

# UNIT 1: WAVES

One of the main features of quantum mechanics is that particles can behave like waves, so we first start with a description of classical waves, like sound. These waves are typically generated by a source, such as a speaker for sound waves, or a laser. The fundamental object is a function of space and time, which we will call  $y(x, t)$  in this section\*.  $y$  may represent the magnitude of the electric field for light, or the pressure in a sound wave, or the height of the water in a water wave.

## After this unit, you should be able to

- Identify the basic properties of a harmonic wave.
- Compute the intensity and average intensity for harmonic waves.

## Harmonic waves

To further simplify matters, we will consider harmonic waves of a single frequency. Such a wave propagating in the  $+x$  direction may be written as

$$y(x, t) = A \cos(kx - \omega t + \phi), \quad (1)$$

where  $\omega$  is the angular frequency and  $k$  is the wavenumber. For this class we will be considering waves either just in 1D or along a path in 3 dimensions, so you will not have to consider vector quantities. A summary is available in Table 1.

For concreteness, let's consider the classical (PHYS 212) description<sup>1</sup> of light waves polarized in the  $x$  direction. In this case, the wave equation describes the value of the electric field at a given position and time.

$$E_x(x, t) = E_{max} \cos(kx - \omega t + \phi) \quad (2)$$

Let's break this equation down. Since  $\cos$  always returns a value between  $\pm 1$ , the maximum electric field at any position or time is  $E_{max}$ . The electric field varies between  $\pm E_{max}$ . We will call this the **amplitude** of the wave.

Now let's consider the part inside the  $\cos$ :  $kx - \omega t + \phi$ . Recall that if we have a function  $f(x)$ , then  $f(x + a)$  shifts the entire function to the left by  $a$ .  $\phi$  serves this role for Eqn 2. The easiest way to read off  $\phi$  is to look at the value of the electric field at  $t = 0$  and  $x = 0$ . Then

$$\phi = \cos^{-1}(E_x(0, 0)/E_{max}). \quad (3)$$

Now let's consider  $t = 0$ . The function is then  $E_{max} \cos(kx + \phi)$ .  $k$  measures the rate at which the **wave repeats in space**; the wavelength  $\lambda$  is equal to  $2\pi/k$ , since the value of the wave is the same for  $x + n\lambda$ .

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<sup>1</sup>This description must be modified because light is actually *quantized*, which we will get to later in the course.

Symbol	Description	SI units	Light wave quantity
$k$	Wave number	$\text{m}^{-1}$	
$\lambda$	Wavelength	$\text{m}$	
$\omega$	Angular frequency	$\text{s}^{-1}$	
$\phi$	Phase offset	radians (unitless)	
$T$	Period	$\text{s}$	
$f$	Frequency	$\text{s}^{-1}$	
$I$	Intensity	$\text{W/m}^2$	
$A$	Amplitude	$\sqrt{\text{W/m}^2}$	

Table 1: Parameters that describe harmonic waves.

Now take  $x = 0$ ; the function is then  $E_{\max} \cos(-\omega t + \phi) = E_{\max} \cos(\omega t - \phi)$ .  $\omega$  is like  $k$  but for time; it's the rate at which the function oscillates in time. We call  $\omega$  the angular frequency, because the function has the same value for  $t + 2\pi/\omega$ . We also sometimes use the frequency  $f = \omega/2\pi$ , and the period  $T = 1/f$ . The period is the equivalent of the wavelength  $\lambda$  for time; it's how often the function repeats itself.

We define the speed of a harmonic wave by tracking how quickly a maximum value moves through space. Eqn 2 is at a maximum where  $kx_{\max} - \omega t + \phi = 2\pi n$ , where  $n$  is an integer. Let's consider  $n = 0$  to track one maximum in particular:

$$x_{\max} = \frac{\omega t - \phi}{k} \quad (4)$$

$$v = \frac{dx_{\max}}{dt} = \frac{\omega}{k} \quad (5)$$

So the speed of such a wave is given by  $v = \omega/k$ , which may also be written as  $\lambda f$ .

## Amplitude and Intensity

For many waves of interest, we don't directly detect the wave amplitude  $y$  at a given position and time (e.g., the instantaneous pressure of a sound wave, or the electric field strength of an electromagnetic wave). Instead, a quantity of interest is the average intensity, which describes how loud the sound is or how bright the light is. For light, it tells us the power per square meter incident on a surface. The intensity of the wave at a given time and position is  $I(x, t) = |y(x, t)|^2$ .<sup>2</sup> We will average the intensity over a period  $T$ :

$$I_{\text{average}}(x) = \frac{1}{T} \int_0^T |A|^2 |\cos(kx - \omega t + \phi)|^2 dt = \frac{|A|^2}{2}, \quad (6)$$

for a harmonic wave. For a pure harmonic wave, the **average** intensity is the same at all places in space.

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<sup>2</sup>For some variable  $x$ ,  $|x|^2$  is the absolute value squared. The absolute value is there because sometimes  $y$  is complex, which we will see later in the course.

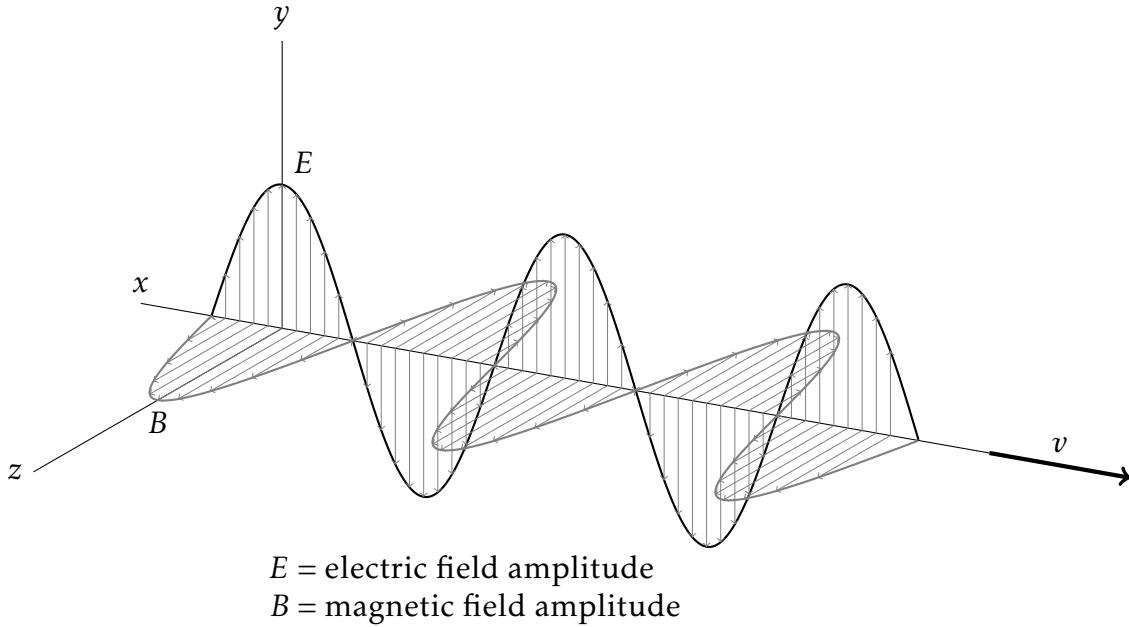


Figure 1: An electromagnetic wave. The fields oscillate in both space (wavelength  $\lambda$ ) and time (frequency  $f$ ).

In the next unit, we will consider what happens when we *superimpose* two harmonic waves. Using light waves as an example, depending on the location and time, the electric field may add or subtract, which will make the time-averaged intensity depend on position. This adding and subtracting of the field value is called interference.

## Example: Light waves

In electromagnetism, light is described as a wave in the electric and magnetic field. The amplitude of the wave is proportional to the maximum electric field<sup>3</sup>, and the wavelength and frequency are related by  $\lambda f = c$ , where  $c$  is the speed of light. Note that the electric field is a vector, which means that it oscillates between pointing one direction and the opposite direction, as diagrammed in Fig 1.

The frequency/wavelength determine the properties of the light. For example, visible light has wavelengths between around 400 and 700 nm (1 nm is  $10^{-9}$  m!), about 1/50 the width of a human hair. This is actually a very narrow proportion of all possible wavelengths! The classification of light waves depends on the reference you look at (it's really a continuum, so classifications are arbitrary), so be sure to check your references. We've provided a rough list in Table 2.

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<sup>3</sup>The maximum magnetic field is required to be proportional to the maximum electric field, so we usually just track the electric field.

	Wavelength range	Frequency range	Example use
Radio	> 1m	0-300 MHz	Communication
Microwaves	1 mm - 1 m	300 MHz-300 GHz	Communication (i.e, WiFi 5.4 GHz)
Infrared	700 nm - 1 mm	300 GHz-430 THz	Thermography
Visible	400 nm - 700 nm	430 THz - 750 THz	Sight..
Ultraviolet	10 nm - 400 nm	750 THz - 30 PHz	CPU manufacturing
X-ray	0.1 nm - 10 nm	30 PHz - 30 EHHz	Medical imaging
Gamma ray	< 0.1 nm	> 30 EHHz	Cancer treatment

Table 2: Wavelength and frequency of various types of light.

## UNIT 2: INTERFERENCE

### After this unit, you should be able to

- Compute the phase difference at an observer's position between the waves emanated from two sources, then compute the intensity that the observer experiences.
- Apply interference rules to two-slit, interferometer, and other interference problems where the path length and source phases differ.

### Superposition of waves

In the previous section\*, we considered a single harmonic wave generated by a source. Now suppose that there are two sources (1 and 2) generating two waves. For this class, for simplicity, we will only consider waves with the same wavelength, amplitude, and speed, so they have the same  $A$ ,  $\omega$ , and  $k$ :

$$y_1(x, t) = A \cos(kx - \omega t + \phi_1) \quad (1)$$

$$y_2(x, t) = A \cos(kx - \omega t + \phi_2). \quad (2)$$

In many cases (you can always assume this in this course), the total wave is given by superposition<sup>1</sup>, so

$$y_{\text{total}}(x, t) = y_1(x, t) + y_2(x, t). \quad (3)$$

At some times and positions,  $y_1$  and  $y_2$  might be either the same sign or different signs. So at some locations the summed amplitude will be larger than either of the waves by themselves, and at other locations it will be smaller. We refer to this as **interference**. If the waves are the same sign, they will interfere *constructively* and if they are opposite signs, they will interfere *destructively*. A picture of this is shown in Figure 1.

Using the trigonometric identity

$$\cos \alpha + \cos \beta = 2 \cos\left(\frac{\alpha - \beta}{2}\right) \cos\left(\frac{\alpha + \beta}{2}\right) \quad (4)$$

we can find that

$$y_{\text{total}}(x, t) = 2A \cos\left(\frac{\phi_1 - \phi_2}{2}\right) \cos\left(kx - \omega t + \frac{\phi_1 + \phi_2}{2}\right) \quad (5)$$

So the result is a new cos wave with a new amplitude related to the difference in phase,  $2A \cos\left(\frac{\phi_1 - \phi_2}{2}\right)$ . That means that the average intensity is given by  $2A^2 \cos^2\left(\frac{\phi_1 - \phi_2}{2}\right)$ , so the difference in phase between the waves is the key to knowing the total intensity. There are a few ways of getting differences in the phase.

<sup>1</sup>Waves that do this are called “linear” because they add.

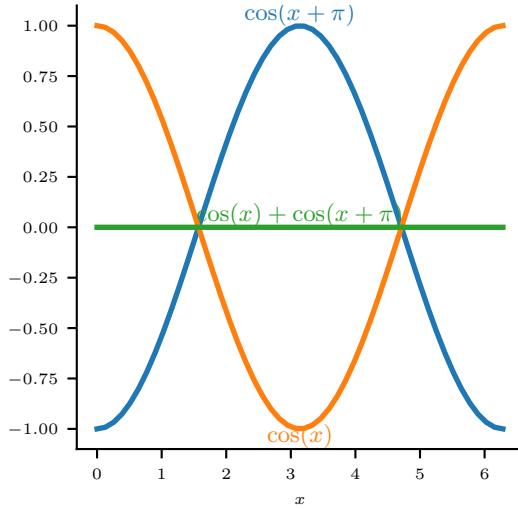


Figure 1: Destructive interference between two waves

## Phasors

What if the amplitudes of the waves are different? In that case, we cannot use the trigonometric identity in Eqn 4. Luckily, there is a graphical way of adding harmonic waves, called phasors.

