Quantum Mechanics

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1 Introduction

Until this point in the course, we have always started with physical laws that you learned in your earlier courses on mechanics and electricity and magnetism and worked carefully, step by step through their consequences. Now, we shall use the framework which we have built to describe waves to reveal new physical laws for systems which you have not yet studied. The result will be the laws of quantum mechanics.

Quantum mechanics is a fascinating subject. It teaches that much of what you accept as common sense is wrong and that most everything you have learned so far in physics is not correct. The following three statements summarize the main intellectual content of quantum mechanics.

- **Anything can happen (almost[1]).**

  It is entirely possible for a person to run towards a wall — even without enough energy to break through it — and end up on the other side. A ball thrown perfectly straight through a door — even in vacuum so that there is nothing to deflect it — can take a sharp turn to the upon exiting the door. The moon could suddenly appear on the other side of its orbit from where you calculate it should be using Newton's laws. None of these things violates the laws of physics; all have a non-zero probability of happening. The world is indeed a magical place.

- **No one can say what will happen.**

  In addition to all sorts of unexpected things being possible, the world is also quite mysterious. It is impossible under the laws of physics ever to predict what will happen.

- **We can give the probabilities of the different possibilities.**

  Without this, there would be very little more to say, and physics would be a truly useless subject. It turns out that even with all of this unpredictability it is possible to determine the chances of different things happening. The subject of quantum mechanics consists mostly of learning to compute these probabilities and understanding what they mean for the world around us.

Classical limit — From the perspective of the scientific method, any new theory must be able to explain the predictions of previous theories. We resolve the unpredictability described in quantum mechanics with the reliability of the physics which you learned and verified in lab in your previous classes through the concept of the *classical limit*. In quantum mechanics, it turns out that the prediction of traditional or *classical physics* is by far the most likely possibility with all of the weird things mentioned above having extremely low probabilities, *unless* the objects involved happen to be very "small" in a sense we will quantify in Section 3. This idea gets the name *classical limit* because it is usually phrased mathematically: in the limit as the size of things becomes large, the probability of the classical result approaches one (certainty).

Elementary particles — There are many situations which do not fall under the classical limit and for which quantum mechanics becomes quite important. Usually these situations involve the smallest possible objects, *elementary particles*, things like electrons, photons and quarks. Often people get hung up on whether these *elementary particles* are really "particles" or "waves." But, *particle* and *wave* are concepts of classical physics, which has very little to do with such objects. Indeed, some things which *elementary particles* do may remind us of our classical concepts of particle or wave behavior, but we should always keep in mind that *elementary particles* are *elementary particles*, neither *waves* nor *particles*. The task of quantum mechanics is to observe and determine what these objects do and then to learn how to describe this behavior without bringing in our own prejudices. When we do this, we see that it turns out that the *elementary particles* have much more in common with each other than they do with our concepts of *particles* and *waves*.

2 Electron diffraction experiment

In the spirit of observing and characterizing the behavior of *elementary particles* without prejudice, we performed an experiment in lecture on electrons where we observed their trajectories in vacuum after being sent through a series of slits formed by atoms of aluminum.

Figure 1 shows the experiment. The experiment takes place in a cathode ray tube (crt) similar to almost all computer monitors before the advent of the lcd flat panel display. Such a tube is filled with vacuum and has on one end a source of electrons and on the other end an observation screen coated with a chemical which gives a little flash of light at the location where each electron hits it. In general, the source emits

[1] As we will see, sometimes the probability of something happening "accidently" turns out to be zero (See Section 3.), but the *possibility* must always be considered.

