

# Probability, Wave Functions, and the Copenhagen Interpretation

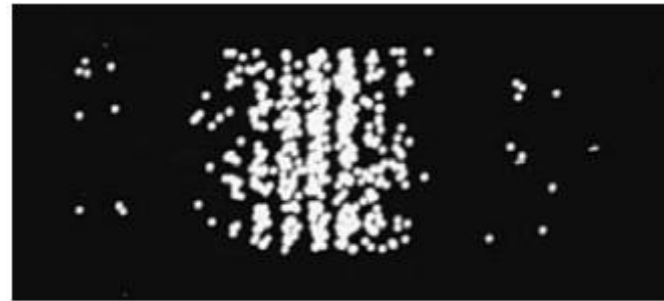
- We learned in elementary physics that the **instantaneous wave intensity of electromagnetic radiation** (light) is  $\epsilon_0 c E^2$  where  $E$  is the electric field.
- Thus the probability of **observing light** is proportional to the **square of the electric field**.
- In the **double-slit light experiment**, the electric field of the light wave is relatively large at the bright spots on the screen and small in the region of the dark places.
- After only 20 flashes we cannot make any prediction as to the eventual pattern, but we still know that the probability of observing a flash is proportional to the square of the electric field.



(a) 20 counts



(b) 100 counts



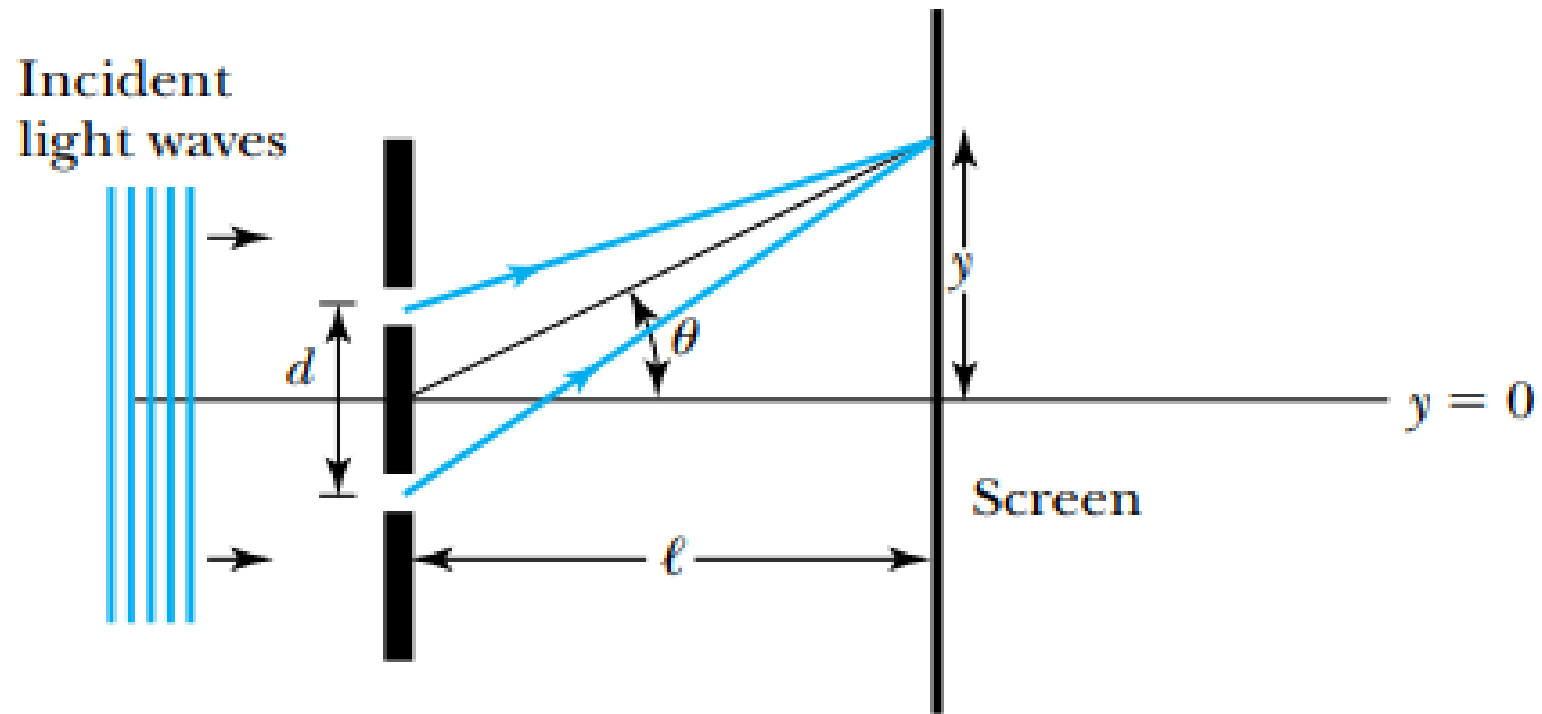
(c) 500 counts



(d) ~4000 counts

Young's double slit  
experiment

- We now briefly review this calculation that is normally given in introductory physics courses.
- If the **distance from the central ray** along the screen we are observing in an experiment is denoted by  $y$ , the **probability** for the photon to be found between  $y$  and  $y + dy$  is proportional to the intensity of the wave ( $E^2$ ) times  $dy$ .



- For **Young's double-slit experiment**, the value of the electric field  $\vec{E}$  produced by the two interfering waves is large where the flash is likely to be observed and small where it is not likely to be seen.
- By counting the **number of flashes** we relate the energy flux  $I$  (called the intensity) of the light to the number flux,  $N$  per unit area per unit time, of photons having energy  $hf$ .
- In the wave description, we have  $I = \epsilon_0 c \langle E^2 \rangle$ , and in what appears to be the particle description,  $I = Nh f$ .
- The **flux of photons**  $N$ , or the **probability**  $P$  of observing the photons, is **proportional** to the average value of the square of the electric field  $\langle E^2 \rangle$ .