An observer at a given position will see an amplitude from a given source that varies like  $A_1 \cos(\phi_1 - \omega t)$ . Phasors map this onto a two dimensional vector (Figure 2) with amplitude  $A_1$  and an angle from the  $x$ -axis given by  $\phi_1 - \omega t$ . Then the amplitude at any given time is given just by the  $x$  coordinate of the vector, by trigonometry. It turns out that you can add phasors as if they are vectors, and the  $x$  coordinate of the summed vector will give the amplitude of the wave at a given time. The length of the phasor squared, divided by two, will give the average intensity of the summed wave.

## Example: Two speakers

Now let's consider the intensity of waves emitted by two sources, as measured by an observer. We will consider an observer that is  $r_1$  away from source 1 and  $r_2$  away from source 2 (Figure 3) For simplicity, let's suppose that the sources have exactly the same amplitude. For example, this could be a person listening to music from two speakers. Our objective will be to compute how loud the observer perceives the sound to be. The waves that the observer experiences<sup>2</sup> from each source are:

$$y_1(x, t) = A \cos(kr_1 - \omega t + \phi_1) \quad (6)$$

$$y_2(x, t) = A \cos(kr_2 - \omega t + \phi_2). \quad (7)$$

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<sup>2</sup>This is the amplitude *at the observer's position*.

$$y_1(t) = 5 \cos(\omega t + \frac{\pi}{4}) \quad y_2(t) = 4 \cos(\omega t + \frac{\pi}{3})$$

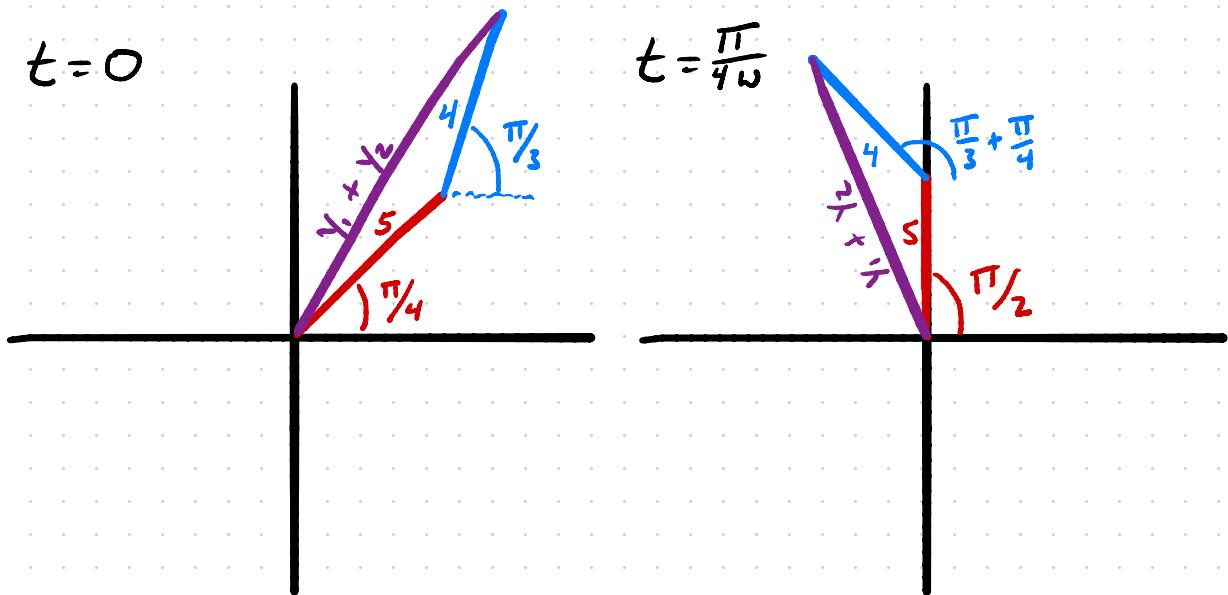


Figure 2: A figure that shows the relationship between phasors and harmonic waves.

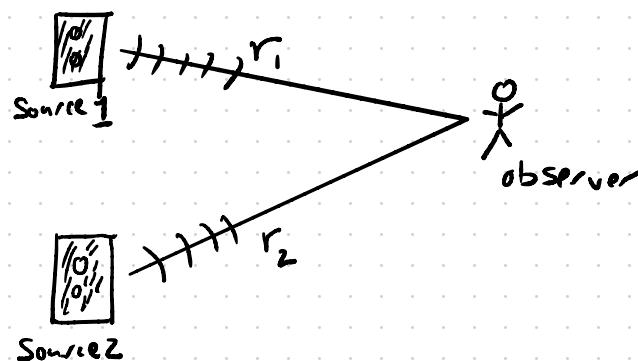


Figure 3: An observer experiencing the intensity of waves generated from two sources in phase.

Then, using the trigonometric identity from Eqn 4,

$$y_1(x, t) + y_2(x, t) = 2A \cos\left(\frac{kr_1 + \phi_1 - kr_2 - \phi_2}{2}\right) \cos\left(\frac{kr_1 + \phi_1 + kr_2 + \phi_2}{2} - \omega t\right). \quad (8)$$

and the total average intensity for that observer is

$$I_{\text{total}} = 2A^2 \cos^2\left(\frac{kr_1 + \phi_1 - kr_2 - \phi_2}{2}\right). \quad (9)$$

So the measured intensity depends on the relative phase offsets of the speakers ( $\phi_1, \phi_2$ ) as they are emitting the sound and the position of the observer relative to the two speakers.

Let's suppose that  $\phi_1 = \phi_2$  (when this is true, we say that the sources are in phase), so that

$$I_{\text{total}} = 2A^2 \cos^2\left(k \frac{r_1 - r_2}{2}\right) = 4I_1 \cos^2\left(k \frac{r_1 - r_2}{2}\right). \quad (10)$$

The intensity is maximal ( $2A^2$ ) when  $r_1 - r_2 = m\lambda$ , where  $m$  is an integer, and it is zero when  $r_1 - r_2 = (m + \frac{1}{2})\lambda$  for some (possibly other) integer  $m$ .

Because amplitudes add, and intensity is amplitude squared, the maximal intensity is actually **four** times as large as the intensity of a single source. Energy is still conserved here, because there are places with zero intensity. Interference is just redistributing the total energy compared to the two sources operating independently.

## Example: Two slits

An important example of interference is the two-slit experiment, shown in Fig 4. In this experiment, we aim a laser at an opaque barrier with two slits made in it. There is a screen placed a distance  $L$  away from the barrier. We measure the intensity of light on the screen as a function of the position on the screen.

We use the physics of interference to analyze this situation.

- We treat the slits as if they are sources of waves.
- Since both slits are equidistant from the laser, the waves at each slit are in phase; that is,  $\phi_1 = \phi_2$  when considered at the slit.
- The variation of intensity measured on the screen will be due to the fact that different points on the screen are different distances from the slits.
- If the slits are the same size, then the amplitude measured at the screen will be the same from each slit ( $A_1 = A_2$ ).
- The wavelength coming from both slits is the same, since the same laser is incident ( $k_1 = k_2$  and  $\omega_1 = \omega_2$ )

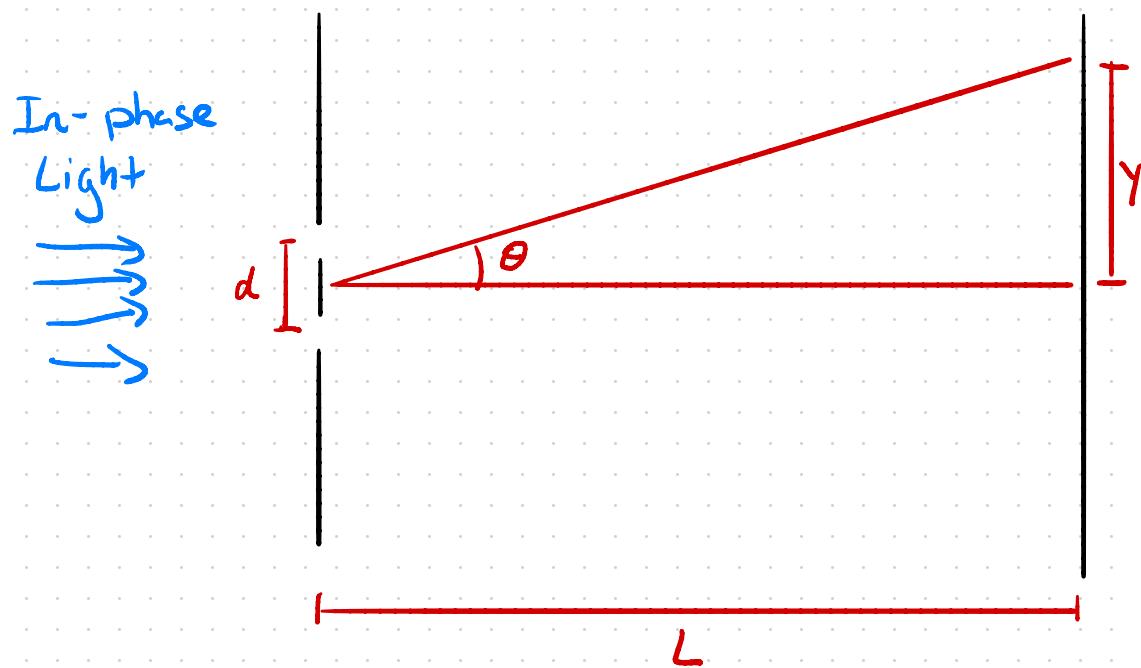
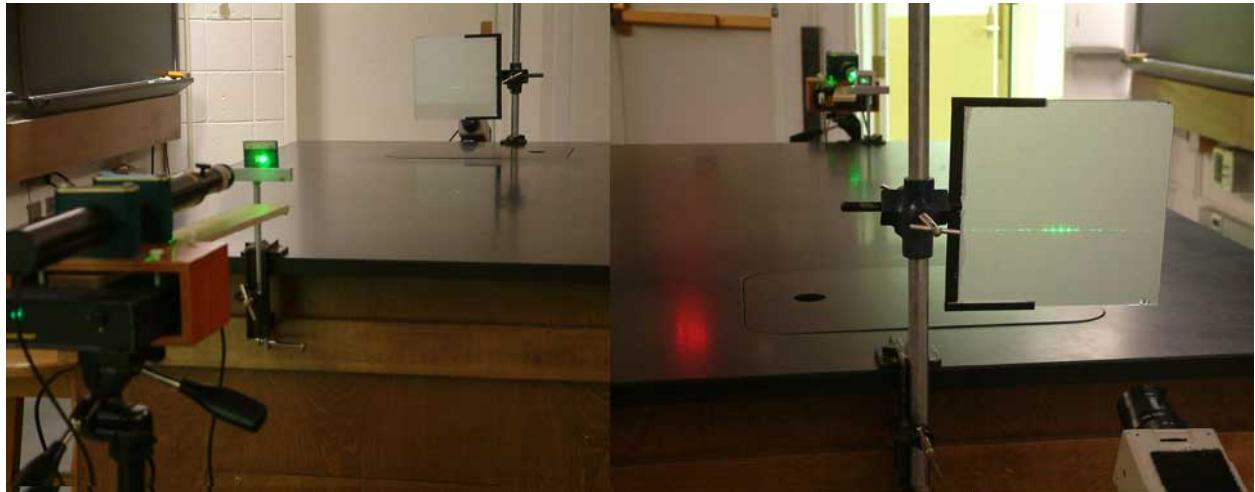


Figure 4: Geometric setup of a two-slit experiment. The card in the pictures has slits separated by a distance  $d$  (usually a few  $\mu\text{m}$ ). The screen is placed  $L$  (a meter or two) away from the card. Then the intensity varies on the screen as we can see from a pattern of bright and dark spots. The position on the screen is  $y$ .