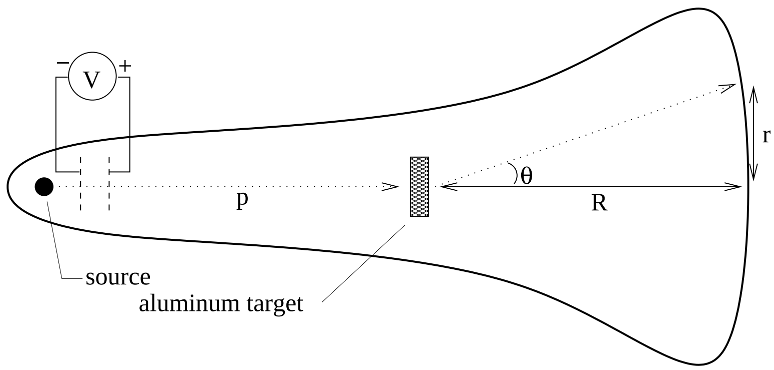

Figure 1: Schematic of electron diffraction experiment performed in lecture

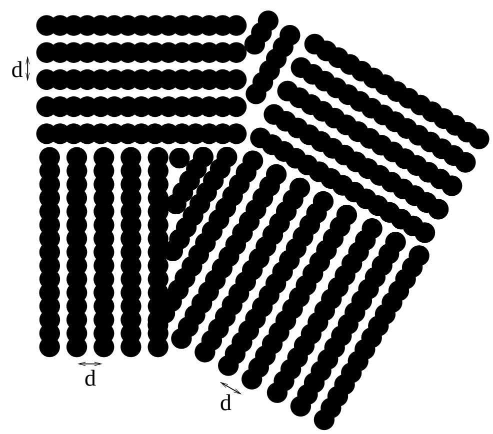

Figure 2: Small section of target from electron beam's head-on viewpoint

electrons at such a high rate that we do not perceive the individual flashes; we just see a glow with brightness proportional to the rate or, equivalently, *probability* at which electrons arrive at each point.

After emerging from the source, the electrons pass through a parallel plate capacitor, made from two metal screens rather than solid plates so that the electrons can pass through. A knob controls the voltage V across the capacitor so that the electrons can be accelerated to different speeds, ultimately picking up a kinetic energy equal to the electron charge e times the voltage V,

$$KE = \frac{1}{2}mv^2 = eV. \tag{1}$$

Some additional equipment (not shown) focuses the accelerated electrons into a narrow beam which impinges on a target of aluminum metal (Al). Finally, after interacting with the aluminum metal, the electrons travel off to the observation screen at a distance $R = 0.20$ m from the target.

Aluminum metal is generally *polycrystalline*, consisting of many tiny *crystallites* of aluminum stuck together at all different random angles, where each little crystal is a nearly perfect periodic array of atoms of aluminum. Figure 2 illustrates a tiny portion of such a polycrystal, showing five crystallites stuck together. We will not be going into three-dimensional crystal structure in any detail in this course other than to say that aluminum forms a so-called face centered cubic (fcc) crystal in which the atoms are arranged tightly into planes of spacing $d = 2.34$ Å.[2]

[2]For completeness, we note here that the full three-dimensional arrangement is somewhat more complicated than implied

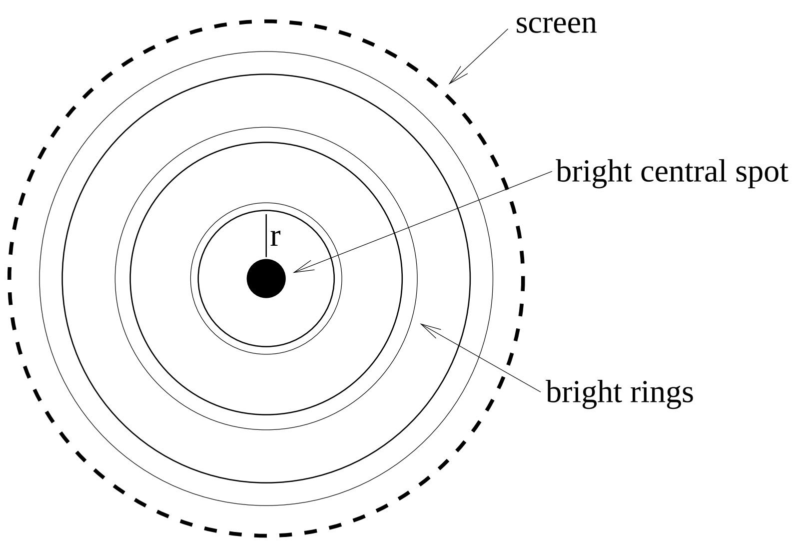

Figure 3: Image on surface of cathode ray tube

Upon sending the electrons through this series of slits, we observed something truly remarkable (Figure 3). The probability of finding electrons arranges itself into thin circles of narrowly defined radii. The geometry of the experiment (Figure 1), means that the narrowly defined radius of each of these circles implies that electrons emerging from each crystallite come out at certain specific highly preferred angles, with the arrangement into circles coming from the fact that the crystallites occur at all possible angles. The radii which we see, in addition to be very narrowly defined, also always seem to occur in multiples: if there is a circle of radius r, we also find circles of radii $2r$, $3r$, $\ldots$. This is extremely reminiscent of the sharply defined principle maxima of the intensity pattern for N-slits and leads to the hypothesis that *the probability of finding an electron emerging at an angle θ from one of the crystallites is exactly what we would compute for the intensity pattern of interfering waves passing through the slits formed by the planes of atoms in the crystal.* We are *not* saying that the electrons are waves, only that we can compute the probabilities using the same methods which we have already developed for computing intensities of waves.

