## A Free Particle in One-Dimension

For a particle bound in a box, we saw "non-classical" results:

- quantization of energy levels ( $E$ not continuous)
- zero-point energy
- nodes, or points where there is zero probability of finding the particle, even though there is a finite probability of finding the particle on either side of the node!

We'll now examine the quantum mechanical description of a free particle.

From this description, we will see several important and practical quantum mechanical effects that also defy every day common sense.

## A Free Particle in One-Dimension

## What is a "free" particle?

A free particle is one which is not confined in space as was the particle in a box.

We will first consider the case where the particle experiences no potential anywhere in space. More specifically:


Essentially, the particle is free to go anywhere in one-dimension without any impediments.

## What is the Quantum Mechanical Description of the Free Particle?

As with the particle in a box, (or any system), we need to find the wave function for the system.

Because our potential is not time-dependent, we can use Schrödinger's time independent equation to find the wave function.

$$
\hat{H} \psi(x)=E \psi(x)
$$

If the potential is zero everywhere, our Hamiltonian operator for this system is given by:

$$
\hat{H}=-\frac{h^{2}}{8 \pi^{2} m} \frac{\mathrm{~d}^{2}}{\mathrm{~d} x^{2}}+0
$$

$$
-\infty<x<\infty
$$

The Schrödinger equation for this problem is therefore:

$$
\begin{gathered}
-\frac{h^{2}}{8 \pi^{2} m} \frac{\mathrm{~d}^{2}}{\mathrm{~d} x^{2}} \psi(x)=E \psi(x) \\
\frac{\mathrm{d}^{2}}{\mathrm{~d} x^{2}} \psi(x)+\frac{2 E m}{(h / 2 \pi)^{2}} \psi(x)=0 \\
\frac{\mathrm{~d}^{2}}{\mathrm{~d} x^{2}} \psi(x)+k^{2} \psi(x)=0
\end{gathered}
$$

rearranging

$$
\frac{\mathrm{d}^{2}}{\mathrm{~d} x^{2}} \psi(x)+k^{2} \psi(x)=0 \quad k^{2}=\frac{2 E m}{(h / 2 \pi)^{2}}
$$

This is the identical differential equation that we had to solve for the particle in a box. Will we obtain the same wave function?

The general solution to the differential equation is:

$$
\psi(x)=A e^{i k x}+B e^{-i k x}
$$

In full we have:

$$
\psi(x)=A e^{i \sqrt{2 m E} x /(h / 2 \pi)}+B e^{-i \sqrt{2 m E} x /(h / 2 \pi)}
$$

What boundary conditions might we impose?

Let's go back to the requirements for a well behaved wave function. The wave function must be bound. In other words, it can't go to an infinite value as $x$ tends towards plus or minus infinity.

If we impose this condition, then the energy can only be positive or zero.

$$
E \geq 0
$$

If $E$ is negative, then the wave function becomes unbound.

For our free particle, the energy was all kinetic energy, which is consistent with the conclusion that:

$$
E \geq 0
$$

Notice that the only restriction on the energy is that it is positive or zero.
It turns out the energy of the free particle is not quantized. It can assume any positive energy. The allowed energies of a free particle are continuous just as they are in classical mechanics.


## Physical interpretation of the Free Particle Wave Function

We can further specify our wave function if we examine its physical interpretation.

Let's break up our wave function into two parts:

$$
\psi(x)=A e^{i k x}+B e^{-i k x}
$$

$\psi_{+}(x) \quad$ represents the particle moving in the $+x$ direction
$\psi_{-}(x) \quad$ represents the particle moving in the $-x$ direction
Show that $\psi_{+}$represents the particle moving in the $+x$ direction. (Hint: Show that $\left.p_{x}=-(i h / 2 \pi) \mathrm{d} \psi_{+}(x) / \mathrm{d} x>0\right)$

Going back to our wave function, we still have two arbitrary constants.

$$
\psi(x)=A e^{i k x}+B e^{-i k x}
$$

Because the particle is free, nothing can change the direction of the particle. This would require a force and therefore a potential!