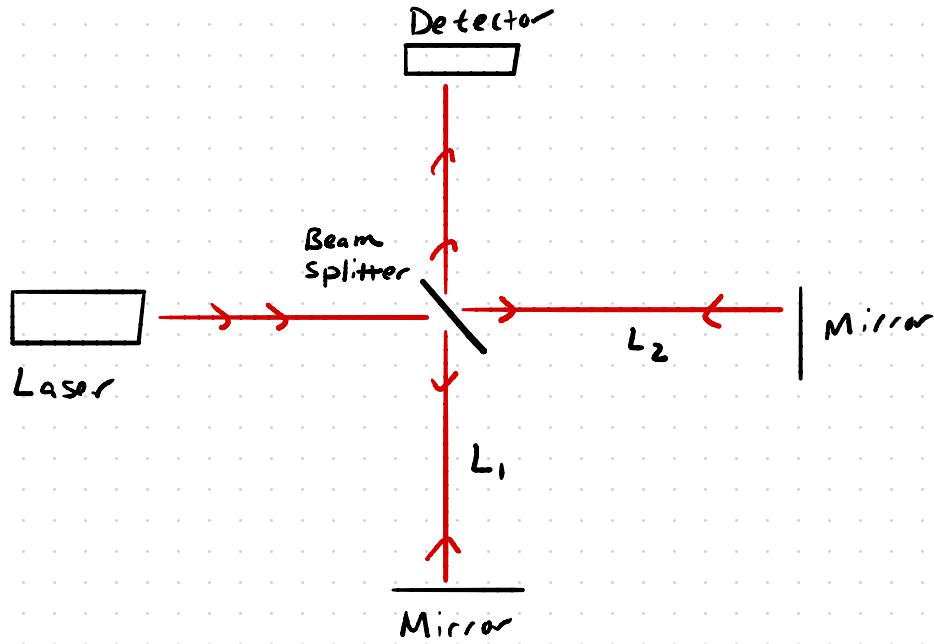


Figure 5: Interferometer optical setup

Because of these observations, we can use Eqn 10 to compute the intensity at a point in the screen. All that has to be done is to compute the difference in distance to the slits,  $\delta = r_1 - r_2$ .

The calculation of  $\delta$  can be done by assuming that  $L$  is much larger than the separation between the slits,  $d$ . In that case,  $\delta = d \sin \theta$ . So the angles at which the intensity is maximal will be when  $d \sin \theta = m\lambda$ , with  $m$  an integer. There will be minima between each of the maxima!

## Example: Interferometer

The interferometer uses interference to measure distances very accurately, as you might be able to tell from the name (interfero - meter). In this setup, a laser is sent down a path where it encounters a half-silvered mirror set at a 45 degree angle. This mirror reflects half of the light and allows half of the light to pass through. The **intensity** is reduced by a factor of two for each path, but then recombines. The light then travels down two separate paths, of length  $L_1$  and  $L_2$ , and rejoin at the mirror. We place a detector as noted in the figure.

Since the mirrors typically absorb some of the light, we typically don't work the intensity of the laser, but instead use the intensity of the light with one path blocked:  $I_1$ . Since the two paths are in phase, we can use Eqn 10, so

$$I = 4I_1 \cos^2 \left( k \frac{r_1 - r_2}{2} \right). \quad (11)$$

$r_1$  is the distance traveled on one path, and  $r_2$  is the distance traveled on the second path. It actually doesn't matter the total values of  $r_1$  and  $r_2$ ; we can compute  $r_1 - r_2$  knowing just the *difference* between the arm lengths:

$$r_1 - r_2 = 2(L_1 - L_2) \quad (12)$$

The factor of two occurs because the light travels the arms twice, once to the terminal mirror, and again on the way back.

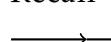
## UNIT 3: DIFFRACTION

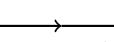
Consider light passing through a single slit, incident on a screen a distance  $L$  away. Previously, we assumed that the slits acted as if they were infinitesimally thin and acted as point sources. For slits of a finite width, *each location* along the slit acts as if it were a point source; this principle is known as **Huygen's principle**. This will create a spot on the screen due to the interference between all the points on the slit. Thinner slits lead to larger spots and thicker slits lead to smaller spots.

### After this unit, you should be able to

- Compute the size of spots that a single slit or a single circular aperture makes on a screen.
- Be able to construct phasor diagrams that lead to destructive interference and compute the angle between the phasors.
- For a diffraction-limited optical setup, suggest changes that will decrease/increase the size of the spots.

### Phasors for more than two sources

Recall that the phasor diagram for two sources in constructive interference looks like . The angle between the phasors is  $2\pi m$ , with  $m$  an integer. This is achieved when  $k(r_2 - r_1) = 2\pi m$ , assuming the sources were in phase. For the two-slit experiment,  $r_1 - r_2 = d \sin \theta$ , which combined with before gives us the relationship  $d \sin \theta = m\lambda$ .

Phasors become particularly useful when there are more than two sources. Suppose that there are now three slits equally spaced  $d$  apart. Then  $r_1 - r_2 = d \sin \theta$  and  $r_2 - r_3 = d \sin \theta$ . Then we can get constructive interference between *all three* if we have a phasor diagram like the following: . In analogy to the two-slit problem, this happens when  $k(r_2 - r_1) = 2\pi m$  and  $k(r_3 - r_2) = 2\pi m$ , for the same  $m$ . This can happen if  $d \sin \theta = m\lambda$ , the same condition for maxima of the two slit situation. You can likely see that the same condition will hold no matter how many evenly spaced slits we have.

It turns out (we will not prove this in this course) that the maxima get sharper the more slits are participating. This fact is used to produce **diffraction gratings**, which have many slits and are used to perform spectroscopy. Spectroscopy<sup>1</sup> allows us to measure precisely what wavelengths are present in a given light source.

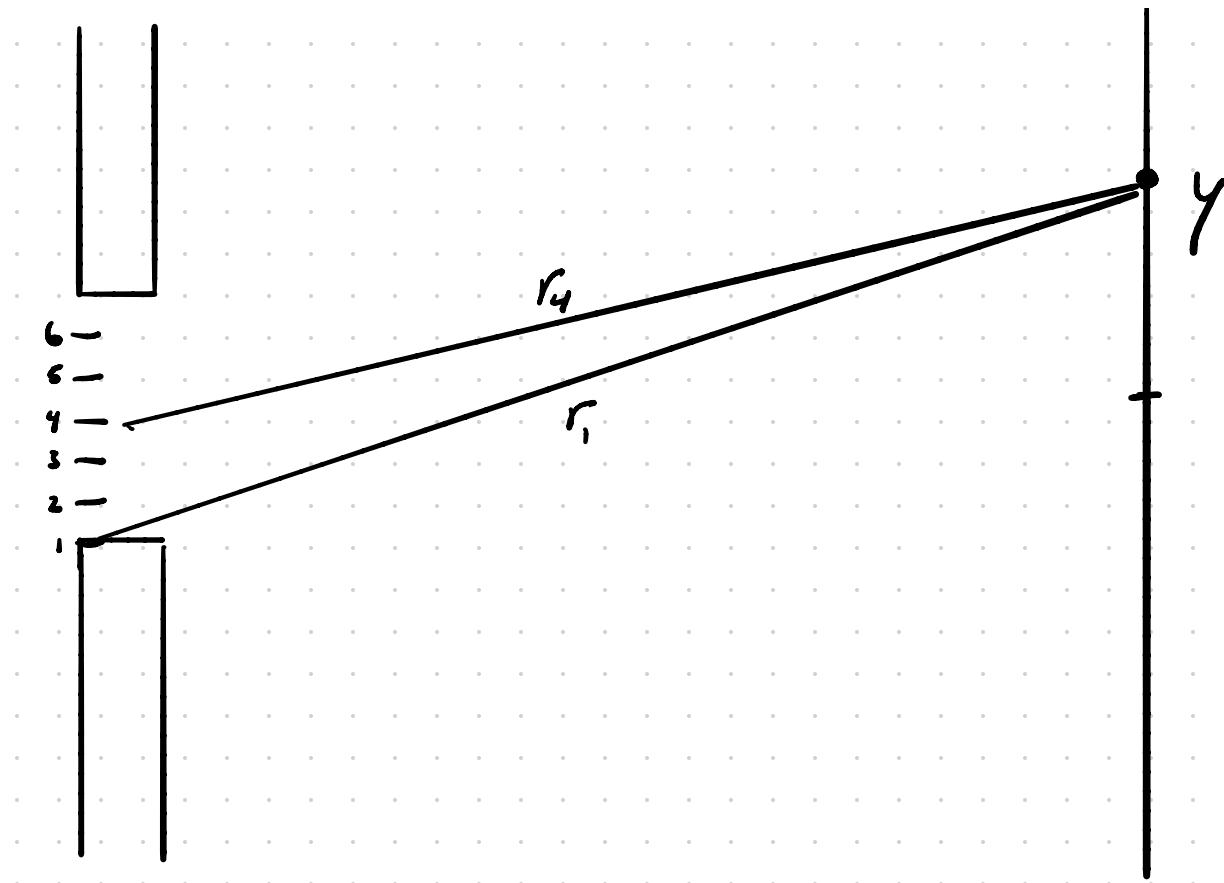


Figure 1: The partitioning of a single slit into 6 point sources.

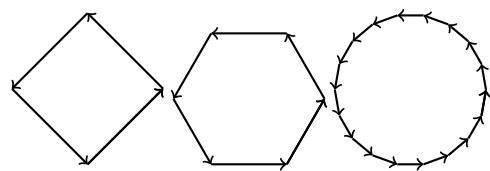


Figure 2: Phasor diagrams that lead to destructive interference for different numbers of point sources.

## Diffraction from a single slit

Our goal in this section<sup>\*</sup> will be to compute the intensity of light at a given position  $y$  on the screen. For our purposes, we will really just be satisfied in finding where the intensity goes to zero the first time, so we know how big the spot is. It's easier to consider the angle  $\theta_0$  at which the intensity is zero. To do this, let's pretend that the single slit (width  $a$ ) is actually made up of  $N$  point sources, separated by a distance  $d = a/N$ . We will take the limit as  $N \rightarrow \infty$ .

There is complete destructive interference when the phasor diagrams complete a full loop, since the sum of all the phasors is zero (the sum ends up back where we started, so the total is zero). This is shown in Fig 2 for a few different values of  $N$ .

We will follow the same strategy as before; first we need to know what angle  $\phi_0(N)$  leads to a closed phasor diagram. This is  $2\pi/N$ ; that way  $N$  angles add up to one complete rotation,  $2\pi$  radians. There is destructive interference when

$$k(r_2 - r_1) = \frac{2\pi}{N} \quad (1)$$

Plugging in  $2\pi/\lambda$  for  $k$  and  $a/N \sin \theta$  for  $(r_2 - r_1)$ , we get

$$a \sin \theta_0 = \lambda \quad (2)$$

Note that this result does not depend on  $N$  at all! So the limit as  $N \rightarrow \infty$  does not change the result. Remember that this is the angle of the first zero in the spot.

The position of the zero on the screen is given by  $y_0 = L \tan \theta_0$ . The **size** of the spot is  $2y_0$ , since it extends in the positive and negative direction.

## Diffraction for a circular aperture

For a slit geometry, the zero of the spot satisfies the equation  $a \sin \theta_0 = \lambda$ . For a circular geometry, the derivation is very similar to the single slit case. We will not derive this quantity in this class; it's a little complicated and does not offer much insight. The result is that for a circle of diameter  $D$ , the first zero in the pattern is  $D \sin \theta_0 = 1.22\lambda$ .<sup>2</sup>

## Diffraction-limited optics

The presence of diffraction puts fundamental physical limits on how tightly we can focus light. Consider a point source of light, which is far away. The light from the point source is incident on a lens, which focuses the light onto a screen. This is how telescopes and cameras capture their images. The main point here is that even if a lens is used, diffraction will occur, so a point source will create on the screen a spot as large as we derived above.

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<sup>1</sup>In Latin, spectrum means "image" and the -scopy relates to the study of a subject.

<sup>2</sup>If you want to know more, this is called the Airy disk

## Example: diffraction and lithography

Lithography<sup>3</sup> is the technique used to draw tiny nanometer resolution circuits on semiconductors to create computers, phones, and other electronics. A laser is sent through a lens to focus it onto a given spot, which removes material from the silicon. The important question is how large the spot will be; this determines how narrow the lines are and how closely they can be drawn to one another.