The above hypothesis has been verified in detail many times. In fact, the radii of the different sets of rings correspond precisely to the spacings of the various planes of atoms in a truly three-dimensional treatment of the fcc crystal of aluminum. Moreover, many different types of barrier (other than crystals) have been tried, and each and every time the above hypothesis has held true. No one has yet to see a violation of it, for electrons or any other particle. It has even been verified for composite particles like helium atoms.

To turn the hypothesis into something useful for the central task of quantum mechanics, calculating probabilities, the final thing needed is to know the wave vector k to use in the phase factors in the sum over histories prescription for evaluating intensities. To understand what affects k, we observed how the radius of the innermost circle, which corresponds to the first-order principle maximum of the interference from the planes of spacing $d = 2.34$ Å, depends on the applied voltage. To relate this to the radius, we first note that from the N-slit interference formula, the nth-order principle maximum occurs at angle θ, where

$$kd \sin\theta = 2\pi n. \tag{2}$$

Then, to convert the observed radius r to the angle θ, we use the geometry in Figure 1 to find

$$\tan\theta = \frac{r}{R}. \tag{3}$$

here. It consists of multiple sets of planes at various spacings, with the spacing $d = 2.34$ Å being the most prominent.

V (volts)	r (m)	θ (rad)	k (m^{-1})	p (kg·m/s)	$\hbar$ (J·s)
10,000	0.93×10^{-2}	4.6×10^{-2}	58×10^{10}	5.4×10^{-23}	0.93×10^{-34}
5,000	1.36×10^{-2}	6.7×10^{-2}	40×10^{10}	3.8×10^{-23}	0.95×10^{-34}

Table 1: Data on smallest ring from electron diffraction experiment

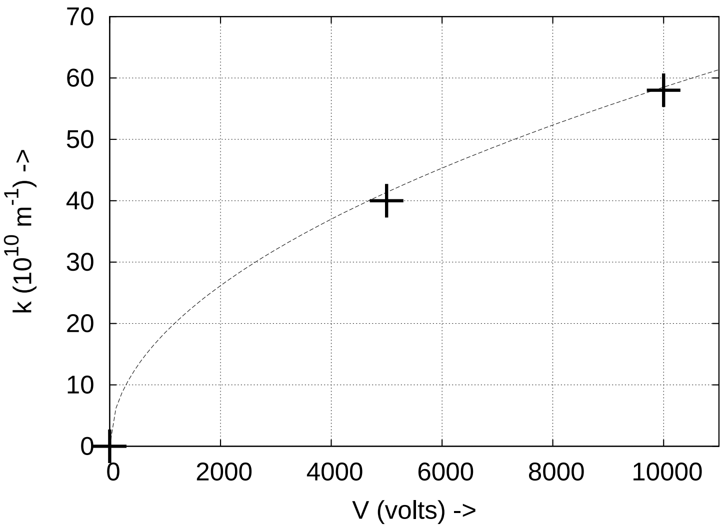

Figure 4: Plot of results from Table 1 (crosses) with sketch of square-root function for comparison (curve)

The first two columns of Table 1 summarize the raw results from one lecture for the radius of the smallest ring r for two different values of the applied voltage V. Then, to produce the third column we use $\theta = \tan^{-1}(r/R)$ from Eq. (3). To produce the forth column, we solve Eq. (2) with $n = 1$ (for the first-order principle maximum) to find $k = 2\pi/(d \sin\theta)$. The results for k show that it does depend on the voltage V.

To determine the functional dependence, Figure 4 shows the value of k as a function of V where we have added the additional data point (found by continuing to decrease V) that indeed $k \to 0$ as $V \to 0$. The data in the figure approach the origin with increasing slope, something characteristic of the square-root function (curve sketched in the figure), suggesting that the dependence is as the square-root of the voltage,

$$k \propto \sqrt{V}. \tag{4}$$

The difficulty with Eq. (4) as a new general physical law is that the quantity V is quite specific to our experiment and that there are many other ways to accelerate electrons. As a reflection of this, the proportionality constant in Eq. (4) turns out to be different for nearly every particle. To find a truly general law of physics, it is better to relate the intrinsic property k to some intrinsic property which the voltage controls. One possible choice would be to use the electron's velocity, but it turns out that using the momentum, which is even more fundamental as it is a *conserved* quantity, leads to a much more general relation that applies to all known particles. To relate k to the momentum p of the electrons, we first relate the kinetic energy of the electrons directly to the momentum,

$$KE = \frac{1}{2}mv^2 = \frac{1}{2}m\left(\frac{p}{m}\right)^2 = \frac{p^2}{2m}. \tag{5}$$

This form for the kinetic energy turns out to be very useful in advanced applications because it actually relates two conserved quantities, energy and momentum. It is in fact the form for kinetic energy always used in quantum mechanics and even more advanced courses on mechanics. It is worth memorizing.