- **How can we interpret the probability of finding the electron in the wave description?**
- First, the **localization of a wave** can be accomplished by using a wave packet.
- We used a **wave function  $\Psi(\mathbf{x},t)$**  to denote the superposition of many waves to describe the wave packet.
- **In the case of light**, we know that the electric field  $\vec{E}$  and magnetic field  $\vec{B}$  satisfy a wave equation.
- In electrodynamics either  $\vec{E}$  or  $\vec{B}$  serves as the wave function  $\Psi$ .
- For particles (say electrons) a similar behavior occurs.
- In this case the wave function  $\Psi(\mathbf{x},t)$  **determines the probability**, just as the flux of photons  $N$  arriving at the screen and the electric field  $\vec{E}$  determined the probability in the case of light.

- For **matter waves** having a **de Broglie wavelength**, it is the wave function  $\Psi$  that determines the probability of finding a particle at a particular position in space at a given time.
- The value of the wave function  $\Psi$  has no physical significance itself, and it can have a **complex** value (containing both **real** and **imaginary** numbers).
- The quantity  $|\Psi|^2$  is called the **probability density** and represents the probability of finding the particle in a given unit volume at a given instant of time.

- In general,  $\Psi(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{t})$  is a **complex** quantity and depends on the spatial coordinates  $x, y$ , and  $z$  as well as time  $t$ .
- The complex nature will be of no concern to us: we use  $\Psi$  times its complex conjugate  $\Psi^*$  when finding **probabilities**.
- We are interested here in only a single dimension  $y$  along the observing screen and for a given time  $t$ .
- In this case  $\Psi^*\Psi dy = |\Psi|^2 dy$  is the **probability** of observing an electron in the interval between  $y$  and  $y + dy$  at a given time, and we call this  **$P(y) dy$** .

$$P(y)dy = |\Psi(x, y)|^2 dy$$

- Because the electron has to have a probability of unity of being observed somewhere along the screen, we integrate the probability density over all space by integrating over  $y$  from  $-\infty$  to  $\infty$ .
- This process is called **normalization**.

$$\int_{-\infty}^{\infty} P(y)dy = \int_{-\infty}^{\infty} |\Psi(y, t)|^2 dy = 1$$

- Max Born (Nobel Prize, 1954), one of the founders of the quantum theory, first proposed this **probability interpretation of the wave function** in 1926.
- The determination of the wave function  $\Psi(\mathbf{x}, t)$  is discussed in much more detail later.
- The use of wave functions  $\Psi(\mathbf{x}, \mathbf{y}, \mathbf{z}, t)$  rather than the classical positions  $x(t)$ ,  $y(t)$ ,  $z(t)$  represents a clean break between classical and modern physics.
- Physicists have developed a **set of rules and procedures in quantum theory** to determine physical observables like position, momentum, and energy.

# The Copenhagen Interpretation

- **Schrödinger and Heisenberg** worked out independent and separate mathematical models for the quantum theory in 1926.
- Schrödinger's theory is somewhat easier to understand and is based on waves.
- Paul Dirac reported his relativistic quantum theory in 1928.
- Today there is little disagreement about the mathematical formalism of quantum theory.
- We want to examine the ***Copenhagen interpretation***, because it is the mainstream interpretation of quantum theory.
- Heisenberg announced his uncertainty principle in early 1927.
- **Bohr and Heisenberg** had many discussions in 1927 formulating the interpretation of quantum mechanics now known as the “Copenhagen interpretation,” “Copenhagen school,” or sometimes unkindly as “Copenhagen orthodoxy.”
- It was strongly supported by Max Born and Wolfgang Pauli.

- There are various formulations of the interpretation, but it is generally **based on the following:**

**1.The uncertainty principle of Heisenberg**

**2.The complementarity principle of Bohr**

**3.The statistical interpretation of Born, based on probabilities determined by the wave function**

- Together these three concepts form a **logical interpretation of the physical meaning of quantum theory.**
- According to the *Copenhagen interpretation*, physics depends on the outcomes of measurement.

- Consider a **single electron passing through the two-slit experiment**.
- We can determine precisely **where the electron hits** the screen by noting a flash.
- The Copenhagen interpretation rejects arguments about **where the electron was** between the times it was emitted in the apparatus (and subsequently passed through the two slits) and when it flashed on the screen.
- The measurement process itself **randomly** chooses one of the many possibilities allowed by the wave function, and the wave function instantaneously changes to represent the final outcome.
- Bohr argued that it is not the task of physics to find out how nature is, because we can never understand the quantum world or assign physical meaning to the wave function.
- **Bohr and Heisenberg argued that measurement outcomes are the only reality in physics.**

- Many physicists objected (and some still do!) to the Copenhagen interpretation for widely varying reasons.
- One of the basic objections is to its **nondeterministic nature**.
- Some also object to the vague measurement process that converts probability functions into nonprobabilistic measurements.
- Famous physicists who objected to the Copenhagen interpretation were Albert Einstein, Max Planck, Louis de Broglie, and Erwin Schrödinger.
- **Einstein** and **Schrödinger** never accepted the Copenhagen interpretation.
- **Einstein** was particularly bothered by the reliance on probabilities, and he wrote Born in 1926 that “**God does not throw dice.**”
- Nonetheless, it is fair to say that the great majority of physicists today accept the **Copenhagen interpretation as the primary interpretation of quantum mechanics.**