So the particle can only be moving in one direction.
On physical grounds, this means that either $A$ or $B$ is zero.
(It can be shown more rigorously that either $A$ or $B$ must be zero, but our physical interpretation is good enough for now.)

Now we have our wave function for the free particle as:
$\psi_{+}(x)=A e^{i \sqrt{2 m E} x /(h / 2 \pi)}$ or $\psi_{-}(x)=B e^{-i \sqrt{2 m E} x /(h / 2 \pi)}$
This now leaves us with one more unknown constant, either $A$ or $B$.

Recall the Born interpretation of the wave function.

$$
\begin{aligned}
& P(x) \mathrm{d} x=|\psi(x)|^{2} \mathrm{~d} x=\psi^{*}(x) \psi(x) \mathrm{d} x \\
& \quad=A^{*} A e^{-i k x} e^{i k x} \mathrm{~d} x=|A|^{2} e^{0} \mathrm{~d} x=|A|^{2} \mathrm{~d} x
\end{aligned}
$$

So the probability of finding the particle between $x$ and $x+\mathrm{d} x$ is independent of $x$ (the same everywhere).

$$
P(x) \mathrm{d} x=|A|^{2} \mathrm{~d} x
$$

The wave function of the free particle is not normalizable in the usual sense (but this is not actually required for unbound particles)

On physical grounds this might be expected because there is no reason for the probability to go to zero as $x$ goes to $\pm \infty$.
In other words, there is no point in space that is favored by the particle over any other point in space.

If the wave function is not normalizable, then isn't it an invalid wave function according to our first postulate?

Yes, according to our original statement of the condition of normalizability.

However, we should modify that condition to be a requirement only for bound states. The free particle is an unbound state, a special case.

What are bound states? This is were the particle is localized by a potential $V(x)$. This does not apply to a free particle.

If the particle is localized, then the following should hold:

$$
\text { as } x \rightarrow \pm \infty \text { then } \psi(x) \rightarrow 0
$$

NOTE: Be careful not to confuse the meaning of an bound/unbound function and a bound/unbound state.

If the probability of finding the particle is equal for all $x$ as given by:

$$
P(x) \mathrm{d} x=|A|^{2} \mathrm{~d} x
$$

we say that the position of the particle is completely uncertain.
This state of affairs is indeed very strange! But it is consistent with the uncertainty principle

$$
\Delta x \Delta p_{x} \geq \frac{h}{4 \pi}
$$

because the linear momentum of the particle is completely certain or definite:

$$
\sigma_{p_{x}}^{2}=\left\langle p_{x}^{2}\right\rangle-\left\langle p_{x}\right\rangle^{2}=0
$$

therefore:

$$
\Delta p_{x}=0
$$

Thus, for the uncertainty condition to be satisfied, the particle's position is completely uncertain (infinite standard deviation in $x$ ).

The final constant $A$ or $B$ can only be further specified with some initial conditions (e.g., how did we shoot the particle out into free space).

So our free particle wave functions are:

For a particle moving in the positive $x$-direction:

$$
\psi_{+}(x)=A e^{i \sqrt{2 m E} x /(h / 2 \pi)} \quad-\infty<x<\infty
$$

For a particle moving in the negative $x$-direction:

$$
\psi_{-}(x)=B e^{-i \sqrt{2 m E} x /(h / 2 \pi)} \quad-\infty<x<\infty
$$

where the energy $E$, is zero or positive and is NOT quantized.

## Free Particle Hitting a Step Potential

Let' examine a problem which exhibits distinctly non-classical results.

Consider a particle of mass $m$ and energy $E$, coming from the left that approaches the following step potential.


Note: it is equally valid to interpret this problem as a single particle incident on the step potential or as a beam of non-interacting particles incident on the potential. Sometimes the latter is useful for interpretative proposes.

$$
V(x)=0 \xrightarrow{\text { Zone I }} \begin{aligned}
& \text { Zone II } \\
& \\
& \hline
\end{aligned}
$$

## Classical Picture

- All particles with $E<V_{0}$ will be reflected back.
- All particles with $E>V_{0}$ will be pass through into zone II.