The final relation between V and p we find by using $KE = eV$ from Eq. (1) and solving Eq. (5) for p,

$$p = \sqrt{2meV}. \tag{6}$$

Thus, we have that $p \propto \sqrt{V}$ from basic considerations of energy and momentum, and we also have from our experimental observations (Figure 4) that $k \propto \sqrt{V}$. Therefore, we conclude that $k \propto p$ in our experiment. In fact, this relation has been observed in many different experiments for electrons and every other known elementary particle, *with the same constant of proportionality for all particles!*.[3] The standard form for writing the proportionality is

$$k = \frac{p}{\hbar}, \tag{7}$$

where the proportionality constant $\hbar$ is a universal constant of nature known as *Planck's constant*. The symbol for this constant is an 'h' with a bar through the top and is pronounced "'h'-bar". This is to distinguish it from another constant unfortunately also known as *Planck's constant* but written as a plain 'h'. This other constant, which you may find in tables of physical constants, is directly related to the constant appearing in Eq. (7) through $h = 2\pi\hbar$. The reasons for this are purely historical. In this course, we shall always use the version with the bar.

Now that we have the general relation (7), the last thing we need is the value of $\hbar$. We could look this up in a table, but we can also determine an approximate value right from the experiment which we did in lecture. To do so, the fifth column of Table 1 lists the values of p determined from Eq. (6) using the voltage from the first column and the known values for the mass $m = 9.11 \times 10^{-31}$ kg and charge $e = 1.602 \times 10^{-19}$ C of the electron. Finally, the sixth column gives the value for $\hbar$ determined by solving Eq. (7) to give $\hbar = p/k$. The values are not quite the same because of errors in our experiment and the difference between them gives some idea of our experimental errors. We find a value of about 1×10^{-34} J·s, which is quite close to the official value of $\hbar = 1.055\ldots \times 10^{-34}$ J·s, especially considering how roughly we did all of the measurements!

The following statement summarizes the lessons learned from our experiment in a form that has been verified in many experiments and never yet observed to be violated.

> *de Broglie hypothesis (generalized)*: The probability $\mathcal{P}(x)$ of finding a particle at point x is proportional to the intensity $I(x)$ we would compute for waves of wave vector $k = p/\hbar$ (and frequency $\omega = E/\hbar$) at x, where p and E are the momentum and energy of the particle, respectively.

We call this form of the hypothesis "generalized" because de Broglie did not spell out the connection between probabilities and intensities quite so clearly. He was mostly responsible for the connections between momentum and wave vector and energy and frequency. The frequency-energy connection is not something that we will deal with in this course. It comes from other experiments (such as the photo-electric effect) which we will not cover; we include it here only for completeness.

3 Heisenberg Uncertainty Principle

From the de Broglie hypothesis, we can quickly predict the outcome of many experiments with elementary particles. The first experiment we shall consider demonstrates something very unusual about elementary particles known as the *Heisenberg Uncertainty Principle*. This principle what we mean by "small" in the idea of the classical limit and is useful in giving quick estimates of quantum mechanical effects.

The basic idea comes from what we already know about the intensity of waves after passing through any opening. The notes on interference show that the intensity of waves passing through a finite slit exhibit the phenomenon of diffraction: no matter how straight the waves approach the opening, on the other side the intensity spreads out over a range of angles. From the de Broglie hypothesis, we expect the same behavior for the probability of finding particles. This has some unusual implications.

[3] Once you accept this as experimental fact for all elementary particles, you can prove as a theorem that the same relation holds for the center of mass motion of any object composed of such particles. Thus, you can also use the same value of the constant for a baseball or yourself.