Suppose the lens has diameter  $D$  and is a distance  $L$  from the silicon. The wavelength of the laser is  $\lambda$ . Then the first zero is at  $\theta_0 = \sin^{-1}(1.22\lambda/D)$ . The thickness of the line is  $2L\tan\theta_0$ . Plot these functions; you can see that if  $\lambda$  is increased, then the thickness of the line increases, while if  $D$  increases, then the thickness decreases. Similarly,  $L$  should be as small as possible to make the line as thin as possible.

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<sup>3</sup>The litho prefix means ‘stone,’ and the -graph suffix means to write or draw, so lithography literally means ‘to draw on stone.’

## UNIT 4: PHOTONS

Here's the conclusion: it turns out that light comes in discrete packets (quanta) of energy. We call one of these discrete packets a photon. For a given frequency of light, the quantum of energy is given by  $E = hf$ , or  $\hbar\omega$ , where  $h$  is a fundamental physical constant equal to  $6.626 \times 10^{-34} \text{ m}^2 \text{ kg/s}$  and  $\hbar = h/2\pi$ . The momentum of a photon is  $p = h/\lambda = \hbar k$ . In this unit, we will explore how we know this to be true.

### After this unit, you should be able to

- Explain why only certain wavelengths of light cause electrons to be ejected from materials
- Compute the kinetic energy of electrons ejected from a material
- Use the energy of a photon to compute the number of photons that arrive per second for a given intensity of light.
- Use the momentum of a photon to solve simple kinematics problems involving photons.
- Solve problems that use the relationships between wavelength, frequency, momentum, and energy of photons.

### Photoelectric effect

The photoelectric effect is one of the simplest physical situations in which we can observe the quantization of light. The experiment is as follows. Light is incident on a metal or other material, and there is a metallic electrode nearby. Electrons that are emitted from the material hit the electrode and cause a current to be measured.

Figure 1 shows the current observed for a fixed intensity of light, as a function of the frequency. We will explain three observations using the concept of photons:

1. There is a threshold below which no current is emitted, and then current appears.
2. For a fixed intensity of light, the current is maximal at the lowest frequency, and decreases as  $1/f$  as the frequency increases.
3. However, the *kinetic energy* of emitted electrons depends linearly on the frequency of light.

It turns out that one can explain this and many other experiments by proposing that energy can be added and removed to the electromagnetic field in **quanta** with energy  $\hbar\omega = hf$ . We call these discrete packets photons.

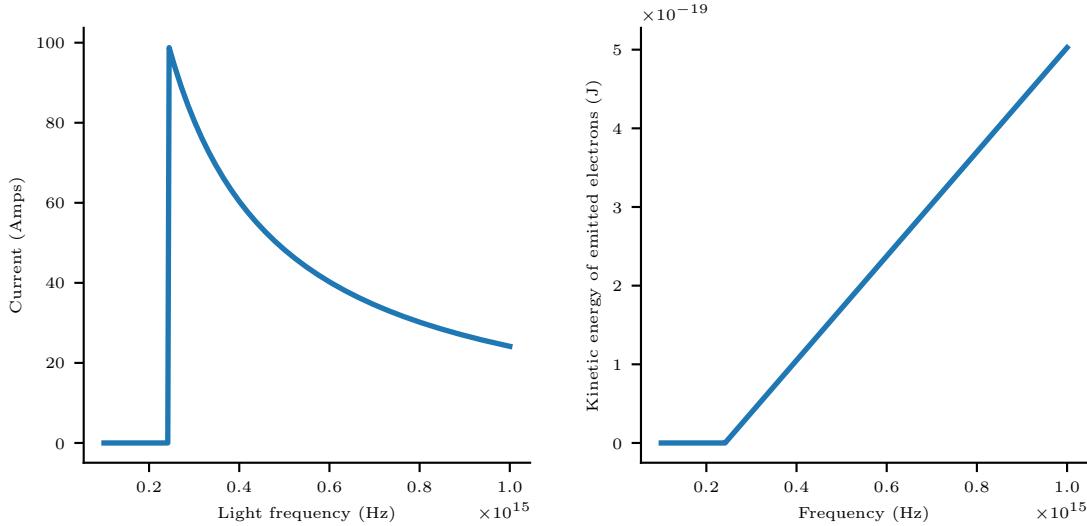


Figure 1: Sketches of the photoelectric effect. (left) The current observed for a fixed intensity of light of a given frequency. (right) The kinetic energy of ejected electrons as a function of the frequency of incident light.

The **threshold effect** is explained because it takes a certain amount of energy to eject an electron from a metal. This energy is called the **work function**,  $\Phi$ . The energy balance equation is

$$E_{\text{initial}} = hf - \Phi \quad (1)$$

$$E_{\text{final}} = KE_{\text{electron}}, \quad (2)$$

where  $KE_{\text{electron}}$  is the kinetic energy of the ejected electron. If  $hf < \Phi$ , then the kinetic energy is negative, which is impossible, so the electron cannot make it out of the material. We begin to get a current when  $hf = \Phi$ , so that is where the current goes from zero to non-zero. The **linear relationship between kinetic energy and frequency** is also explained by Eqn 2. To compute  $h$ , we can plot the kinetic energy of the ejected electrons versus the frequency of the light. The slope is  $h$ .

The **decrease in current** is explained because each electron is ejected by a single photon. The number of photons arriving per second in a light beam with power  $P$  is given by  $\frac{P}{hf}$ . Therefore, for a constant  $P$ , the electrons per second ejected will go as  $1/f$ , as shown in Fig 1.

Photons can independently be verified by setting up a very sensitive photodetector and finding that the energy comes in discrete packets; for light of frequency  $f$ , the energy always arrives in amounts of  $hf$ .<sup>1</sup>

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<sup>1</sup>For more experiments that show the existence of photons, look up blackbody radiation and Compton scattering. Lasers are also based on the properties of photons!

Table 1: Ways to write the momentum and energy of the photon

$$\text{Energy} \quad E \quad hf = \hbar\omega = \frac{hc}{\lambda} = \hbar ck$$

$$\text{Momentum} \quad p \quad h/\lambda = \hbar k = \frac{hf}{c} = \frac{\hbar\omega}{c}$$

## Energy and momentum of a photon

We determined that the quantum of energy for light is equal to  $hf$ . There is also a corresponding momentum associated with that energy, which is given by  $p = h/\lambda$ . This can be determined by performing similar types of experiments to those that determined the energy of the photon. There are various relationships that are valid for a photon's momentum and energy, summarized in Table 1.

## The relation between intensity and number of photons

We can use unit analysis to determine how many photons are incident on an object. Suppose that light of frequency  $f$  is incident on an object, with observed intensity  $I$ . In SI units,  $I$  is given in  $\text{W/m}^2$ . We can compute the total power incident by multiplying  $I$  by the area of the object, so  $P = IA$ , which has units of  $\text{W}$ . One photon has energy  $hf$ , so the number of photons incident *per second* is  $N = \frac{IA}{hf}$ .

There is a force exerted by this light on the object, since the photons also have momentum. Newton's second law is  $F = \frac{dp}{dt}$  ( $F = ma$  is only true if mass is constant, but photons don't have mass!). Suppose that the photons are absorbed. Then the momentum imparted per second is  $pN = \frac{hN}{\lambda} = F$ . If the photons are reflected (say a mirror), then the force is twice that.

# UNIT 5: PROBABILITY AND COMPLEX NUMBERS

At this point, we note that we have a tension: we describe light as a wave in that it exhibits interference, but light arrives in what appears to be discrete packets that come at random. This is sometimes referred to as “wave-particle duality;” however, the real answer is much more revolutionary. The resolution to this duality is that everything is described using *probability waves* that interfere just like the waves we have been studying earlier in the class, and allow us to compute the probabilities of events (such as observing a photon at a particular location).

The probability waves are written in terms of complex numbers, and are used to compute probabilities. At this point in their career, many students have not had a lot of experience with this mathematics, so we will spend this unit discussing these concepts.

## After this unit, you should be able to

- Given a probability density  $\rho(x)$  for the position of a particle, compute the probability of observing that particle within a given range  $a < x < b$ .
- Using the probability for a particle of a given kinetic energy hitting a detector and the flux of particles, compute the total power incident on the detector.
- Manipulate complex numbers to find the magnitude squared and complex conjugate, and use Euler’s equation.

## Probability density

A probability is a number between 0 and 1. A probability density is a function, often called  $\rho(x)$ , that represents the probability **per unit length**. This is similar to the relationship between intensity and power; intensity is the power per unit area, and the power is the total amount of energy per second.

Probability densities have the following properties:

$$\rho(x) \geq 0 \quad (1)$$

and so-called normalization

$$\int_{-\infty}^{\infty} \rho(x) dx = 1. \quad (2)$$

Normalization ensures that the probability of the particle being *somewhere* is equal to 1.

The probability for  $x$  to be between two points  $a$  and  $b$ , assuming  $a < b$ , is

$$P(a < x < b) = \int_a^b \rho(x) dx. \quad (3)$$

Because of Eqns. 1 and 2, this probability is always between 0 and 1. Note that  $\rho$  can actually have a value greater than 1, as long as it is normalized.

## Probability density examples

### Normalization

Suppose a probability density is given by  $\rho(x) = Ne^{-x}$  for  $0 < x < \infty$ , and is zero elsewhere. What must  $N$  be to ensure the probability density is normalized?

**Solution:** We must have

$$\int_{-\infty}^{\infty} \rho(x)dx = \int_0^{\infty} Ne^{-x}dx = 1. \quad (4)$$

The integral starts at zero because  $\rho = 0$  for  $x < 0$ . The integral

$$\int_0^{\infty} e^{-x}dx = -e^{-x}|_0^{\infty} = 1. \quad (5)$$

So therefore  $N \cdot 1 = 1$  and  $N = 1$  to normalize this probability density.

### Number of particles per second

Suppose that we place a detector between  $x = a$  and  $x = b$   $\mu\text{m}$ . Suppose that the normalized probability density of a particle hitting the detector in that region is given by  $\rho(x) = (0.1 + Cx) \mu\text{m}^{-1}$  in that region, with  $C = 0.05 \mu\text{m}^{-2}$ . The probability density must have units of inverse length because when we integrate it, it must equal a unitless number.

#### Question part 1

What is the probability that a single particle hits the detector?

**Solution:** The probability is given by

$$P(a < x < b) = \int_a^b 0.1 + Cxdx = 0.1(b-a) + \frac{C}{2}(b^2 - a^2) \quad (6)$$

#### Question part 2

Suppose that 1000 particles are sent at the detector per second. How many will hit the detector on average per second?

**Solution:** The number is  $1000 \cdot P(a < x < b)$  particles per second, since each particle has probability  $P(a < x < b)$  to hit the detector.

## Complex numbers

In quantum mechanics, we describe the interference of particles using complex numbers. This is very similar to the phasor description of waves. Some rules:

- $i = \sqrt{-1}$ .

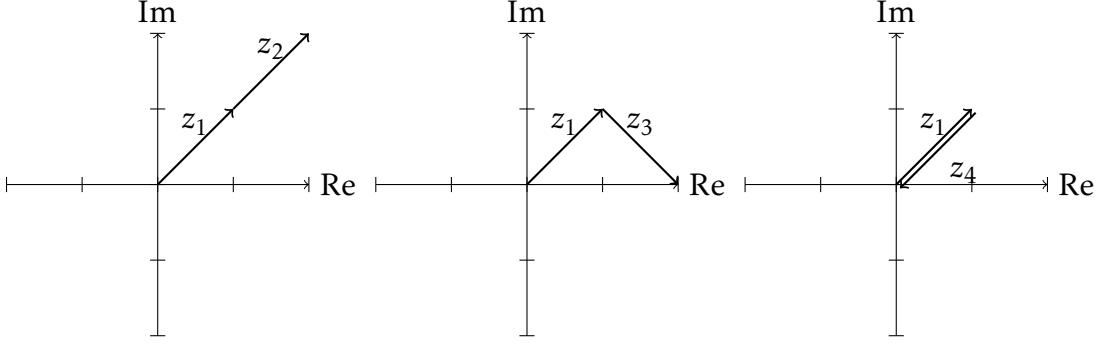


Figure 1: Adding complex numbers. For  $z = x + iy$ , the real part is  $x$ , labeled Re, and the imaginary part is  $y$ , labeled Im.