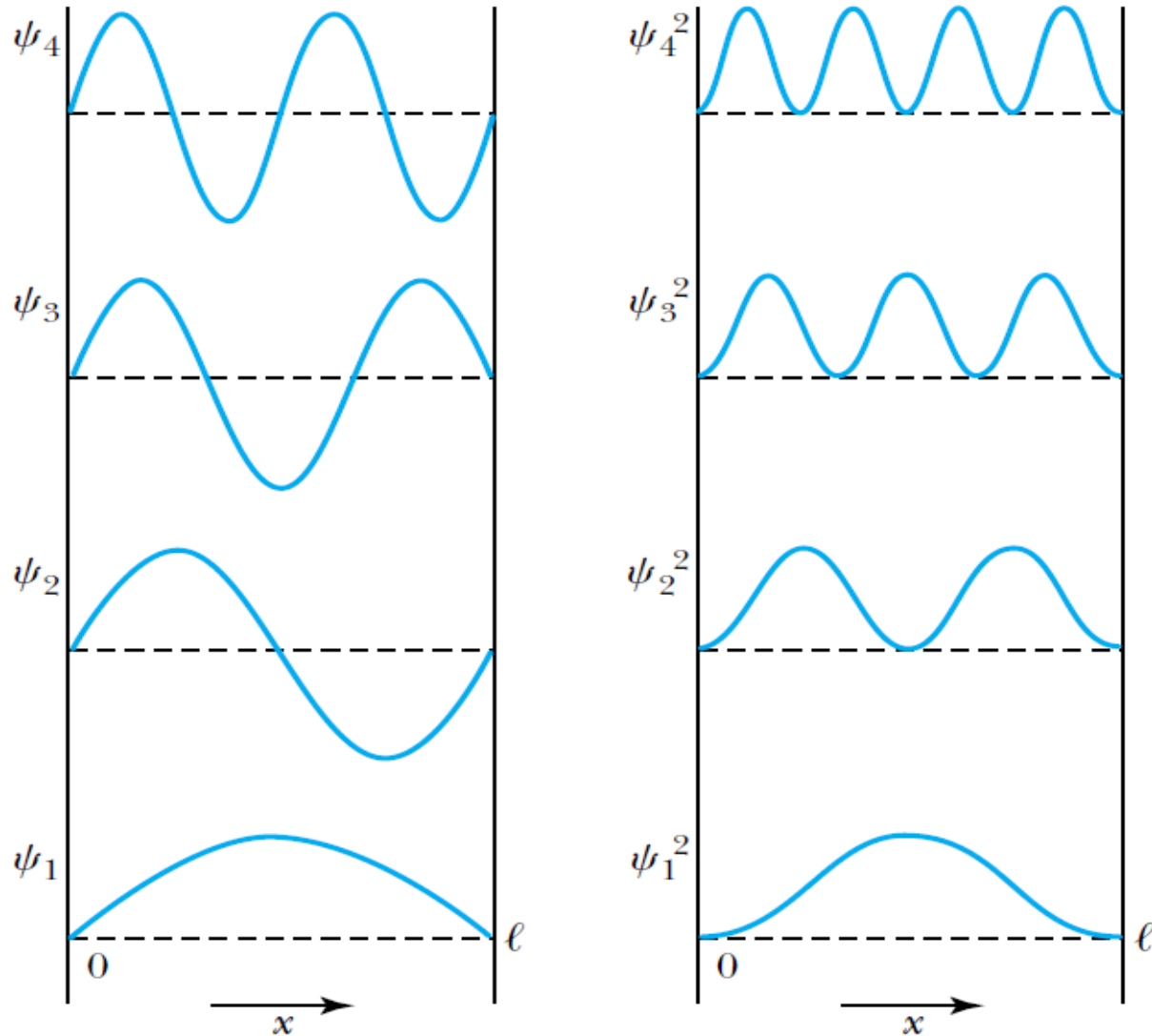
- Several paradoxes have been proposed by physicists to refute the Copenhagen interpretation.
- They include the famous Schrödinger cat paradox, the Einstein-Podolsky-Rosen paradox, and Bell's theorem (or inequality).
- Space does not allow us to describe these paradoxes.
- A Princeton University graduate student, Hugh Everett III, announced an alternate interpretation to the Copenhagen view in 1957.
- In Everett's "**Many Worlds**" interpretation, the concept of parallel universes is invoked—in itself such a weird idea that it has not gained wide acceptance, but it overcomes some objections to the Copenhagen interpretation.
- Since 1957 there have been several versions of the Many Worlds interpretation presented, and some physicists prefer it over the Copenhagen interpretation.
- Nevertheless, the **Copenhagen interpretation remains the favored interpretation.**

# Particle in a Box

- Let's now consider the situation of a **particle of mass  $m$  trapped** in a one-dimensional box of width  $l$ .
- We used the uncertainty principle to calculate the minimum kinetic energy of such a particle.
- Now let's determine the possible energies of such a particle.
- Because of our discussion in the previous section **we want to use the wave nature of the particle in this determination.**
- First, what is **the most probable location of the particle in the state with the lowest energy** at a given time, say  $t = 0$ , so that  $\psi(x, 0) = \psi(x)$ ?

- To find the probable location, **we will treat the particle as a sinusoidal wave.**
- **The particle cannot be physically outside the confines of the box, so the amplitude of the wave motion must vanish at the walls and beyond.**
- In the language of the **wave function**, its probability of **being outside is zero**, so the wave function must vanish outside.
- **The wave function must be continuous, and the probability distribution can have only one value at each point in the box.**
- **For the probability to vanish at the walls, we must have an integral number of half wavelengths  $\lambda/2$  fit into the box.**

# Particle in a Box



All the possible ways of fitting waves into a **one dimensional box** of length  $\ell$ .

The **left** side shows the wave functions for the four lowest energy values.

The **right** side shows the corresponding **probability distributions**.

- The requirement of an integral number of half wavelengths  $\lambda/2$  means that

$$\frac{n\lambda}{2} = l \quad \text{or} \quad \lambda_n = \frac{2l}{n} \quad (n = 1, 2, 3, \dots)$$

- **The possible wavelengths are quantized, and the wave shapes will have  $\sin(n\pi x/l)$  factors.**
- If we treat the problem **nonrelativistically** and assume there is no potential energy, the energy  $E$  of the particle is

$$E = K.E. = \frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}$$

- If we insert the values for  $\lambda_n$ ,

$$E_n = \frac{h^2}{2m} \left( \frac{n}{2l} \right)^2 = n^2 \frac{h^2}{8ml^2} \quad (n = 1, 2, 3, \dots)$$