## Quantum Mechanical Highlights

- Particles with $E<V_{0}$ can penetrate the barrier and make it into zone II.
- For particles with $E>V_{0}$ there is a finite chance that they will be reflected.


The Schrödinger equation for the problem can be divided into two parts, one for each zone.

## ZONE I

Here, because there is zero potential energy in this region, the Hamiltonian is given by:

$$
\stackrel{\hat{H}}{\mathrm{by}}=\hat{T}=-\frac{h^{2}}{8 \pi^{2} m} \frac{\mathrm{~d}^{2}}{\mathrm{~d} x^{2}}
$$

and the Schrödinger equation is:

$$
-\frac{h^{2}}{8 \pi^{2} m} \frac{\mathrm{~d}^{2}}{\mathrm{~d} x^{2}} \psi_{I}(x)=E \psi_{I}(x)
$$

$$
\begin{aligned}
& \qquad \frac{\mathrm{d}^{2}}{\mathrm{~d} x^{2}} \psi_{I}(x)+K_{I}^{2} \psi_{I}(x)=0 \quad K_{I}=\frac{\sqrt{2 m E}}{h / 2 \pi} \\
& \text { Again the general solution is given by: }
\end{aligned}
$$

$$
\psi_{I}(x)=A e^{i K_{I} x}+B e^{-i K_{I} x}
$$

This is the same as the free particle, so again we make the argument that:

$$
E \geq 0
$$

In this case, we cannot set $A$ or $B$ equal to zero because there is the possibility of reflection of the particle at the barrier (then $B$ is $>0$ ).

$$
\psi_{I}(x)=A \psi_{+}(x)+B \psi_{-}(x)
$$

The amount of reflection can be given by the relative magnitudes of $B$ versus $A$. (the amplitudes)


## ZONE II

Here, the potential is constant and equal to $V_{0}$

$$
\hat{H}=-\frac{h^{2}}{8 \pi^{2} m} \frac{\mathrm{~d}^{2}}{\mathrm{~d} x^{2}}+V_{0}
$$

the Schrödinger equation is then:

$$
-\frac{h^{2}}{8 \pi^{2} m} \frac{\mathrm{~d}^{2}}{\mathrm{~d} x^{2}} \psi_{I I}(x)+V_{0} \psi_{I I}(x)=E \psi_{I I}(x)
$$

rearranging we have:

$$
\frac{\mathrm{d}^{2}}{\mathrm{~d} x^{2}} \psi_{I I}(x)+K_{I I}^{2} \psi_{I I}(x)=0
$$

$$
K_{I I}=\frac{\sqrt{2 m\left(E-V_{0}\right)}}{h / 2 \pi}
$$

Again the general solution is given by:

$$
\psi_{I I}(x)=C e^{i K_{I I} x}+D e^{-i K_{I I} x}
$$

Because particles that make it into the barrier will only be traveling in the positive $x$-direction, $D=0$.

$$
\psi_{I I}(x)=C e^{i K_{I I} x}+D e_{0}^{-i K_{I I} x}
$$

## Summary of Zone I and II Wave Functions

Now we have the general form for our wave function in the two regions:

ZONE I $\quad \psi_{I}(x)=A e^{i K_{I} x}+B e^{-i K_{I} x} \quad K_{I}=\frac{\sqrt{2 m E}}{h / 2 \pi}$
ZONE II $\quad \psi_{I I}(x)=C e^{i K_{I I} x}$

$$
K_{I I}=\frac{\sqrt{2 m\left(E-V_{0}\right)}}{h / 2 \pi}
$$

$$
E \geq 0
$$

Due to the restriction that the wave function is continuous, singlevalued and smooth, we have continuity relationships that connect the wave functions in the two regions.