- $e^{i\theta} = \cos(\theta) + i \sin(\theta)$
- For a complex number  $z = x + iy$ , the complex conjugate  $z^* = x - iy$
- For a complex number  $z = x + iy$ , the magnitude squared (also known as the absolute value squared) is  $|z|^2 = zz^* = (x + iy)(x - iy) = x^2 + y^2$

For complex conjugation, the main thing is to remember that the  $i$  gets a minus sign.

We will sometimes write complex numbers as  $Ae^{i\theta}$ , where  $A$  is some positive real overall amplitude. This has the advantage that the magnitude squared is  $Ae^{i\theta}Ae^{-i\theta} = A^2$ .

You can think of complex numbers as being better phasors. As implied by  $z = x + iy$ , the numbers can be drawn on a 2D plot, and added component-wise in the same way as 2D vectors:

$$z_1 + z_2 = x_1 + iy_1 + x_2 + iy_2 = (x_1 + x_2) + i(y_1 + y_2) \quad (7)$$

The main difference between complex numbers and phasors is that we can multiply complex numbers to get another complex number:

$$z_1 \cdot z_2 = (x_1 + iy_1)(x_2 + iy_2) = x_1x_2 + iy_1x_2 + ix_1y_2 - y_1y_2 \quad (8)$$

## Example: interference using complex numbers

Consider the four complex numbers:

$$\begin{aligned} z_1 &= 1 + i \\ z_2 &= 1 + i \\ z_3 &= 1 - i \\ z_4 &= -1 - i \end{aligned}$$

Some sums are shown in Fig 1. What is the magnitude squared of the complex numbers  $z_{1i} = z_1 + z_i$  for  $i = 2, 3, 4$ ?

**Solution:** First let's compute the sums

$$z_{12} = 2 + 2i,$$

$$z_{13} = 2,$$

$$z_{14} = 0.$$

Now using the definition of the magnitude squared,

$$|z_{12}|^2 = z_{12}z_{12}^* = (2 + 2i)*(2 - 2i) = 4 + 4 = 8, \quad (9)$$

$$|z_{13}|^2 = z_{13}z_{13}^* = (2)*(2) = 4, \quad (10)$$

$$|z_{14}|^2 = z_{14}z_{14}^* = (0)*(0) = 0. \quad (11)$$

You may be able to see the reason for the definition  $|z|^2 = zz^*$ ; it is equivalent to the definition of length for a 2D vector  $|v|^2 = v_x^2 + v_y^2$ .

## Example 2: Euler's equation

We can also write  $z = Re^{i\theta} = R\cos\theta + iR\sin\theta$ , with  $R$  a positive real number. This is the equivalent of writing a 2D vector in polar coordinates. Show that  $|z|^2 = R^2$ .

**Solution:** We must use the identity  $z^* = Re^{-i\theta}$ , where we used the rule of replacing  $i$  with  $-i$  to take the complex conjugate. Then

$$|z|^2 = zz^* = Re^{i\theta}Re^{-i\theta}. \quad (12)$$

Using the identity  $e^a e^b = e^{a+b}$ ,

$$|z|^2 = R \cdot R = R^2, \quad (13)$$

which is the desired relationship.

# UNIT 6: THE WAVE FUNCTION

In this unit, we will introduce the wave function, which is how we describe the state of a system in quantum mechanics. The idea is that the concept of a wave function can describe the two-slit experiment with electrons. However, as the class continues, we will see that quantum mechanics can describe much more, including discrete energy levels in atoms and molecules, the existence of metals and insulators, and many other physical effects.

## After this unit, you will be able to

- Given the wave function of a particle  $\Psi(x)$ , compute the probability of finding the particle between two locations  $a$  and  $b$ .
- Normalize simple wave functions.
- Use the relationship between a free particle's momentum and wavelength to compute the outcome of interference experiments on matter.

## Two slit experiment for electrons

Suppose that we send electrons (one at a time) with a given momentum  $p$  towards two slits. You can do this by using x-rays to eject electrons from a metal, then sending them through a magnetic field, which will cause them to bend due to the Lorenz force  $qv \times B$ , as sketched in is shown in Fig 1.<sup>1</sup> After many electrons have passed through, we count how many electrons were incident on each part of the screen. The peaks look clearly like the interference maxima we saw with light earlier in the class.

In the experiment, the electrons arrive one at a time—the detector at the screen goes off in discrete amounts at discrete times. So they are also quantized, just like light is. There is something wave-like: the probability of the electron appears to exhibit interference, and something sort of particle-like: the electrons arrive in discrete packages. This is a lot like our observations of photons from the previous chapters; in fact electrons have **exactly the same relationship between momentum and wavelength:**  $p = \hbar k = h/\lambda$ . To describe this, quantum mechanics uses a wave, called the wave function, which then is used compute probability of arrival.

## Probability density from wave functions

**Important:** Here's how quantum mechanics works. The state of a particle is described using a *wave function*, which at some particular time is a function of position  $\Psi(x)$ <sup>2</sup>. The

<sup>1</sup>For a real implementation of this, see Frabboni et al. Ultramicroscopy 116, 73 (2012).

<sup>2</sup>Time dependence will come in a later class!

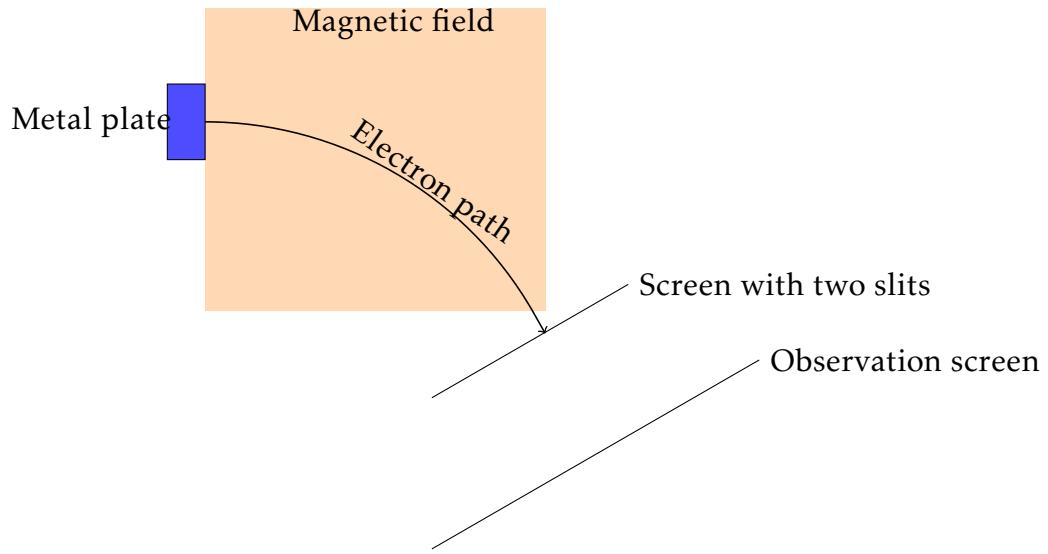


Figure 1: Experimental setup for sending electrons with a known momentum through a two-slit experiment. On the observation screen, we observe interference fringes as if the electrons had wave number  $k = p/\hbar$ .

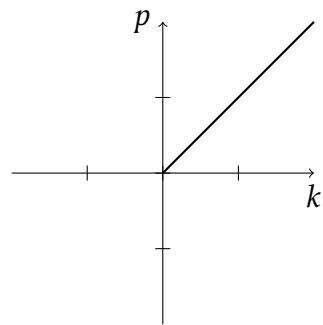


Figure 2: The relationship between the incident momentum of the electron and the wave number  $k$  inferred from the spacing of the peaks.

value of the wave function is a complex number. When we place a detector which occupies some region  $a < x < b$ , we say that we are measuring the position of the particle. The probability density is  $\rho(x) = |\Psi(x)|^2 = \Psi^*(x)\Psi(x)$ . So the probability that the detector goes off is

$$P(a < x < b) = \int_a^b \rho(x)dx = \int_a^b \Psi^*(x)\Psi(x)dx. \quad (1)$$

This rule replaces what you have known from classical mechanics. At the beginning, you were likely taught that the state of the particle is described by its position  $x$  at a given time. If we have a detector in the region  $[a, b]$ , then if  $x$  is in that region, the detector will go off, and if it is not, then it won't. In the quantum mechanical description, at any given time the particle has a *probability* of setting the detector off, which is computed from the wave function. Interference comes from the fact that a wave function is a complex number.

Just a note about the philosophy of this. There is no way to derive quantum mechanics from the things we know about classical physics. Quantum mechanics *includes* classical physics as a special case; it's broader. The existence of the wave function is similar to the existence of the electric and magnetic field; it is used because it describes the world very accurately.

## Explaining the two-slit experiment using electrons

We now have the concept of a wave function, but we don't know how to compute it yet. For the moment, we are just going to make a guess<sup>3</sup> for the wave function and show that it can describe the experiment above. We will assume that the wave function at a given position  $x$  on the screen is given by

$$\Psi(x) = A(e^{ikr_1} + e^{ikr_2}), \quad (2)$$

where  $A$  is a normalization constant. Remember that  $r_1$  and  $r_2$  are functions of  $x$ , the position on the screen. Review Unit 2 for this geometry. It's often useful to pull out a factor of  $e^{ikr_1}$  from this wave function:

$$\Psi(x) = Ae^{ikr_1}(1 + e^{ik(r_2-r_1)}) \quad (3)$$

To compare to experiment, we compute the probability density that a detector will go off:

$$\rho(x) = \Psi^*(x)\Psi(x) \quad (4)$$

$$= [A^*e^{-ikr_1}(1 + e^{-ik(r_2-r_1)})][Ae^{ikr_1}(1 + e^{ik(r_2-r_1)})] \quad (5)$$

$$= |A|^2(2 + e^{-ik(r_1-r_2)} + e^{ik(r_1-r_2)}) \quad (6)$$

---

<sup>3</sup>Often called an *ansatz*, which is German for guess. Many german words are used in quantum mechanics since much of the development was done in Germany in the early 20th century.

Using Euler's formula that  $e^{i\theta} = \cos \theta + i \sin \theta$ , we get

$$\rho(x) = |A|^2(2 + 2\cos(k(r_2 - r_1))), \quad (7)$$

which can be simplified using a trigonometric identity to give

$$\rho(x) = 4|A|^2 \cos^2\left(\frac{k(r_2 - r_1)}{2}\right). \quad (8)$$

This should look very familiar; in fact it is the same relationship we derived for light back in Unit 2. We know that the peaks in probability will occur at angles such that

$$d \sin \theta = m\lambda, \quad (9)$$

where  $d$  is the distance between the slits.

## Momentum-wavelength relationship

We were able to describe the peaks in the probability for the two-slit experiment using the wave function concept, but we had to guess a wavelength, through the value of  $k$ . It turns out that the wavelength is directly related to the *momentum* of the particle. This is known experimentally, and can be measured by controlling the velocity of the electrons as they head towards the two slits. Depending on the velocity, the peaks have different separation.

As shown in Fig 1, if you plot the wave number  $k$  versus the momentum of the electron, there is a linear relationship such that  $p = \hbar k$ , or alternatively  $p = h/\lambda$ . This is called the *de Broglie wavelength*. Note that this is the same relationship that photons have, and the value of  $h$  is the same as the one for photons. This is a hint that there is something fundamental connecting electrons and photons.

## Normalization of wave functions

The probability of observing the particles *somewhere* is equal to 1. So if the wave function is  $\Psi(x)$ , then

$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x)dx = 1 \quad (10)$$

For example, consider a wave function given by  $Ae^{ikx}$ , for  $0 < x < L$ . Then

$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x)dx = 1 \quad (11)$$

$$A^2 \int_0^L e^{ikx} e^{-ikx} dx = A^2 L. \quad (12)$$

So  $A = \sqrt{1/L}$  in order to keep the wave function normalized. Then the probability of the particle being observed in  $a < x < b$  is

$$\int_a^b \frac{1}{L} dx = \frac{b-a}{L}, \quad (13)$$

as long as  $a, b$  are greater than zero and less than  $L$ . So this wave function represents a particle that has an equal probability to be found anywhere between 0 and  $L$ .

