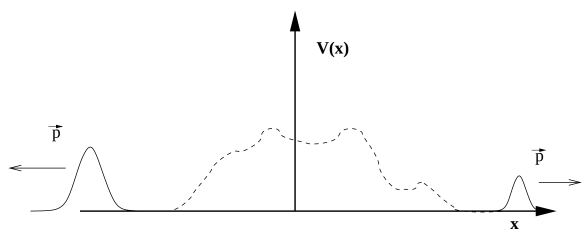


Now consider a wave packet incident on a localized $V(x)$.
The packet can "scatter" from potential (like e^--Atom collision)

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



$t > t_0 \quad \Rightarrow$
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: $\psi(x,t) = Ae^{i(k_0 x - \omega t)}$].
↪ 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 $J_x(x)$

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

↪ 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:

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