At the boundary $(x=0)$ :

$$
\begin{aligned}
\psi_{I} & =\psi_{I I} \\
\frac{\mathrm{~d} \psi_{I}}{\mathrm{~d} x} & =\frac{\mathrm{d} \psi_{I I}}{\mathrm{~d} x}
\end{aligned} \quad \psi_{I}(x)=A e^{i K_{I} x}+B e^{-i K_{I} x}
$$

In other words the wave functions (and slopes) have to match up at the boundary.
So we have two equations and three unknowns. We can only solve for $B$ and $C$ in terms of $A$.

If the particle was confined to some region of space, then a normalization condition would be our third condition. But since our particle can be anywhere, we can not normalize the wave function.

Solve for $B$ and $C$ in terms of $A$ using the continuity relationships.

$$
\begin{array}{rr}
\psi_{I}(x)=A e^{i K_{I} x}+B e^{-i K_{I} x} & x \leq 0 \\
\psi_{I I}(x)=C e^{i K_{I I} x} & x>0
\end{array}
$$

where:

$$
\begin{gathered}
K_{I}=\frac{\sqrt{2 m E}}{h / 2 \pi} \quad K_{I I}=\frac{\sqrt{2 m\left(E-V_{0}\right)}}{h / 2 \pi} \\
C=A+B \quad \quad B=\frac{K_{I}-K_{I I}}{K_{I}+K_{I I}} A \\
E \geq 0
\end{gathered}
$$

The constant $A$ can be specified from the initial conditions (e.g., how fast we shoot our particle at the potential barrier).

## What Happens to the Beam as it Encounters the Step Potential?

This largely depends on if the energy of the particles relative to $V_{0}$.

## Consider the Case $E<V_{0}$

When the energy of the incoming particle is less than the potential, classically we expect all particles to reflect back. Let's look at what happens in the quantum mechanical description.

The wave function in the barrier or Zone II is:

$$
\psi_{I I}(x)=C e^{i K_{I I} x} \quad K_{I I}=\frac{\sqrt{\left(E-V_{0}\right) 2 m}}{h / 2 \pi}
$$

If $E<V_{0}$, then $E-V_{0}$ is negative and we have a negative root in $K_{I I}$.

$$
K_{I I}=\frac{\sqrt{\left(E-V_{0}\right) 2 m}}{h / 2 \pi}=\frac{\sqrt{-1 \bullet\left|\left(E-V_{0}\right)\right| 2 m}}{h / 2 \pi}=\frac{i \sqrt{\left(V_{0}-E\right) 2 m}}{h / 2 \pi}
$$

If we let

$$
K_{I I}=i k \quad \text { where } \quad k=\frac{\sqrt{\left(V_{o}-E\right) 2 m}}{h / 2 \pi}
$$

$k$ is a positive and real valued. This gives:

$$
\psi_{I I}(x)=C e^{i i k x}=C e^{-k x}
$$

Because $k$ is positive and real valued, inside the barrier we have an exponentially decaying wave function.
representation of the real component of the wave function


This is an example of quantum mechanical penetration into a classically forbidden barrier.

$$
\psi_{I I}(x)=C e^{-k x} \quad k=\frac{\sqrt{\left(V_{o}-E\right) 2 m}}{h / 2 \pi}
$$

Notice that the larger $k$ is, the steeper the decay. The larger the mass (or larger $V_{0}-E$ ), the less penetration into the barrier is observed.

For macroscopic particles ("large" $m$ ), barrier penetration is negligible and for all practical purposes zero, no matter what the barrier is.

We can define a penetration depth as:

$$
D_{p}=\frac{1}{k}
$$

This is the depth at which the amplitude of the wave function will diminish to a factor of $\mathrm{e}^{-1}$ of its value at the edge of the barrier.

The penetration depth is proportional to $k^{-1}$ and therefore proportional to $m^{-1 / 2}$. So the penetration depth will be negligible for large $m$.

## Non-Classical Reflection

Consider the case: $E>V_{0}$
Classical picture.

- All particles with $E>V_{0}$ will pass through into zone II.