- The possible **energies of the particle are quantized**, and each of these energies  $E_n$  is a possible energy level.
- Note that the **lowest energy** is  $E_1 = h^2/8ml^2$ .
- Because we assumed the potential energy to be zero,  $E_n$  is also equal to the kinetic energy.
- The probability of observing the particle between  $x$  and  $x + dx$  in each state is  $P_n dx \propto |\psi_n(x)|^2 dx$ .
- Notice that  $E_0 = 0$  is not a possible state, because  $n = 0$  corresponds to  $\psi_0 = 0$ .
- The **lowest energy level is therefore  $E_1$** , with a probability density  $P_1 \propto |\psi_n(x)|^2$ , shown in Figure.
- **The most probable location for the particle in the lowest energy state is in the middle of the box.**

- This **particle-in-a-box model** is more important than it might seem.
- It is our first application of what we call “**quantum theory**” or “**quantum mechanics**.”
- Notice how the **quantization of energy arises from the need to fit a whole number of half-waves into the box** and how we obtained the corresponding probability densities of each of the states.
- The concept of energy levels, as first discussed in the Bohr model, has surfaced in a natural way by using waves.
- The procedure followed is the same as finding the allowed modes of standing waves inside the box.
- We can use all the results that we learned about waves in elementary physics.

# The Schrödinger Wave Equation

- The Austrian physicist Erwin **Schrödinger** (Nobel Prize, 1933) was presenting a seminar at the University of Zurich in November 1925 on **de Broglie's** wave theory for particles when Peter Debye suggested that **there should be a wave equation.**
- Within a few weeks Schrödinger had found a **suitable wave equation** **based on** what he knew about **geometrical and wave optics**.
- In our previous study of elementary physics, we learned that Newton's laws, especially the **second law** of motion, **govern the motion of particles**.
- We need a similar set of equations to describe the wave motion of particles; that is, **we need a wave equation** that is dependent on the **potential field** (for example, the Coulomb or strong force field) that the particle experiences.

- We can **then find the wave function** that will allow us to calculate the probable values of the particle's **position, energy, momentum, and so on.**
- We point out that although our procedure is similar to that followed in classical physics, we will **no longer be able to calculate and specify the *exact* position, energy, and momentum simultaneously.**
- Our calculations now must be consistent with the uncertainty principle and the notion of probability.
- There are several possible paths through which we could plausibly obtain the **Schrödinger wave equation.**
- Because **none of the methods is actually a derivation**, we prefer to present the equation and indicate its usefulness.

- Its ultimate correctness rests on its ability to **explain and describe experimental results**.
- The **Schrödinger wave equation** in its **time-dependent** form for a particle moving in a potential  $V$  in one dimension is

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V\Psi(x, t)$$

- where  $i = \sqrt{-1}$  is an imaginary number and we have used partial derivatives.
- Both the potential  $V$  and wave function  $\Psi$  may be functions of space and time,  $V(x, t)$  and  $\Psi(x, t)$ .
- **The equation in three dimensions** is fairly straightforward.

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + V\Psi(x, y, z, t)$$

- We will restrict ourselves to the **one-dimensional form** now.
- Let's compare the equation with the **classical wave equation** given by

$$\frac{\partial^2 \Psi(x, t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \Psi(x, t)}{\partial t^2}$$

- The wave function may be as varied as the amplitude of a water wave, a guitar-string vibration, or even the electric field  $E$  or magnetic field  $B$ .
- **Notice that the classical wave equation contains a second-order time derivative, whereas the Schrödinger wave equation contains only a first-order time derivative.**
- This already gives us some idea that we are dealing with a somewhat different phenomenon.

- Despite the fact that the Schrödinger wave equation has not been derived, it is still a useful tool because **it describes experimental results.**
- In science, and especially in physics, the **test of a theoretical calculation is that it agrees with what we observe.**
- We apply the Schrödinger wave equation to several simple situations to illustrate its usefulness.
- We discussed wave motion and the formation of wave packets from waves.

- For a wave of **wave number  $k$**  and **angular frequency  $\omega$**  moving in the  $x$  direction, the wave function is

$$\Psi(x, t) = A \sin(kx - \omega t + \phi)$$

- This equation is **not the most general form** of a wave function, which may include both sines and cosines.
- Our wave function is also not restricted to being real.
- **A more general form of wave function including the imaginary part also is given as below:**

$$\Psi(x, t) = Ae^{i(kx - \omega t)} = A[\cos(kx - \omega t) + i \sin(kx - \omega t)]$$

- which also describes a wave moving in the  $x$  direction.
- In general the amplitude  $A$  may also be complex.

# Normalization and Probability

- The **probability**  $P(x)dx$  of a particle being between  $x$  and  $x + dx$

$$P(x)dx = \Psi^*(x, t)\Psi(x, t)dx$$

- The **probability of the particle** being between  $x_1$  and  $x_2$  is given by

$$P = \int_{x_1}^{x_2} \Psi^* \Psi dx$$

- The **wave function must also be normalized** so that the probability of the particle being somewhere on the  $x$  axis is 1.

$$\int_{-\infty}^{\infty} \Psi^*(x, t)\Psi(x, t)dx = 1$$

- The **wave function**  $e^{i(kx-wt)}$  represents a particle under **zero net force** (constant  $V$ ) moving along the  $x$  axis.
- There is a problem with this wave function, because if we try to normalize it, we obtain an **infinite result** for the integral.
- This occurs because there is a **finite probability** for the particle to be anywhere along the  $x$  axis.
- Over the **entire  $x$  axis**, these **finite probabilities** add up, when integrated, to **infinity**.
- The only **other possibility** is a **zero probability**, but that is not an interesting physical result.

- Because this wave function has **precise  $k$  and  $\omega$  values**, it represents a particle **having a definite energy and momentum**.
- According to the uncertainty principle, because  $\Delta E=0$  and  $\Delta p=0$ , we must have  $\Delta t=\infty$  and  $\Delta x=\infty$ .
- **We cannot know where the particle is at any time.**
- We can still use such wave functions if we restrict the particle to certain positions in space, such as in **a box or in an atom**.
- We can also form wave packets from such functions in order to localize the particle.