# UNIT 7: MOMENTUM AND POSITION

## After this unit, you should be able to

- Explain whether a wave function has definite momentum.
- From a superposition of eigenstates, compute the probability of a measurement outcome.
- Apply the Heisenberg Uncertainty Principle to determine the limits of what can be predicted about measurement outcomes.

## Wave function of a particle with definite momentum

We can explain the electron double slit experiment (and many other similar experiments) if we assume that the wave function of a particle with momentum  $p^1$  is:

$$\Psi(x, t) = A e^{i(kx - \omega t)}, \quad (1)$$

where  $k = p/\hbar$ . We don't yet know how to determine  $\omega$  (we will do that in Unit 10). As a simplification, if we suppose that the particle is in a large box of length  $L$ , then  $A = \sqrt{\frac{1}{L}}$  from the normalization condition. So for the moment, let's just consider the wave function at a given time  $t = 0$ , so

$$\Psi(x) = A e^{ikx}. \quad (2)$$

The wave function tells us the probability of measuring quantities. This is one of the very fundamentally different things about the quantum mechanical description as opposed to the classical mechanics description.

For the wave function in Eqn 2, if we measure the momentum, say by measuring the change in momentum the particle imparts on some other thing when it impacts it, we will always find that the particle has momentum  $p$ . On the other hand, if we measure the location of the particle, then we will find that it can be anywhere within that large box, since

$$\rho(x) = \Psi(x)\Psi^*(x) = |A|^2. \quad (3)$$

This is referred to as *uncertainty* in quantum mechanics. For this particular wave function, we can predict the outcome of a measurement of the momentum very precisely (it's always  $p$ ), but we cannot predict the outcome of a measurement of the position very precisely. We would find it somewhere in the box, but it's completely random where we will find it!

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<sup>1</sup>In quantum mechanics, we work with momentum rather than velocity. Part of the reason is that the math is easier this way. Another reason is that momentum is actually more fundamental to physics than velocity. For example, the more general formula for Newton's first law is  $F = \frac{dp}{dt}$ .

## Eigenstates

The wave function in Eqn 2 is called an *eigenstate*<sup>2</sup> of momentum. This means that when we measure the momentum of the particle with that wave function, we can predict that we will obtain one particular value of the momentum,  $\hbar k$ . We will also sometimes say that such a wave function has **definite** momentum.

One can also have eigenstates of position, which are wave functions that are only non-zero in one location. The mathematics of this is a little bit beyond this course,<sup>3</sup> so we will not cover this. In later units, we will learn how to find *energy eigenstates*, which are very important in quantum mechanics.

## Superposition of wave functions

Suppose we have a particle which we confine to a box of side  $L$  with wave function

$$\Psi(x) = A(e^{ik_1 x} + e^{ik_2 x}) \quad (4)$$

with  $k_1 = \frac{2\pi}{L}$  and  $k_2 = \frac{4\pi}{L}$ . What will happen when we measure the momentum of a particle with this wave function? Since the wave function is an equal superposition of two wave functions with different momenta, we have an equal probability of measuring  $\hbar k_1$  and  $\hbar k_2$ . This is not a momentum eigenstate since two different momenta could be measured.

In general, if the wave function is given by

$$\Psi(x) = A(ae^{ik_1 x} + be^{ik_2 x}), \quad (5)$$

we will obtain  $\hbar k_1$  with probability  $\frac{a^2}{a^2+b^2}$  and  $\hbar k_2$  with probability  $\frac{b^2}{a^2+b^2}$ . The denominator ( $a^2 + b^2$ ) ensures that the probabilities add to 1 (normalization).

What about measuring the position of the particle? From Fig 1, we can see that as we add together more momentum eigenstates, the position is more likely to be measured near the middle of the box than near the edges. So this wave function has more uncertainty in momentum than the momentum eigenstate, but less uncertainty in position.

## Heisenberg uncertainty principle

It turns out that there is a general relationship between the spread of the momentum values and the spread of position values, which is encoded in the Heisenberg uncertainty principle:

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \quad (6)$$

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<sup>2</sup>“Eigen” is from German, where it means ‘same.’

<sup>3</sup>Dirac delta functions

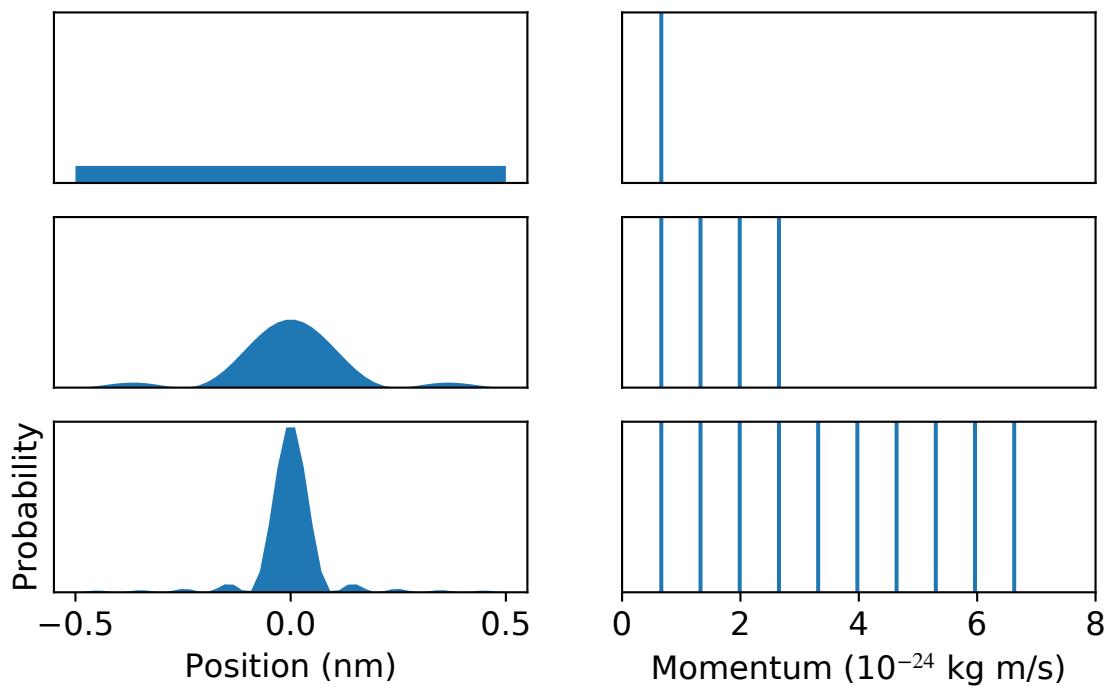


Figure 1: Making a localized wave function using a sum of momentum eigenstates. Each row is one wave function; the left is the probability density for position, while the right is the probability density for momentum. The momentum probability density is a bunch of spikes because it is a sum of momentum eigenstates. To make a wave function with high probability to be in one position, it's necessary to include many possible momenta.

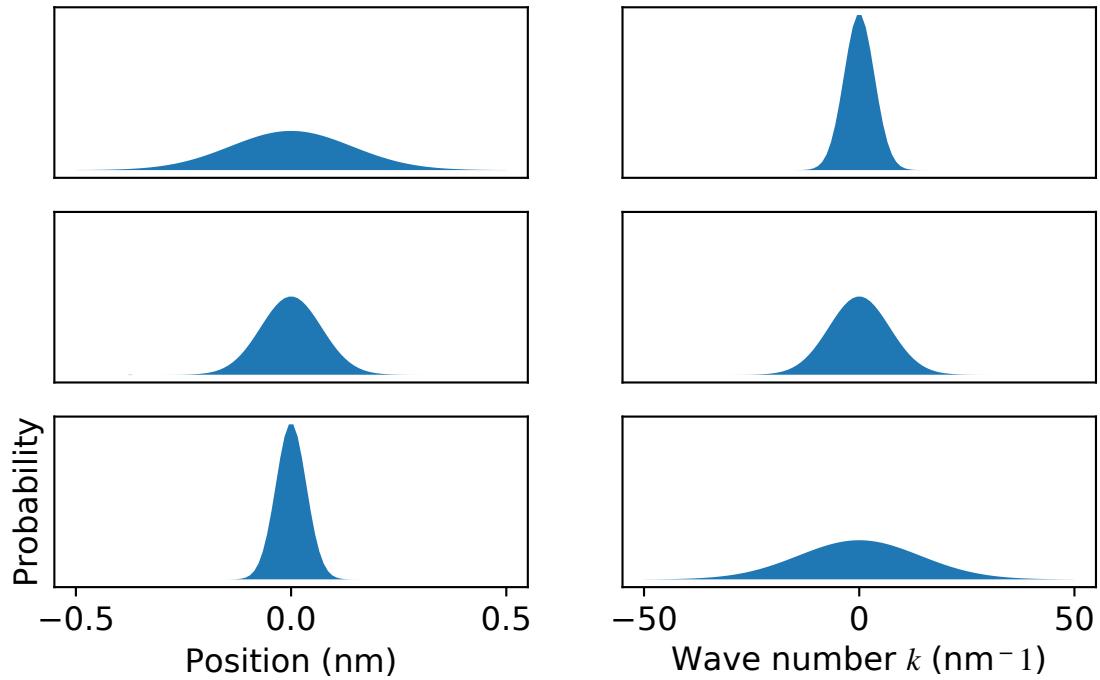


Figure 2: The position and momentum probabilities for various wave functions. Each row corresponds to one wave function with form proportional to  $\exp(-x^2/2\sigma^2)$ , and the probability of measuring position and momentum is given in each column.

This relationship puts fundamental physical limits on how well we can predict the outcome of an experiment.<sup>4</sup>

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<sup>4</sup>If you are paying extremely close attention, you might notice that a particle in a box with wave function  $e^{ikx}$  seems to violate this. This is because we ignored boundary conditions. This is ok if the box is very large.

# UNIT 8: ENERGY OF QUANTUM PARTICLES

To summarize the last few section\*s, in the quantum mechanics description of physics, the primary description of the state is the wave function,  $\Psi$ . For a particle moving in one dimension, the wave function is  $\Psi(x, t)$ . The wave function determines the **probability** of a measurement, which is given by the absolute square of the wave function. So far, we discussed how wave functions give the probability of measuring a particle at a given position and momentum.

In this section\*, we consider how to compute the result of an energy measurement. We will find out that in many situations, the energy we can measure in a quantum system will only be one of several discrete amounts, or quanta. This is the origin of the name of quantum mechanics!

## After this unit, you should be able to

- Check whether wave functions satisfy the time-independent Schrödinger equation.
- Explain how the Schrödinger equation is consistent with experimental observations of the relationship between wavelength, momentum, and energy for a free particle.
- For a particle in an infinite square well of length  $L$ , compute the allowed energies that could be measured.
- If the particle is in an energy eigenstate of the infinite square well with quantum number  $n$ , compute the probability of it being found between  $x = a$  and  $x = b$ .

## Energy of a free particle

- The energy of a free particle with wave function  $Ae^{ikx}$  is  $\frac{\hbar^2 k^2}{2m}$

From the last section\*, recall that if a particle has a definite momentum, then its wave function is given by

$$\Psi(x) = Ae^{ikx}. \quad (1)$$

If we measure the momentum of this particle, say by observing how it bends in a magnetic field, then with probability 1 the momentum will come out to  $\hbar k$ . We will write this as  $p_k = \hbar k$ , where the  $k$  subscript represents that the wave function of the particle is from Eqn 1.

What is the energy of a free particle with the wave function of Eqn 1? You may recall from classical mechanics that it is  $\frac{1}{2}mv^2$ . Since our formula is in terms of  $p_k = mv = \hbar k$ , we write the energy as

$$E_k = \frac{p_k^2}{2m} = \frac{\hbar^2 k^2}{2m}. \quad (2)$$

## The momentum equation

To review the logic of the previous section's, we know empirically that we describe the state of a particle using a wave function, and the wave function of a particle with momentum  $p$  is  $Ae^{ikx}$ , with  $k = p/\hbar$ . We find the possible values of momentum by expanding any wave function as a superposition of momentum eigenstates, and then reading the probabilities off the expansion.