- Classically, $100 \%$ of the particles are transmitted into the barrier region. $0 \%$ of the particles are reflected.
But according to quantum mechanics, there is a finite chance of reflected particles, even if $E>V_{0}$.

$$
V(x)=V_{0}
$$

$$
\psi_{I}(x)=A e^{i K_{I} x}+B e^{-i K_{I} x} \quad \psi_{I I}(x)=C e^{i K_{I I} x}
$$

Here it can be useful to interpret our problem as a beam of noninteracting particles incident on the potential.

The magnitudes of the constants $A, B$ and $C$ can be interpreted as amplitudes of the beam of particles. For example, the larger $|A|$ the larger the amplitude the beam of particles. (More particles)

Recall we could not specify $A, B$ and $C$ without the 'initial' conditions, but we could specify their ratios.

$$
\psi_{I}(x)=A e^{i K_{I} x}+B e^{-i K_{I} x} \quad \psi_{I I}(x)=C e^{i K_{I I} x}
$$

The ratio:

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

can be defined as the reflection coefficient. It gives the fraction of particles that are reflected by the barrier.

Recall that for this problem we derived:

$$
\frac{B}{A}=\frac{K_{I}-K_{I I}}{K_{I}+K_{I I}}
$$

so we have

$$
R=\frac{|B|^{2}}{|A|^{2}}=\frac{\left(K_{I}-K_{I I}\right)^{2}}{\left(K_{I}+K_{I I}\right)^{2}}
$$

$$
R=\frac{|B|^{2}}{|A|^{2}}=\frac{\left(K_{I}-K_{I I}\right)^{2}}{\left(K_{I}+K_{I I}\right)^{2}}
$$

Using our definitions for $K_{\mathrm{I}}$ and $K_{\mathrm{I}}$,

$$
K_{I}=\frac{\sqrt{2 m E}}{h / 2 \pi} \quad K_{I I}=\frac{\sqrt{2 m\left(E-V_{0}\right)}}{h / 2 \pi}
$$

It is simply a matter of algebra to derive an expression for the reflection coefficient for $E>V_{0}$ :

$$
R=\frac{2 \frac{E}{V_{0}}-2 \sqrt{\frac{E}{V_{0}}\left(\frac{E}{V_{0}}-1\right)}-1}{2 \frac{E}{V_{0}}+2 \sqrt{\frac{E}{V_{0}}\left(\frac{E}{V_{0}}-1\right)}-1}
$$

Notice that the reflection coefficient $R$ depends on the size of the $V_{0}$ barrier relative to the energy $E$ of the particles.

Consider how the reflection coefficient changes as we vary $E / V_{0}$.


Therefore, even when $E>V_{0}$, there is a finite chance of reflection. This is a non-classical result and it is sometimes called non-classical reflection.

The amount of reflection decreases rapidly as $E$ increases over $V_{0}$.


The amount of transmission through the barrier is defined as:

$$
T=1-R
$$

Notice that if $E<V_{0}$, there is zero chance of transmission. This is different from 'penetration'.

Barrier penetration is NOT transmission ("keeps going to $x=\infty$ ").

## Visualization of the Probabilities, $\Psi^{\star} \Psi$

Below the probability density is plotted for increasing energy of the particle, but where $\boldsymbol{E}<\boldsymbol{V}_{0}$.

$$
P(x)=|\psi(x)|^{2}
$$

The probability oscillates in zone I due to interference with the reflected particles.

Notice that the penetration depth of the particle into the barrier increases as the energy increases.

$$
\begin{array}{r}
\boldsymbol{E}>\boldsymbol{V}_{\mathbf{0}} \\
P(x)=|\psi(x)|^{2}
\end{array}
$$

The probability oscillates in zone I due to interference with the reflected particles. In zone II, they are only moving in one direction so the probability is constant. (remember the free particle with no barrier)

Notice that the amplitude in zone I diminishes as the energy increases. This is because there is less non-classical reflection as $E$ increases.