# Properties of Valid Wave Functions

- The Schrödinger wave equation, there are certain properties (often called boundary conditions) that an acceptable wave function must also satisfy:
  1. In order to avoid infinite probabilities, **must be finite everywhere**.
  2. In order to avoid multiple values of the probability, **must be single valued**.
  3. For finite potentials,  $\Psi$  and  $\frac{\partial \Psi}{\partial x}$  **must be continuous**. This is required because the second-order derivative term in the wave equation must be single valued. (There are exceptions to this rule when  $V$  is infinite.)
  4. In order to normalize the wave functions,  **$\Psi$  must approach zero as  $x$  approaches  $\pm\infty$** .
- Solutions for  $\Psi$  that do not satisfy these properties do not generally correspond to physically realizable circumstances.

# Time-Independent Schrödinger Wave Equation

- In many cases, the **potential** will **not depend** explicitly **on time**.
- **The dependence on time and position can then be separated in the Schrödinger wave equation.**

$$\Psi(x, t) = \psi(x)f(t)$$

- We obtain

$$i\hbar\psi(x)\frac{\partial f(t)}{\partial t} = -\frac{\hbar^2 f(t)}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x)f(t)$$

- We divide by  $\Psi(x) f(t)$  to yield

$$i\hbar\frac{1}{f(t)}\frac{df(t)}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + V(x)$$

- The **left** side depends only on time, and the right side depends only on spatial coordinates.
- We have changed the partial derivatives to ordinary derivatives, because each side depends on only one variable.
- It follows that each side must be equal to a constant (which we label  $B$ ), because one variable may change independently of the other.
- We integrate the left side in an effort to determine the value of  $B$ .

$$i\hbar \frac{1}{f} \frac{df}{dt} = B$$

- We integrate both sides and find

$$i\hbar \int \frac{df}{f} = \int B dt$$

- where  $C$  is an integration constant that we may choose to be 0.

$$i\hbar \ln f = Bt + C \qquad \ln f = \frac{Bt}{i\hbar}$$

- From this equation we determine  $f$  to be

$$f(t) = e^{Bt/i\hbar} = e^{-iEt/\hbar}$$

- If we compare this function for  $f(t)$  to the free-particle wave function that has the time dependence  $e^{-i\omega t}$ , we see that  $B = \hbar\omega = E$ .
- **This is a general result.**
- We now have,

$$i\hbar \frac{1}{f(t)} \frac{df(t)}{dt} = E$$

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

- This equation is known as **the time-independent Schrödinger wave equation**, and it is a fundamental equation in quantum mechanics.

- $f(t)$  can be rewritten as

$$f(t) = e^{-i\omega t}$$

- and the wave function  $\Psi(x, t)$  becomes

$$\Psi(x, t) = \psi(x)e^{-i\omega t}$$

- We will restrict our attention for the present to time-independent potentials in one space dimension.
- Many important and useful results can be obtained from this nonrelativistic and one-dimensional form of quantum mechanics, because usually only the **spatial part of the wave function  $\Psi(x)$**  is needed.
- Therefore, we need to use the time-independent form of the Schrödinger wave equation.

- Let's examine the probability density  $\Psi^*\Psi$ .
- For the case where the potential does not depend on time, we have

$$\Psi^*\Psi = \psi^2(x)(e^{i\omega t}e^{-i\omega t})$$

$$\Psi^*\Psi = \psi^2(x)$$

- The probability distributions are constant in time.
- We have seen in introductory physics the phenomenon of *standing waves* (for example, oscillations of strings fixed at both ends).
- Such standing waves can be **formed from traveling waves** moving in opposite directions.
- In quantum mechanics, we say the system is in a **stationary state**.

# Comparison of Classical and Quantum Mechanics

- **Newton's second law** ( $\vec{F} = d\vec{p}/dt$ ) and **Schrödinger's wave equation** are both **differential equations**.
- They are both postulated to explain certain observed behavior, and **experiments show that they are successful**.
- Newton's second law can **be derived from** the Schrödinger wave equation.
- Newton's laws may seem more **fundamental**—because they describe the **precise values** of the system's parameters, whereas the wave equation only produces wave functions that **give probabilities**—but by now we know **from the uncertainty principle that it is not possible to know simultaneously precise values of both position and momentum and of both energy and time**.
- Classical mechanics only appears to be more precise because it deals with macroscopic phenomena.
- The underlying **uncertainties in macroscopic measurements are just too small** to be significant.

- It was shown early in the 1800s that **wave optics** was needed to explain the observed phenomena of diffraction and interference.
- Ray optics is a good approximation as long as the wavelength of the radiation is much smaller than the dimensions of the apertures and obstacles it passes.
- **Rays of light are characteristic of particle-like behavior.**
- In order to describe interference phenomena, wave optics is required.
- Similarly for macroscopic objects, the de Broglie wavelength is so small that wave behavior is not apparent.
- However, advances in instrumentation and experimentation made it possible to observe behavior at the atomic level, and eventually the wave descriptions and quantum mechanics were required to understand all the data.
- **Classical mechanics is a good macroscopic approximation** and is accurate enough in the limit of large quantum numbers, but as far as we know now, there is only one correct theory, and that is **quantum mechanics**.

# Expectation Values

- The wave equation formalism must be able to determine values of measurable quantities, including **position, momentum, and energy**.
- Now we will discuss how the wave function is able to provide this information.
- We will do this here in only one dimension.
- We will also evaluate the values of the physical quantities for a given time  $t$ , because in general the whole system, including the values of the physical quantities, **evolves with time**.
- Consider a measurement of the position  $x$  of a particular system.
- If we make three measurements of the position, we are likely to obtain three different results.

- If our method of measurement is accurate, then there is some physical significance to the average of our measured values of  $x$ .
- The precision of our result improves as more measurements are made.
- In quantum mechanics we use wave functions to calculate the expected result of the average of many measurements of a given quantity.
- We call this result the **expectation value**; the expectation value of  $x$  is denoted by  $\langle x \rangle$ .
- Any measurable quantity for which we can calculate the expectation value is called a **physical observable**.
- The expectation values of physical observables (for example, position, linear momentum, angular momentum, and energy) must be real, because the experimental results of measurements are real.