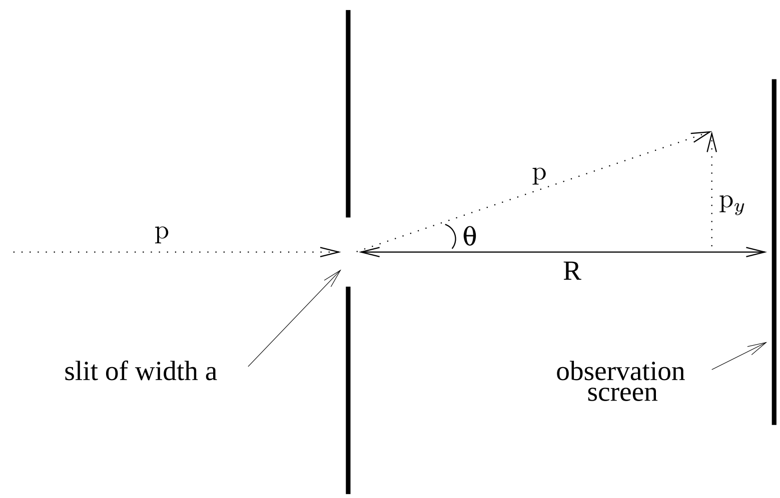

Figure 5: Particle of momentum p sent directly through slit of width a

Figure 5 shows an experiment where particles of momentum p are sent directly toward a slit of width a and then collected on a observation screen at a large distance $R \gg a$ from the slit. From the de Broglie hypothesis we have the immediate result that particles arrive at the screen with all possible random angles θ with the same pattern we found for the interference pattern from a single slit (from LN "Wave Phenomena II: Interference")

$$\mathcal{P} = \mathcal{P}_{max} \frac{\sin^2 \frac{\Delta\Phi}{2}}{\left(\frac{\Delta\Phi}{2}\right)^2}, \tag{8}$$

where $\Delta\Phi \equiv ka \sin\theta$ with k now given by the de Broglie hypothesis to be $k = p/\hbar$. Figure 6 shows the probability pattern.

For this type of experiment, the classical physics prediction is that all particles should arrive on the screen at the angle $\theta = 0$. Consistent with the concept of the *classical limit*, this is the most probable outcome. However, some particles will hit the screen at almost all angles, with the exception of just a few special points where the probability just happens to be zero. This means that every time a baseball is thrown through a door, even in vacuum so that there is nothing to disturb the path of the ball, there is some chance that it will take a sharp turn on the other side.

To see how this is not inconsistent with the observations of our daily lives, it helps to figure out what range of angles are most likely. The probabilities in Figure 5 tend to be rather small after the first minima bounding the central maximum. In fact, over 90% of the area under the curve is contained in the main peak between these first minima. Thus, with better than 90% certainty, we can say that the particle will arrive at angles in the range $|\Delta\Phi/2| < \pi$, so that $|\Delta\Phi| < 2\pi$. Using the definitions of $\Delta\Phi$ and k above, this gives $|ka \sin\theta| = \frac{pa}{\hbar} |\sin\theta| < 2\pi$. Thus, the reasonably expected range of angles is

$$|\theta| \approx |\sin\theta| \leq \frac{2\pi\hbar}{pa}, \tag{9}$$

where remind ourselves of the small angle approximation. The key to Eq. (9) is that $\hbar$ is extremely small in standard units, approximately 10^{-34} J·s, so that the range of likely angles thus will be very small for normal objects. For instance, if we toss ($v \approx 10$ m/s) a baseball ($m \approx 0.1$ kg) through a door ($a \approx 1$ m), we find $pa = mva = 1$ kg·m^2/s $= 1$ J·s and thus $|\theta| < 2\pi \times 10^{-34}$ radians, an angle so small that we never notice it in everyday life. On the other hand, if the objects and distances involved are small enough so that pa approaches $\hbar = 10^{-34}$ J·s, then a wide range of angles becomes likely. This answers the question of how small is "small enough" so that classical physics begins to break down.