## Visualization of the Wave Functions

Plotted below are the real parts of the stationary state wave functions of the particle incident on the barrier of infinite width at various energies.

$$
E<V_{0}
$$

$\operatorname{Re}[\psi(x)$

$$
\begin{array}{r}
\boldsymbol{E}>\boldsymbol{V}_{\mathbf{o}} \\
\operatorname{Re}[\psi(x)]
\end{array}
$$

Although the probability is constant in zone II, the real component of the wave function in the zone II still oscillates. Again consider the free particle wave function with no barrier.

Notice that there is a change in the wave length of the oscillations.
Why does the wavelength in zone II decrease as the energy increases? (Ignore the wave length in zone I)

## Finite Width Barrier and Quantum Mechanical Tunneling



Consider a particle of mass $m$ and energy $E$, coming from the left.

Classical picture.

- All particles with $E<V_{0}$ will be reflected back.
- All particles with $E>V_{0}$ will be pass through the barrier into Zone III.


## Finite Width Barrier and Quantum Mechanical Tunneling



The quantum mechanical treatment of this problem will show that particles with energies less than the barrier can tunnel through to the other side!

In other words when $E<V_{0}$ there will be a finite transmission coefficient through to zone III.

Quantum mechanical tunneling is important in many areas of chemistry.

electron $\square$
$\square$

We can again set up our Hamiltonian and Schrödinger equation in each of the regions. We get wave functions for each zone given by:

$$
\begin{gathered}
\psi_{I I}(x)=C e^{i K_{I I} x}+D e^{-i K_{I I} x} \\
\psi_{I}(x)=A e^{i K x}+B e^{-i K x} \prod_{\text {Zone I }}^{V(x)=V_{0}} \quad \psi_{I I I}(x)=F e^{i K x} \\
V(x)=0 \xrightarrow{x=0 \quad x=L} \quad V(x)=0 \\
K=\frac{\sqrt{2 m E}}{h / 2 \pi} \\
\psi_{I}=\psi_{I I} \quad \psi_{I}^{\prime}=\psi_{I I}^{\prime} \quad \text { at the boundary } x=0 \\
K_{I I}=\frac{\sqrt{2 m\left(E-V_{0}\right)}}{h / 2 \pi} \quad \psi_{I I}=\psi_{I I I} \quad \psi_{I I}^{\prime}=\psi_{I I I}^{\prime} \quad \text { at the boundary } x=L
\end{gathered}
$$

Again, by applying the continuity relationships, it's just a matter of algebra to derive analytic expressions for the transmission and reflection coefficients. Let's not worry about these derivations, but rather focus on interpreting the results.

## Non-classical reflection

The results are similar to that of the step-potential problem. But now, even if $E>V_{0}$, there is a finite chance of reflection at both boundaries.


## Quantum Mechanical Tunneling

When $\boldsymbol{E}<\boldsymbol{V}_{\mathbf{0}}$, there is a non-zero probability that particles will make it all the way through the barrier, into zone III. This is called quantum mechanical tunneling because particles are 'observed' to tunnel through barriers they could not get through classically.

For this system, an expression for the transmission coefficient can be derived that shows that tunneling can occur.

$$
T=\left(1+\frac{V_{0}^{2}}{16 E\left(V_{0}-E\right)}\left(e^{\beta}-e^{-\beta}\right)^{2}\right)^{-1} \quad \beta=\frac{L \sqrt{2 m\left(V_{0}-E\right)}}{h / 2 \pi}
$$

Once again the transmission coefficient depends on $V_{\mathrm{o}}$ and $E$, but now also on the particle mass, $m$, and the width of the barrier, $L$.

Plot of the Tunneling probability as a Function of the kinetic energy of the incoming particle relative to the barrier height, $E / V_{\mathrm{o}}$ for $\boldsymbol{E}<V_{0}$


As the energy $E$ approaches the barrier height, or $E / V_{0}$ approaches 1, the more tunneling we have.