- Let's first determine **average values**.
- Consider a particle that is constrained to move along the  $x$  axis.
- If we make many measurements of the particle, we may find the particle  $N_1$  times at  $x_1$ ,  $N_2$  times at  $x_2$ ,  $N_i$  times at  $x_i$ , and so forth.
- The **average value of  $x$** , denoted by  $\bar{x}$  [or  $(x)_{av}$ ], is then

$$\bar{x} = \frac{N_1x_1 + N_2x_2 + N_3x_3 + N_4x_4 + \cdots}{N_1 + N_2 + N_3 + N_4 + \cdots} = \frac{\sum_i N_i x_i}{\sum_i N_i}$$

- We can change from **discrete to continuous variables** by using the probability  $\mathbf{P(x, t)}$  of observing the particle at a particular  $x$ .
- The previous equation then becomes

$$\bar{x} = \frac{\int_{-\infty}^{\infty} xP(x)dx}{\int_{-\infty}^{\infty} P(x)dx}$$

- In quantum mechanics we must use the probability distribution  $\mathbf{P(x)dx = \Psi^*(x, t) \Psi(x, t)dx}$ , to determine the average or expectation value.

- The **expectation value**  $\langle x \rangle$  can be found by

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x \Psi^*(x, t) \Psi(x, t) dx}{\int_{-\infty}^{\infty} \Psi^*(x, t) \Psi(x, t) dx}$$

- The denominator is the normalization equation.
- If the wave function is normalized, the denominator **becomes 1**.
- The **expectation value** is then given by

$$\langle x \rangle = \int_{-\infty}^{\infty} x \Psi^*(x, t) \Psi(x, t) dx$$

- The same general procedure can be used to find the **expectation value** of any function  $g(x)$  for a normalized wave function  $\Psi(x, t)$ .

$$\langle g(x) \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) g(x) \Psi(x, t) dx$$

- The wave function can provide only the expectation value of a given function  $g(x)$  that can be written as a function of  $x$ .
- **It cannot give us the value of each individual measurement.**
- When we say the wave function provides a complete description of the system, we mean that the expectation values of the physical observables can be determined.

- The **simultaneous values** of the position  $x$  and momentum  $p$  must be consistent with the uncertainty principle.
- To find the expectation value of  $p$ , we first need to represent  $p$  in terms of  $x$  and  $t$ .
- As an example, let's consider once more the wave function of the free particle,  $\Psi(x, t) = e^{i(kx - \omega t)}$ .
- If we take the derivative of  $\Psi(x, t)$  with respect to  $x$ ,

$$\frac{\partial \Psi}{\partial x} = \frac{\partial}{\partial x} [e^{i(kx - \omega t)}] = ike^{i(kx - \omega t)} = ik\Psi$$

- because  $k = p/\hbar$ , this becomes

$$\frac{\partial \Psi}{\partial x} = i \frac{p}{\hbar} \Psi$$

- After rearrangement, this yields

$$p[\Psi(x, t)] = -i\hbar \frac{\partial \Psi(x, t)}{\partial x}$$

- An **operator** is a mathematical operation that **transforms one function into another**.
- For example, an operator, denoted by  $\hat{Q}$ , transforms the function  $f(x)$  by  $\hat{Q}f(x) = g(x)$ .
- In the previous wave function equation, the quantity  $-i\hbar(\partial/\partial x)$  is operating on the function  $\Psi(x, t)$  and is called the **momentum operator**  $\hat{p}$ , where the ^ sign over the letter  $p$  indicates an operator.

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}$$

- The existence of the momentum operator is not unique.
- **Each of the physical observables** has an associated **operator** that is used to find that observable's expectation value.
- In order to compute the expectation value of some physical observable  $Q$ , the operator  $\hat{Q}$  must be placed between  $\Psi^* \Psi$  and so that it *operates* on  $\Psi(x, t)$  in the order shown:

$$\langle Q \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \hat{Q} \Psi(x, t) dx$$

- Thus, the **expectation value of the momentum** becomes

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \Psi^*(x, t) \frac{\partial \Psi(x, t)}{\partial x} dx$$

- The position  $x$  is its own operator.
- Operators for observables that are functions of both  $x$  and  $p$  can be constructed from  $x$  and  $\hat{p}$ .
- Now let's take the **time derivative of the free-particle wave function**.

$$\frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t} [e^{i(kx - \omega t)}] = -i\omega e^{i(kx - \omega t)} = -i\omega \Psi$$

- We substitute  $\omega = E / \hbar$ , and then rearrange to find

$$E[\Psi(x, t)] = i\hbar \frac{\partial \Psi(x, t)}{\partial t}$$

- We call the quantity operating on  $\Psi(x, t)$  the **energy operator**.

$$\hat{E} = i\hbar \frac{\partial}{\partial t}$$

- It is used to find the **expectation value**  $\langle E \rangle$  of the energy.