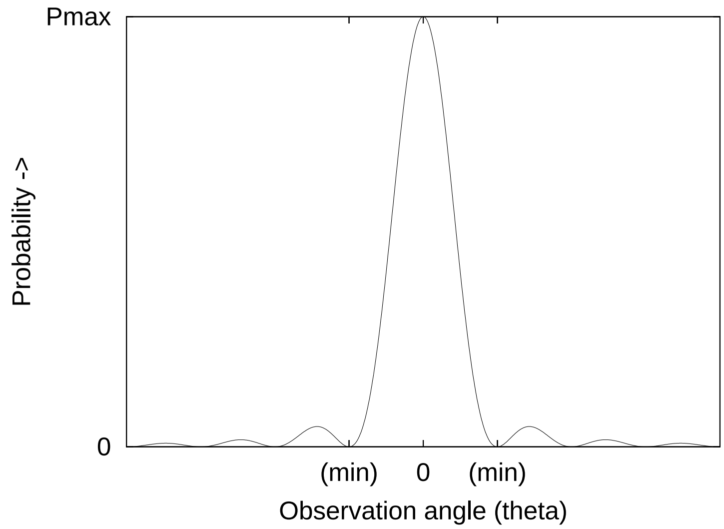

Figure 6: Probability of observing particle on screen at deflection angle θ

Heisenberg realized that this phenomenon of spreading out after being restricted through an aperture is very general and found a very useful way of expressing the result in terms of classical concepts about particles. The slit in Figure 5 restricts the particles to a range of values $\Delta y = a$ in the y-direction. The fact that the particles can then be found on the screen at angles θ means that after being restricted by the slit in the y-direction, the particles now pick up random (!) momenta p_y in the y-direction of value which the geometry of Figure 5 determines to be $p_y = p \sin\theta$.[4] The likely range in these random momenta is thus $\Delta p_y = p|\sin\theta| = \frac{2\pi\hbar}{a}$, where we have used the likely range of angles from Eq. (9). Note that this range becomes greater and greater in inverse proportion as a decreases. Heisenberg described this effect by saying that the act of constraining a particle to a region of size Δy along the y-direction results in an uncertainty in its momentum Δp_y so that $\Delta y\,\Delta p_y$ is at least as big as some constant. (He said "at least" as big because it is always possible to introduce additional sources of uncertainty beyond the fundamental limit.) In this case, multiplying our results, we find the constant to turn out to be $2\pi\hbar$.

A few technical notes are in order. In defining the uncertainty Δp_y, we used the range of momenta for which we have 90% confidence. The precise definition used in advanced courses in quantum mechanics is to use the standard deviation statistic that we use in the analysis of exam scores, which gives a somewhat narrower measure for Δp_y. Also, a "smoother" slit where the particle has some chance of making it through the edges can also lessen the uncertainty in Δp_y. Finally, we could just as easily aligned our slit with the x-axis. When all of this is taken into account, the precise mathematical statement has been shown to be that we have separately for each component x, y and z that

$$\begin{aligned} \Delta x\,\Delta p_x &\geq \frac{\hbar}{2} \\ \Delta y\,\Delta p_y &\geq \frac{\hbar}{2} \\ \Delta z\,\Delta p_z &\geq \frac{\hbar}{2}, \end{aligned} \tag{10}$$

but that there is no restriction when mixing directions,

$$\Delta x\,\Delta p_y \geq 0$$

[4]Because there is nothing in the experiment to add energy to the particles, they all do arrive with the same *magnitude* of momentum p, as the figure shows.

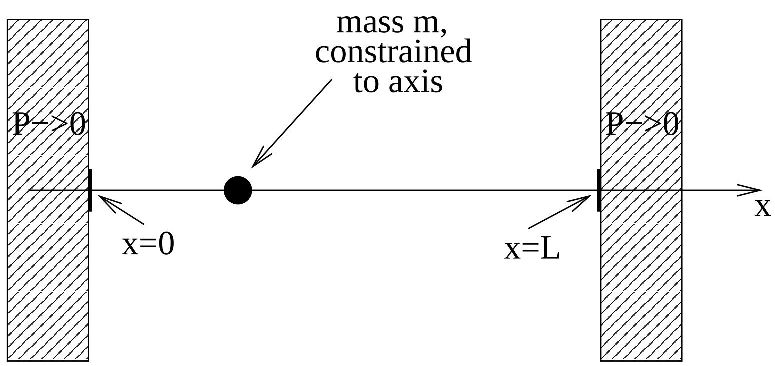

Figure 7: Realization of particle of mass m in a one-dimensional "box"

$$\begin{aligned} \Delta x\,\Delta p_z &\geq 0 \\ \Delta y\,\Delta p_x &\geq 0 \\ &\text{etc.} \end{aligned}$$

More typically, one never quite reaches the fundamental limit in Eq. (10) and one can make reasonably good estimates in problems by setting $\Delta x \Delta p_x, \Delta y \Delta p_y, \Delta z \Delta p_z \sim \hbar$.

4 Particle in a box

Our first application of the de Broglie hypothesis dealt with probability patterns that correspond to waves interfering and diffracting as they traveling through various obstacles. We now consider an application which corresponds to the first phenomenon which we have studied, normal modes. From the general wave behavior of normal modes we will learn several important general lessons about the behavior of elementary particles.

As a first example, we consider a "particle in a (one-dimensional) box" as in Figure 7. Here, a particle of mass m is constrained to move along a frictionless rod oriented along the x axis. A very strong repulsive force is applied at $x = 0$ so that the probability $\mathcal{P}(x)$ of finding the particle at points $x < 0$ becomes extremely small, $\mathcal{P}(x < 0) \to 0$. The "box" is completed by applying a similar repulsive force at $x = L$ so that the probability of finding the particle at locations $x > L$ is also extremely small, $\mathcal{P}(x > L) \to 0$. In general in quantum mechanics, we cannot make these probabilities go exactly to zero, but we can consider the *idealization* that the forces are sufficiently strong to make the probabilities as close to zero as we like.