If we want to know what energies can be measured, we need a way to find **energy eigenstates** when there is a potential energy. For that we will need to generalize our principle beyond just empirically measuring the wave function using diffraction. The principle of quantum mechanics is that you find eigenstates by performing an operation on the wave function, and if the wave function does not change other than a total factor, then the wave function is an eigenstate. This is the 'same' of eigenstate, from German.

For momentum, the operation is the derivative  $-i\hbar \frac{\partial}{\partial x}$ . Applying that to our momentum eigenstate, we get

$$-i\hbar \frac{\partial Ae^{ikx}}{\partial x} = \hbar k Ae^{ikx} = pAe^{ikx}. \quad (3)$$

So we see that we get back the original wave function with a constant factor of the momentum applied. Note that this equation means that it holds for **all** values of  $x$ ; this is an equality of functions.

## The Schrödinger equation: the energy operation

- The time-independent Schrödinger equation tells us which wave functions are energy eigenstates.

For this section\* (and this course), we will just consider a wave function at a given time, which we will write  $\Psi(x)$ . Time propagation in quantum mechanics is a surprisingly advanced topic that you will learn about in your next class. For a particle of mass  $m$  in one dimension, the Schrödinger equation is

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} + U(x)\Psi(x) = E\Psi(x). \quad (4)$$

In this equation,  $U(x)$  is the external potential energy, and  $-\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2}$  is our momentum operation squared, divided by  $2m$ . This is analogous to the energy being written as  $p^2/2m + U$  in classical mechanics.

There are several important things to note about this equation:

- Only certain wave functions satisfy Eqn 4. These special wave functions are called **energy eigenstates**
- $E$  is a number that gives the energy of the wave function.

- If a particle is in an energy eigenstate, any measurement of its energy will result in  $E$ . For many systems, only certain values of  $E$  have a wave function that satisfies Eqn 4.
- Energy eigenstates are also called **stationary states**. Their probabilities don't change in time.
- For the wave function to be an energy eigenstate, it must be true for **all** values of  $x$ , for the same value of  $E$ . You don't get to change  $E$  for different values of  $x$ .

## Example: free particle

Let's describe a free particle using the Schrödinger equation. In that case, the external potential is zero (that's what "free" means!), and the equation is:

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} = E\Psi(x). \quad (5)$$

The most common solution method is to guess a wave function and check whether it satisfies Eqn 5. Let's guess  $\Psi_k(x) = Ae^{ikx}$  as the wave function. Then

$$-\frac{\hbar^2}{2m} \frac{d^2Ae^{ikx}}{dx^2} = -\frac{\hbar^2}{2m}(ik)^2Ae^{ikx} = \frac{\hbar^2k^2}{2m}\Psi_k(x). \quad (6)$$

So this wave function satisfies the Schrödinger equation if the energy  $E = \frac{\hbar^2k^2}{2m}$ , and any wave function of this form is an energy eigenfunction. In this case,  $k$  can be any real number, so the energy can take on any positive value. In quantum mechanics,  $k$  is an example of a **quantum number**, which is a label for the energy eigenstates.

This makes some sense; we said earlier that a particle with wave function  $e^{ikx}$  has momentum  $p = \hbar k$ . For a free particle, all energy is kinetic energy, so we would expect the energy to be

$$\frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m}. \quad (7)$$

So the derivative term is associated with kinetic energy, which matches the  $U(x)$  term that is associated with potential energy.

## Example II: a non-energy eigenstate for a free particle

Now consider the wave function  $\Psi(x) = ae^{ik_1x} + be^{ik_2x}$ . Then

$$-\frac{\hbar^2}{2m} \frac{d^2ae^{ik_1x} + be^{ik_2x}}{dx^2} = \frac{\hbar^2k_1^2}{2m}ae^{ik_1x} + \frac{\hbar^2k_2^2}{2m}be^{ik_2x}. \quad (8)$$

No matter what we do, we cannot get back a constant times  $\Psi$  on the right hand side, since  $k_1 \neq k_2$ . So this wave function is **not** an energy eigenstate. In fact, if we measure the energy of such a particle using a magnetic field, for example, then we will measure:

Energy	Probability
$\frac{\hbar^2 k_1^2}{2m}$	$\frac{a^2}{a^2+b^2}$
$\frac{\hbar^2 k_2^2}{2m}$	$\frac{b^2}{a^2+b^2}$

We can compute this because we have expanded  $\Psi$  in terms of energy eigenstates  $e^{ik_1 x}$  and  $e^{ik_2 x}$ .

## Quantized energy levels: infinite square well

Now we consider a case where  $U$  is not just zero. Imagine creating a well (a 1D box) in which the particle is allowed to move freely from  $x = 0$  to  $x = L$ , but encounters an infinite potential barrier at either side. In this case,

$$U(x) = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{otherwise} \end{cases} \quad (9)$$

Given this, let's look back at Eqn 4 to see what kind of wave function can satisfy the equality. The first thing we can notice is that since  $U$  is  $\infty$  outside the box, the only way for the equality to be satisfied is for either  $\Psi(x)$  to be zero, or have infinite energy. The more physically possible case is for the wave function to be zero outside the box. This makes some sense classically; if a particle is inside a box with infinitely hard walls, there is zero probability to find it outside the box.

Inside the box,  $U = 0$ , so the Schrödinger equation looks a lot like the free particle case. However, we have an additional constraint—the wave function goes to zero at the edges. This has to happen in order for the Schrödinger equation to be satisfied, since the potential energy is infinite there. A guess wave function that works is

$$\Psi(x) = \begin{cases} A \sin\left(\frac{n\pi x}{L}\right) & \text{if } 0 < x < L \\ 0 & \text{otherwise,} \end{cases} \quad (10)$$

where  $n$  is an integer.

We can find  $A$  by enforcing normalization:

$$\int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1. \quad (11)$$

You can verify that if  $A = \sqrt{\frac{2}{L}}$ , then this integral is equal to 1. By plugging our guess  $\Psi$  into the Schrödinger equation, we can get the energy:

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \quad (12)$$

Important things to note about this:

- Because of the boundary conditions ( $\Psi$  must be zero at 0 and  $L$ ), only integer values of  $n$  are allowed.
- The more oscillations in the wave function, the higher the energy.
- Since only certain values of  $n$  are allowed, only certain values of the energy are allowed.

## What it means to have only certain energies allowed

In the previous section\*, we saw that sometimes a quantum system can only be observed to have certain values of the energy. Let's investigate what that means practically. Let's suppose that we have a quantum system (an atom) with two allowed energy levels,  $E_1$  and  $E_2$ , with corresponding energy eigenstates  $\Psi_1$  and  $\Psi_2$ . There may be more energy eigenstates but we will just consider those two for simplicity.

Imagine that the atom has wave function equal to the ground state (lowest energy state),  $\Psi_1$ . As we will find later, if the atom is not disturbed, it will remain in the ground state forever. Suppose now that we disturb the system by allowing a photon to come near it. There is a chance that the photon will interact with the atom. Let's consider the possibilities:

1. At the end of the process, a photon comes out with energy  $\hbar\omega$  and the atom is left with energy  $E_1$ .
2. The photon is absorbed by the atom. No photon comes out and the atom is left with energy  $E_2$ .

While possibility 1 can always happen, possibility 2 can only happen if  $E_2 - E_1 = \hbar\omega$ . This is because energy is still conserved in quantum mechanics; so if we started with  $E_1 + \hbar\omega$  energy, we must end with that much energy when everything is settled. Similarly, if the atom started in  $\Psi_2$ , then it might emit a photon with energy  $\hbar\omega = E_2 - E_1$ .

Atoms, liquids, solids, etc can only absorb photons with energy equal to the difference between their energy levels. This is why glass is transparent, why we can see through air and water. It is why rose-tinted glasses remove all colors but rose. Similarly, quantum systems can only emit photons with energy equal to a difference between their energy levels. This is what gives neon lights their particular color, and in general is what gives objects their color. The list of energies that a given quantum system can obtain is called the **spectrum**. In Latin, spectrum meant ‘image’ and indeed the spectrum of a quantum system determines what type of light it interacts with.

## Application: quantum dot technology

At the time of this writing, new displays are emerging that use quantum dot technology to emit light of very pure frequencies. Here is some data that Samsung<sup>1</sup> published:

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<sup>1</sup><https://news.samsung.com/global/why-are-quantum-dot-displays-so-good>

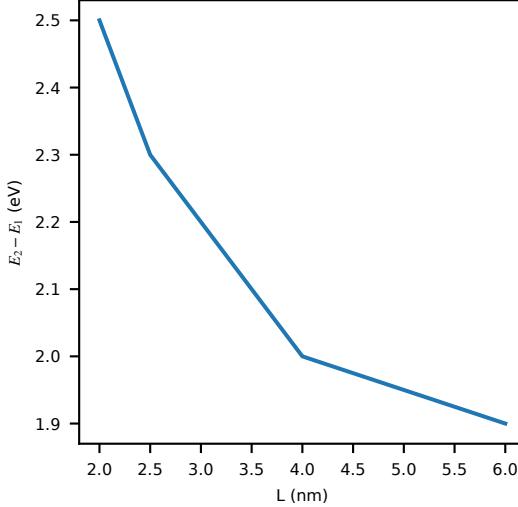


Figure 1: Photon energies emitted by a quantum dot versus the size. It is a reciprocal relationship, as we derived in Eqn 12

Size of the dot (nm)	Wavelength of light emitted (nm)	$E_2 - E_1$ (eV) <sup>2</sup>	Color
2	500	2.5	Blue
2.5	530	2.3	Green
3	570	2.2	Green-yellow
5	610	2.0	Orange
6	640	1.9	Red

shows this same data, where we can see that it matches our model from Eqn 12 pretty well, since we would predict that the energy difference between the lowest energy eigenstate and the next higher energy eigenstate is

$$E_2 - E_1 = \frac{\hbar^2 3\pi^2}{2mL^2}. \quad (13)$$

The fact that the energies are quantized means that the quantum dot *physically cannot* emit light which is not equal to an energy difference between energy eigenstates. This makes the light very highly peaked around a single wavelength, which allows these displays to be very beautiful.

Fig 1

# UNIT 9: QUANTUM HARMONIC OSCILLATOR

## After this unit, you should be able to

- Compute what frequency of light can be emitted and absorbed, given a set of allowed energies for a quantum system.
- Use the allowed energies for a system to explain whether it is more likely that the system is described by a harmonic oscillator or infinite square well potential.
- Determine the potential that led to a given measured spectrum.

## A more realistic potential

While there are some artificially created systems that we can model as something close to an infinite square well, most potential energy functions (force laws) are somewhat different. In this chapter, we will consider the quantum equivalent of a mass on a spring, which you studied in introductory classical mechanics.

One aspect of quantum mechanics is that it is much *harder* to solve for the dynamics of a system than in classical mechanics. For all but some very simple systems, the solution is done numerically using a computer, or we simply learn about quantum systems by observing them experimentally. While this is highly technical, there are some useful things that we can learn about quantum systems by understanding the output of the experiments or numerical calculations. For the remainder of the course, we will just provide you with the energy eigenstates for a given potential, and discuss what they mean.

## Photon emission/absorption

A hydrogen atom has the following energy levels: -13.6 eV, -3.4 eV, and -1.5 eV. Suppose that it starts in the ground (lowest energy) state. It can absorb light with photon energy either  $(-3.4 - (-13.6)) = 10.2$  eV, or  $(-1.5 - (-13.6)) = 12.1$  eV. We can solve for the frequency of that light by using  $hf = E$ , and therefore  $f = E/h$ . Here it is useful to use  $h$  in terms of electron volts (eV) to get:

$$f_1 = \frac{10.2 \text{ eV}}{4.135667 \times 10^{-15} \text{ eV} \cdot \text{s}} = 2.466 \times 10^{15} \text{ s}^{-1} \quad (1)$$

and similarly for  $f_2$ . Those are the frequencies of light that can be absorbed by a hydrogen atom in the ground state.<sup>1</sup> If the hydrogen atom absorbs light of frequency  $f_1$ , then it is now in the state with energy -3.4 eV.