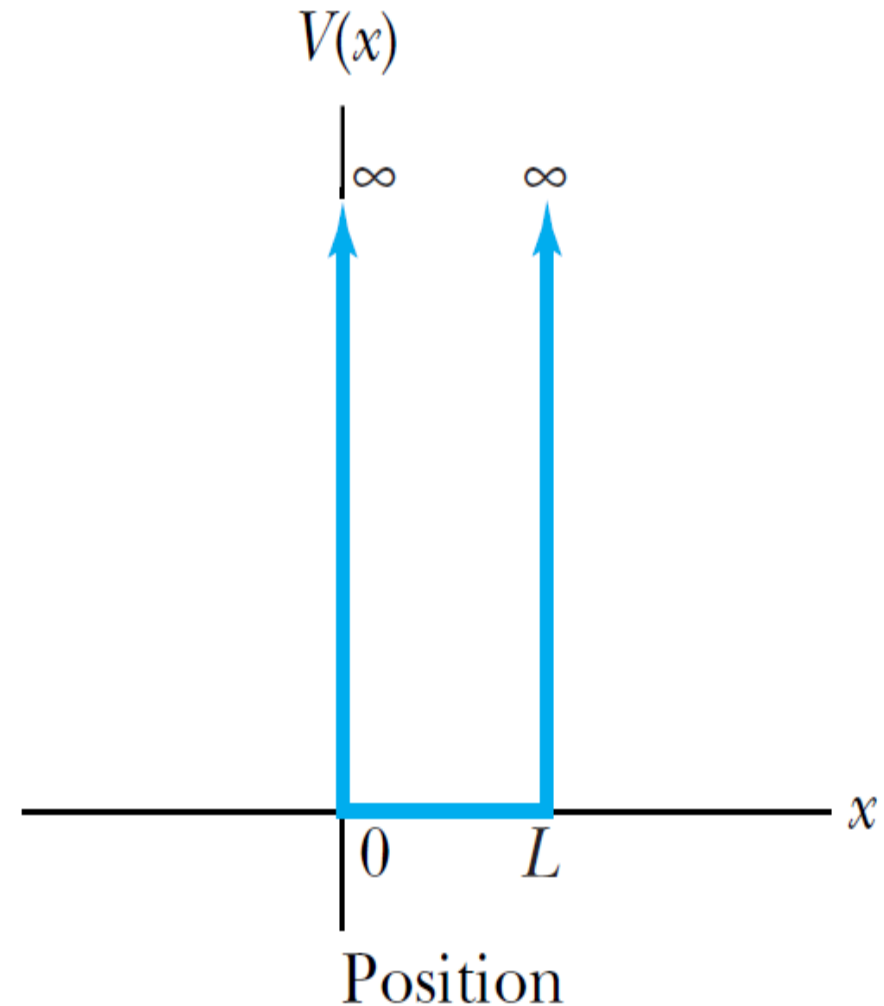
$$\langle E \rangle = i\hbar \int_{-\infty}^{\infty} \Psi^*(x, t) \frac{\partial \Psi(x, t)}{\partial t} dx$$

- Although we have found the **momentum and energy operators for only the free particle wave functions**, they are **general results**.
- Later we will use these operators to determine the physical observables (position, momentum, and energy, for example) and compare with the experimental results.

# Infinite Square-Well Potential

- Now we would like to find the **wave function** for several possible **potentials** and see what we can learn about the behavior of a system having those potentials.
- **We will find that some observables, including energy, have quantized values.**
- We begin by exploring the simplest such system—that of a particle trapped in a box with infinitely hard walls that the particle **cannot penetrate**.
- This is the same physical system as the particle in a box we presented, but now we present the full quantum-mechanical solution.
- The potential, called an ***infinite square well***, is shown in Figure and is given by

$$V(x) = \begin{cases} \infty & x \leq 0, x \geq L \\ 0 & 0 < x < L \end{cases}$$



The potential is  $V = \infty$  everywhere except the region  $0 < x < L$ , where  $V = 0$ .

- The particle is constrained to move only between  $x = 0$  and  $x = L$ , where the particle experiences no forces.
- Although the infinite square-well potential is simple, we will see that it is useful because many physical situations can be approximated by it.
- We will also see that requiring the wave function to satisfy certain boundary conditions leads to energy quantization.
- **We will use this fact to explore energy levels of simple atomic and nuclear systems.**
- As we stated previously, most of the situations we encounter allow us to use the time-independent Schrödinger wave equation.
- If we insert  $V = \infty$  we see that the only possible solution for the wave function is  $\psi(x) = 0$ .
- Therefore, there is zero probability for the particle to be located at  $x \leq 0$  or  $x \geq L$ .
- Because the kinetic energy of the particle must be finite, the particle can never penetrate into the region of infinite potential.
- However, when  $V = 0$ ,

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi$$

- and let the wave number  $k = \sqrt{2mE/\hbar^2}$ .

- A **suitable solution to this equation** that satisfies the properties

$$\psi(x) = A \sin kx + B \cos kx$$

- where  $A$  and  $B$  are constants used to normalize the wave function.
- The wave function must be continuous, which means that  $\psi(x) = 0$  at both  $x = 0$  and  $x = L$  as already discussed.
- The proposed solution therefore must have  $B = 0$  in order to have  $\psi(x = 0) = 0$ .
- If  $\psi(x = L) = 0$ , then  $A \sin(kL) = 0$ , and because  $A = 0$  leads to a trivial solution, we must have

$$kL = n\pi$$

- where  $n$  is a positive integer.
- The value  $n = 0$  leads to  $\psi = 0$ , a physically uninteresting solution, and negative values of  $n$  do not give different physical solutions than the positive values.
- The wave function is now

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right) \quad (n = 1, 2, 3, \dots)$$

- The property that  $d\psi/dx$  must be continuous is not satisfied in this case, because of the infinite step value of the potential at  $x = 0$  and  $x = L$ , and it creates no problem.
- We normalize our wave function over the total distance  $-\infty < x < \infty$ .

$$\int_{-\infty}^{\infty} \psi_n^*(x) \psi_n(x) dx = 1$$

- Substitution of the wave function yields

$$A^2 \int_0^L \sin^2 \left( \frac{n\pi x}{L} \right) dx = 1$$

- This is a straightforward integral and gives  $L/2$ , so that  $A^2(L/2) = 1$  and  $A = (2/L)^{1/2}$ .
- The normalized wave function becomes