Just as there are many possible answers for the intensity of waves moving along a string depending upon how we generate the waves, there are many possible answers for $\mathcal{P}(0 < x < L)$, the probability of finding the particle at any of the allowed points between $x = 0$ and $x = L$, depending upon how exactly we place the particle into the box, the so called "state" of the particle. For the string, although many states of motion are possible, there are a few which are very natural and easy to generate, the normal modes. Similarly, it is quite common to find particles states corresponding to normal modes. Thus, we often find $\mathcal{P}(x) = |\underline{A}(x)|^2$, where $\underline{A}(x)$ is the complex amplitude for a normal mode of classical wave motion. In quantum mechanics, the complex amplitude has a special name, the *wave function* and is usually written with the Greek letter 'psi' so that $\underline{A}(x) \equiv \Psi(x)$. This "wave function" is nothing very mysterious, just the same complex amplitude which we have used throughout the course. The standard way of writing out the probability for finding an electron is thus,

$$\mathcal{P}(x) = |\Psi(x)|^2. \tag{11}$$

For the present situation, the conditions $\mathcal{P}(x = 0) \to 0$, $\mathcal{P}(x = L) \to 0$ mean that the wave function (complex amplitude) $\Psi(x)$ must go to zero at the points $x = 0$ and $x = L$, corresponding to *fixed* boundary conditions. We already found the normal mode solutions for such boundary conditions to be $y(x, t) =$

$A_0 \sin(k_n x)\cos(\omega t)$, where every point under goes simple harmonic motion in phase at the same frequency, and

$$k_n = \frac{\pi}{L} n \quad ; n = 1, 2, 3, \ldots \tag{12}$$

Rewriting this in the complex representation, we have $y(x,t) = \text{Re}\left(A_0 \sin(k_n x) e^{-i\omega t}\right)$ so that the complex amplitude for the nth mode is $\underline{A}(x) = A_0 \sin(k_n x)$. Correspondingly, we expect the probability of finding a particle in a box in one of these "normal mode" states to be given by Eq. (11) with

$$\Psi_n(x) = A_0 \sin(k_n x), \tag{13}$$

where Eq. (12) determines k_n.

Having found for each normal mode n the probability of finding the particle at different points x, we next ask for the momentum of the particle. The de Broglie relation gives the magnitude as $p = \hbar k_n$, but momentum is a vector the de Broglie relation says nothing about the direction or sign of p. To address this issue, we note that any standing wave can be written as a sum of a forward and a backward traveling wave. Mathematically, we can rewrite the solution Eq. (13) using Euler's formula to find

$$\Psi_n(x) = A_0 \frac{e^{+ik_n x} - e^{-ik_n x}}{2i}, \tag{14}$$

so that we see that the particle "state" consists of both a forward $+ik_n x$ and a backward $-ik_n x$ moving part, indicating that it is possible to find either possibility, $p = \pm\hbar k_n$. As probabilities in quantum mechanics are always given by intensities, to determine the probability for each of these two alternatives, we look at the factors multiplying the two component waves and take their square magnitude,

$$\mathcal{P}_{\pm} \propto \left|\pm \frac{A_0}{2i}\right|^2 = \frac{|A_0|^2}{4}. \tag{15}$$

The two possibilities have equal intensities and thus are equally likely. The changes of finding $p = \pm\hbar k_n$ are 50%:50%.

Finally, we consider the energy of the particle in state n. This is tricky because we do not know where we will find the particle or what its momentum will be, and so we must consider all of the possibilities. The total energy is the sum of the potential and kinetic energies. Because the particle is always found in the allowed region $0 < x < L$ where there is no force acting, the potential energy is always $U = 0$. The kinetic energy is given by $KE = \frac{p^2}{2m}$ and the momentum will be either $\pm\hbar k_n$ so that the kinetic energy will also always have a single value, $KE = \frac{\hbar^2 k_n^2}{2m}$. Thus, although the position and momentum are uncertain, we always find a single, well defined value for the energy of

$$E_n = KE + U = \frac{(\pm\hbar k_n)^2}{2m} + 0 = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2} n^2$$

when the particle is in state n.

Having a single, well-defined value for the energy turns out to be a general feature of particles in normal mode quantum states, and so these states are typically called "energy states". Ultimately, this feature results from the frequency-energy part of the de Broglie hypothesis. It arises from the fundamental property of normal modes that every point undergoes harmonic motion at the same frequency frequency, which the frequency-energy relation translates into a single, well-defined value for the energy.