The different plots show that tunneling decreases as:

- as barrier length $L$ increases
- as mass of the particle $m$ increases
- as the barrier height $V_{0}$ increases

Plot of the tunneling or transmission probability as a function of the kinetic energy of the incoming particle relative to the barrier height, $E / V_{0}$ for $\boldsymbol{E}>\boldsymbol{V}_{\mathbf{0}}$


This is the same quantity as plotted in the previous slide but now the particles have $E>V_{0}$.

As the energy becomes larger relative to the barrier, the probability that particles are transmitted increases and there is less chance of non-classical reflection

The wild oscillations are a quantum mechanical effect.

The peaks are called scattering resonances.

## Quantum Mechanical Tunneling and Chemistry

Quantum mechanical tunneling plays an important role in chemistry, biology and physics.

Tunneling is particularly important in proton transfer reactions.

For example, consider our barrier potential as a reaction profile for a chemical reaction.

beta-hydride elimination


Reaction rates of proton transfer reactions can be significantly enhanced by tunneling!

For heavier nuclei, (C, N, O) tunneling is a much smaller effect - almost negligible. For macroscopic phenomena, it is completely negligible.

However, proton transfer reactions are ubiquitous in biological systems and enzymatic reactions.

## Scanning Tunneling Microscope

Works on the principle of quantum mechanical tunneling. A very fine metal tip is placed close to a surface. A small voltage difference is applied across the tip and surface. Electrons tunnel through 'gap' or the vacuum region between the tip and the surface. The tunneling current gives a measure of the distance between the surface and the tip. 0.01 nm vertical resolution! (1986 Physics Nobel Prize)
images of $\mathrm{Si}(100)$ doped with molybdenum


120 A
STM image of same surface at higher resolution. Each spot corresponds to the surface of an individual atom.

## Scanning Tunneling Microscope (STM)



## More on potential boxes, barriers and unbound states

## System in a BOUND particle state

All particles making up the system are localized or "bound" to certain regions of coordinate space.


In all cases:
The energy of the system will be quantized
$|\psi|^{2} \rightarrow 0 \quad \therefore \psi \rightarrow 0 \quad$ as $\quad x \rightarrow \pm \infty$
The probability of finding ANY bound particle will approach zero as $x$ approaches $\pm$ infinity.

The wave functions for bound states are normalizable.

$$
\text { finite value }=\int \psi^{*} \psi d \tau
$$

## System in an UNBOUND particle state

A particle in the system behaves like a free particle in the sense that it is not localized in any particular region of coordinate space.

In all cases:

$$
\underset{\longleftrightarrow}{-\infty} \quad V(x)=0 \quad+\infty
$$

The energy of the system will correspond to a continuum of energy levels. The energy is NOT quantized.

The wave function does not decay to zero as $x \rightarrow \pm \infty$

$$
|\psi|^{2} \nrightarrow 0
$$

We can't normalize the wave function in the usual sense. (Can be handled (normalize per unit length), but not in this course.)

NOTE the confusing terminology. Although we are talking about a UNBOUND state, the wave function is still a bound function of the coordinates (i.e., $\psi$ does not go to infinity).

## Discrete, Continuous and Mixed Spectra of the Energy Levels

discrete energy levels
$\qquad$
$\qquad$
$\qquad$
$\qquad$
Occurs when

$V=0$
continuous energy
levels


Mixed energy levels


Qualitatively, why do mixed energy levels occur?

## Consider a Square Well Potential



When $E<V_{0}$, we will have bound states.

The energy levels will be quantized.
There will be penetration into the nonclassical region.

The wave function of these states is normalizable, notice that:
$|\psi|^{2} \rightarrow 0 \quad \therefore \psi \rightarrow 0 \quad$ as $\quad x \rightarrow \pm \infty$


$$
|\psi(x)|^{2}
$$



## When $E>V_{0}$, We Will Have Unbound States

The allowed energy levels will form a continuum.
There will be non-classical reflection at BOTH boundaries.
Notice the "speed up" of the particles in the well.
in the well.