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad (n = 1, 2, 3, \dots)$$

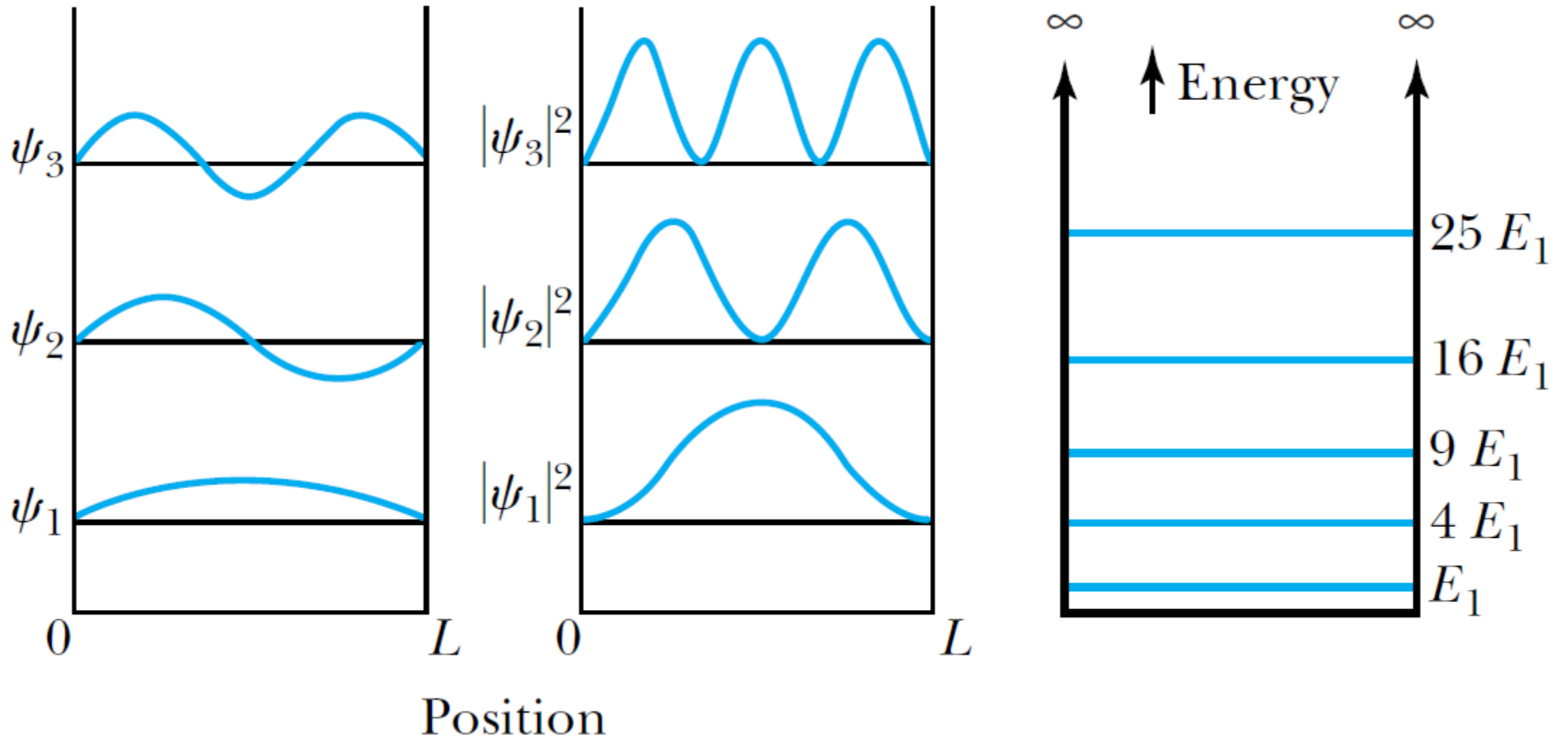
- These wave functions are identical to the ones obtained for a vibrating string with its ends fixed that are studied in elementary physics.
- The application of the boundary conditions here corresponds to fitting standing waves into the box.
- It is not a surprise to obtain standing waves in this case, because we are considering **time-independent solutions**.
- Because  $k_n = n\pi/L$  we have

$$k_n = \frac{n\pi}{L} = \sqrt{\frac{2mE_n}{\hbar^2}}$$

- Notice the subscript  $n$  on  $k_n$  and  $E_n$  denoting that they depend on the integer  $n$  and have multiple values.
- This equation is solved for  $E_n$  to yield

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} \quad (n = 1, 2, 3, \dots)$$

- The possible energies  $E_n$  of the particle are quantized, and the integer  $n$  is a quantum number.
- Notice that the results for the quantized energy levels are identical, when we treated a particle in a one-dimensional box as a wave.
- The quantization of the energy occurs in a natural way from the application of the boundary conditions (standing waves) to possible solutions of the wave equation.
- Each wave function  $\psi_n(x)$  has associated with it a unique energy  $E_n$ .



Wave functions  $\psi_n$ , probability densities  $|\psi_n|^2$ , and energy levels  $E_n$  for the lowest quantum numbers for the infinite square-well potential.

- The lowest energy level given by  $n = 1$  is called the *ground state*, and its energy is given by

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$$

- Note that the lowest energy cannot be zero because we have ruled out the possibility of  $n = 0$  ( $\psi_0 = 0$ ).
- Classically, the particle can have zero or any positive energy.
- If we calculate  $E_n$  for a macroscopic object in a box (for example, a tennis ball in a tennis court), we will obtain a very small number for  $E_1$ .
- Adjacent energy levels would be so close together that we could not measure their differences.
- Macroscopic objects must have very large values of  $n$ .

- Classically, the **particle has equal probability of being anywhere inside the box.**
- The classical **probability density** is  $P(x) = 1/L$  (for  $0 < x < L$ , zero elsewhere) for the **probability to be 1** for the particle to be in the box.
- According to Bohr's correspondence principle, we should obtain the same probability in the region where the classical and quantum results should agree, that is, for large  $n$ .
- The **quantum probability density** is  $(2/L)\sin^2(k_n x)$ .
- For **large values** of  $n$ , there will be **many oscillations** within the box.
- The average value of  $\sin^2\theta$  over one complete cycle is  $1/2$ .

- The average value of  $\sin^2\Theta$  over many oscillations is also  $1/2$ .
- Therefore, the **quantum probability approaches  $1/L$  in this limit**, in **agreement with the classical** result.
- If we had done a calculation, similar to that in the previous example, for an **electron** in the nucleus, we would find energies on the order of  **$10^4$  MeV**, much larger than the rest energy of the electron.
- A correct relativistic treatment is necessary, and it would give electron energies significantly less than  $10^4$  MeV but still much larger than those of electrons actually observed being emitted from the nucleus in  $\beta$  decay.
- **Such reasoning indicates that electrons do not exist inside the nucleus.**

**END OF THE LESSON.**

**THANKS FOR YOUR ATTENTION.**