5 Schrödinger Equation

Figure 8 illustrates the final application we shall consider in this set of notes, finding the probability $\mathcal{P}(x)$ for the energy states of a particle of mass m and energy E moving along the x-axis under the influence of a force $F(x)$ which we describe by the usual potential energy $U(x) \equiv -\int F\,dx$. Unlike the particle in a

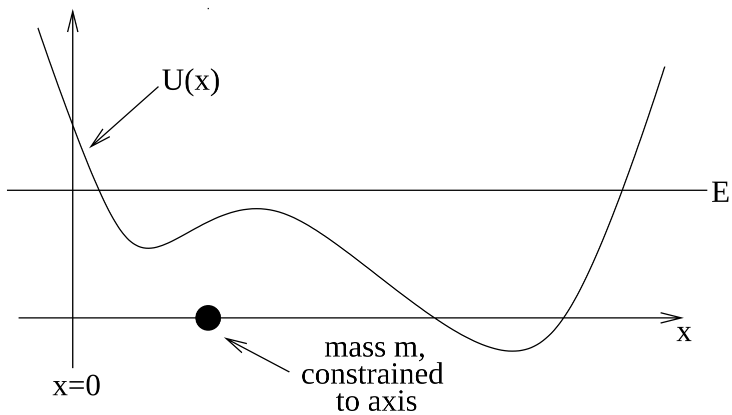

Figure 8: Realization of particle of mass m with energy E moving in potential $U(x)$.

box, this problem cannot be solved by simple analogy to classical waves. It requires our general approach to new problems of (1) identifying the degrees of freedom, (2) finding the equation of motion, (3) solving the equation of motion. The next set of notes explores how to solve the equation of motion. Here, we shall complete the first two of these phases.

Degrees of freedom — From the example of the particle in a box, we learned that the the basic quantity which specifies the state of the system at any instant in time and from which all other quantities can be determined is the wave function $\Psi(x)$. The appropriate choice for the degrees of freedom is thus $\Psi(x)$.

Equation of motion — The equation of motion expresses the controlling physical laws in terms of nothing other than the degrees of freedom, derivatives of the degrees of freedom and given physical quantities and constants. As for the physical laws, the problem involves various types of energy, whose definitions we must invoke, and also involves the quantum mechanical behavior of particles, which the de Broglie hypothesis describes. Thus, we can express the basic physical laws as

$$\begin{aligned} E &\equiv \frac{p(x)^2}{2m} + U(x) \quad \text{; Definitions of energy} \\ &= \frac{(\hbar k(x))^2}{2m} + U(x), \quad \text{; de Broglie hypothesis} \end{aligned} \tag{16}$$

where we have been cautious to note that the presence of the force means that the particle will have different velocities and thus different momenta p and wave vectors k at each point x. This equation expresses all of the physical laws in a single equation; however, it uses $k(x)$ which, unlike all other quantities in the equation, is not a given quantity. To complete the equation of motion, we must find a way to express the wave vector directly in terms of the degrees of freedom $\Psi(x)$ at its derivatives.

To find such an expression, first recall that the wave vector k counts up how many oscillations there are in $\Psi(x)$ per unit length. This kind of counting is difficult to express in terms of the value of $\Psi(x)$ and its derivatives. However, the number of oscillations per unit length is certainly related to the curvature of $\Psi(x)$ – the more curvature, the more oscillations per unit length. To see this mathematically, consider the second derivative (which gives the curvature) of any pure sinusoidal wave of arbitrary amplitude and phase,

$$\begin{aligned} \Psi(x) &= A\cos(kx + \phi_0) \\ \Psi'(x) &= -kA\sin(kx + \phi_0) \\ \Psi''(x) &= -k^2 A\cos(kx + \phi_0) = -k^2\Psi(x). \end{aligned}$$

Thus, we see that we can get a measure of the wave vector k at any point by looking at the ratio of the second derivative to the value of the function,

$$k(x)^2 = -\frac{\Psi''(x)}{\Psi(x)}. \tag{17}$$

Substituting the result Eq. (17) into Eq. (16) gives the final equation of motion,

$$E = -\frac{\hbar^2}{2m}\frac{\Psi''(x)}{\Psi(x)} + U(x).$$

Or, equivalently,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) + U(x)\Psi(x) = E\Psi(x), \tag{18}$$

where in the last line we have rearranged things somewhat to correspond to the standard way of writing the quantum equation of motion, the famous *Schrödinger Equation*.