## Applications of Particle Beams?

## Vacuum Tube Electrical Circuits

## Diode (why Di- ?)

A hot metal cathode emits electrons in an evacuated glass tube.

Electrons are collected at the anode plate.

Electrons flow one way, from cathode to anode.

Why? The anode is cold And emits no electrons.


## Diode

## Circuit diagram symbol for a diode:



Note that electrons flow from the cathode to the anode, opposite to the direction of the arrow!

Why? Electrical engineers use the convention that current transports positive electric charge.

Diodes are used as rectifiers in electronic circuits, turning alternating current (ac) into direct current (dc) flowing in one direction.

Diodes act like check valves in pipeline flow.

## Triode Amplifier

Why Triode?
A grid electrode is placed between the anode and cathode.

A negative grid repels electrons, reduces electron flow from the cathode.

A positive grid attracts electrons,
 increases electron flow from the cathode.

Why Amplifier?
Small changes in a voltage applied to the grid electrode produce large changes in the number of electrons reaching the anode.

## Triode Amplifier

The grid electrode acts like an adjustable gate valve in pipeline flow, increasing or decreasing the current flow.

The grid electrode provides an adjustable potential energy barrier $V_{0}(t)$ for the incoming particles.


## Semiconductor Diode

Vacuum tube diodes, triodes and related devices work well but are bulky, fragile, and require lots of power to operate

Motivated the development of semiconductor diodes, solid-state devices with a junction between n-type and p-type doped semiconductors:

## n-type (excess electrons)

such as $\mathrm{Si}\left(\mathbf{3} \mathbf{p}^{\mathbf{2}}\right.$ ) doped with $\mathrm{As}\left(4 \mathbf{p}^{\mathbf{3}}\right)$
p-type (excess "holes")
such as $\mathrm{Si}\left(\mathbf{3} \mathbf{p}^{\mathbf{2}}\right)$ doped with $\mathrm{Ga}\left(\mathbf{4} \mathbf{p}^{\mathbf{1}}\right)$

## Semiconductor Diode


reverse bias
n-type ${ }^{+}$, $\mathbf{p - t y p e}{ }^{-}$
depletion zone with
no charge carriers,
no current flows

## FET (Field Effect Transistor) Amplifier



## Small changes in the gate voltage produce large changes

 in the source-to-drain current (signal amplification).Negative gate voltage (reverse bias) decreases the number of holes in the p-channel between source and drain electrodes, decreasing the current.

Positive gate voltage (forward bias) increases the number of charge carriers betweel source and drain electrodes. increasing the current.

## Free Electron Laser

- high speed electrons in an undulating magnetic field
- tunable radiation source, from microwaves to X-rays
-Relativistic electron beam in periodic B field
- Wavelength determined by electron energy and $B$ field
- High intensity pulsed output



## The "God" Particle

- Higgs boson
- elementary particle predicted by the Standard Model of physics
- produced experimentally by colliding beams of 4 TeV protons
- discovered at the Large Hadron Collider (near Geneva)
- most expensive scientific instrument ever built (0 billion USD)

$27-\mathrm{km}$ ring of superconducting magnets


## The "Oh My God" Particle

- it came from outer space
- an ultra-high energy (UHE) cosmic "ray"
- probably a proton
- HUGE kinetic energy $3 \times \mathbf{1 0}^{\mathbf{2 0}} \mathrm{eV}$
- equivalent to the kinetic energy of baseball moving at $100 \mathrm{~km} /$
- speed $\mathbf{9 9 . 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 5} \%$ of the speed of light


Detected on 15 October 1991 in the night sky over Utah using the Fly's Eye camera network designed to detect fluorescence from the particle showers caused by incoming cosmic rays.

## Auger Cosmic Ray Observatory

- located in the high plains of Argentina, near the Andes Mounta
- designed to detect UHE cosmic rays
- 24 fluorescent detection telescopes
- an array of 1600 water tanks with photomultiplier detectors
- 3000 km $^{2}$ detection area