On the other hand, suppose that the hydrogen atom is in the first excited state (the one at -3.4 eV). It may be in that state because it absorbed light as in the previous paragraph, or we can induce an excitation using an electric field or temperature. In this case, it can absorb light of energy (-1.5

<sup>1</sup>In reality, this is broadened a little bit by temperature effects.

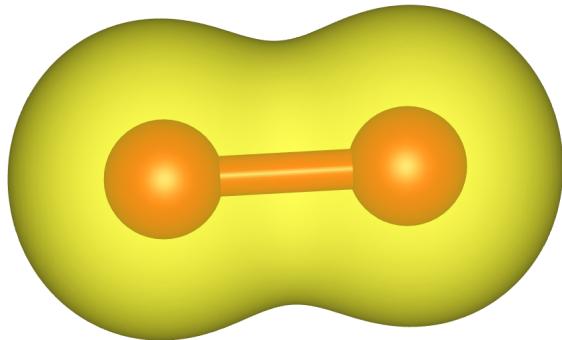


Figure 1: An O<sub>2</sub> molecule, which is present in the air. The electrons (in yellow, this is an averaged view of the electronic wave function) bind the nuclei (in red) together. The nuclei act as if they are connected by a spring, which gives rise to evenly spaced quantized energy levels that can be observed as absorption of infrared light.

- (-3.4)) = 1.9 eV to go to the level at -1.5 eV, or it can emit light of energy 10.2 eV to go back to the ground state. This is the origin of the emission lines of atoms.

## Harmonic oscillator: verifying the ground state

In the previous section, we considered only a very simple and idealized potential,  $U(x)$ . This choice was to make the math relatively tractable. In reality,  $U(x)$  can be more complicated and can require advanced techniques to find the energy eigenstates from the Schrödinger equation. Solving the Schrödinger equation for the general case of many particles is an area of active research in physics, so in this course we will not cover explicit solution of the equation. However, it is much easier to *check* whether a given wave function is an energy eigenstate for a given  $U(x)$ .

Let's go through this for a harmonic oscillator potential. The Schrödinger equation is given by:

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} + \frac{1}{2}kx^2\Psi(x) = E\Psi(x). \quad (2)$$

In contrast to the infinite square well, there are no boundary conditions on this; the wave function can be non-zero everywhere in space.

Let's try a guess wave function:  $\Psi(x) = A \sin(bx)$ , where we use  $b$  because  $k$  is already taken

for the spring constant. Then plugging that into the equation, we get

$$\frac{\hbar^2 b^2}{2m} A \sin(bx) + \frac{1}{2} kx^2 A \sin(bx) = EA \sin(bx) \quad (3)$$

$$\frac{\hbar^2 b^2}{2m} + \frac{1}{2} kx^2 = E \quad (4)$$

(5)

This is **NOT** an energy eigenstate, since there is no way to set  $A$ ,  $k$ , and  $E$  such that this equation is satisfied at all values of  $x$ .

Let's try a better guess<sup>2</sup>:  $\Psi(x) = Ae^{-\alpha x^2}$ . We take the derivative on the left-hand side and find:

$$-\frac{\hbar^2}{2m} A(4\alpha^2 x^2 - 2\alpha)e^{-\alpha x^2} + \frac{1}{2} kx^2 Ae^{-\alpha x^2} = EAe^{-\alpha x^2} \quad (6)$$

$$x^2 \left( \frac{1}{2}k - \frac{4\hbar^2 \alpha^2}{2m} \right) + \left( \frac{\hbar^2 \alpha}{m} - E \right) = 0 \quad (7)$$

The parts in the parentheses must each equal zero for this equation to be true for all values of  $x$ . This means that

$$\alpha = \frac{1}{2\hbar} \sqrt{mk} \quad (8)$$

$$E = \frac{\hbar^2 \alpha}{m} = \frac{\hbar}{2m} \sqrt{mk}. \quad (9)$$

To simplify the equation for energy, often this is written in terms of  $\omega$ , where  $k = m\omega^2$ , so that  $E = \frac{\hbar}{2}\omega$ . Note that when we solved for  $\alpha$ , we could have chosen the negative value. That would not have worked because  $e^{x^2}$  diverges as  $x$  goes to infinity, so  $\alpha$  must be positive for the wave function to be normalizable.

## Harmonic oscillator: spectrum

It turns out that just like the infinite square well, there are an infinite number of discrete solutions to the Schrödinger equation for the harmonic oscillator. The functions are a bit complicated and don't offer a lot of physical intuition, so we will not list them here. However the spectrum is very simple:  $E_n = (n + \frac{1}{2}) \hbar\omega$ , where  $n = 0, 1, 2, \dots$ . Note here that  $n$  can be zero, unlike the infinite square well.

Contrast the harmonic oscillator result with the result for the infinite square well:  $E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$ , with  $n = 1, 2, \dots$ . The harmonic oscillator has evenly spaced energies, called energy levels, while the infinite square well has energies that get farther apart as  $n$  increases. The difference between these two is the potential energy term,  $U(x)$ . This means that by looking at the spectrum; that is, what light is emitted and absorbed by the object, we can tell something about the potential energy in the quantum system! If for example we see evenly spaced levels, then it may be that the potential energy looks like a harmonic oscillator. By measuring the spacing between the levels we can tell what the value of  $k$  is for that oscillator.

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<sup>2</sup>The guess and check method is a long-standing and useful tool in physics!

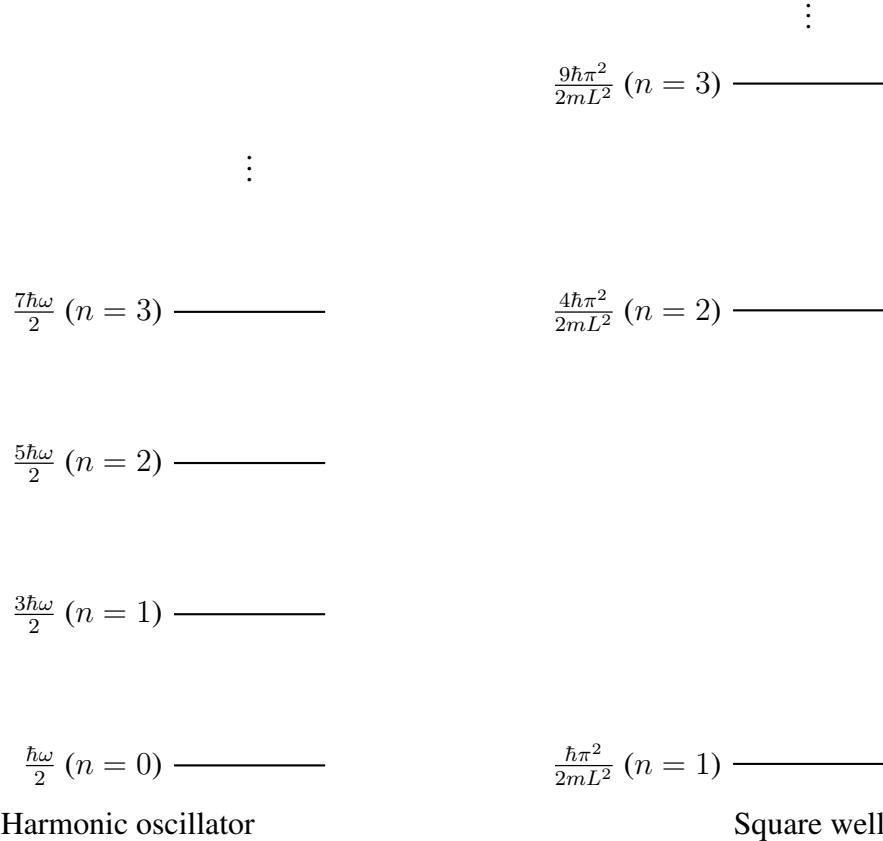


Figure 2: Energy level diagrams for the harmonic oscillator and infinite square well. The energy levels are spaced differently. Light can only be absorbed and emitted in units equal to the difference between the energy levels.

## Energy level diagrams

For the rest of the class, we will be using energy level diagrams to understand the "allowed" energies for a quantum system. In Fig 2, we show diagrams for two different potentials: a harmonic oscillator and square well. The *differences* between the energy levels tell us what frequencies of light can be absorbed by the system.

## Using energy levels to determine the potential

A common way of understanding the vibrations in molecules is to send infrared light through a gas, and measure what frequencies are absorbed by the vibrations of atoms. These vibrations are often well-described as harmonic oscillators. Each type of vibration has its own effective mass and spring constant.

As an example, when infrared light is passed through the atmosphere, which is filled with water, some frequencies are absorbed by the water. By reading off the frequency of light, we can

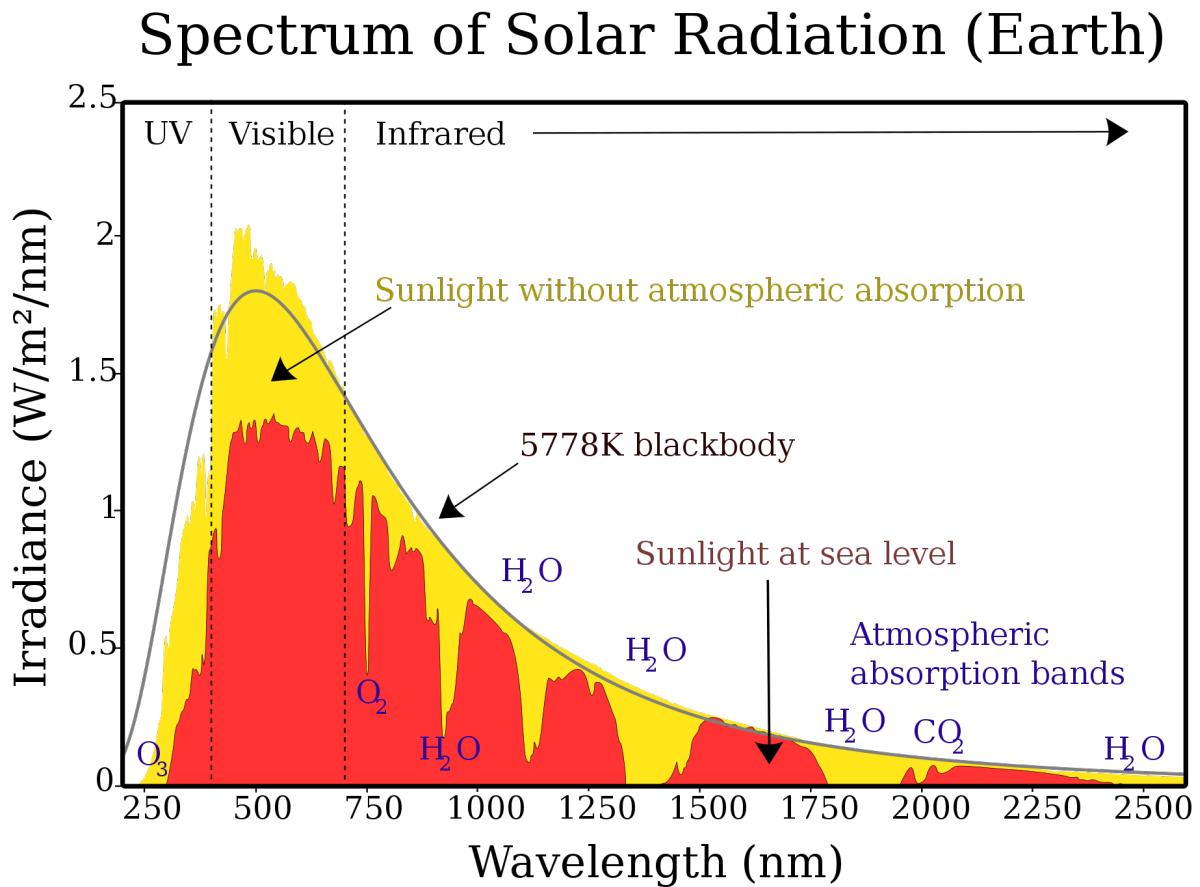


Figure 3: Solar irradiation at the Earth's surface, filtered by frequency. Image credit. By Nick84 - File:Solar\_spectrum\_ita.svg, CC BY-SA 3.0, <https://commons.wikimedia.org/w/index.php?curid=24648395>

tell  $\omega$  by using

$$E_{\text{photon}} = hf \quad (10)$$

$$E_{\text{photon}} = \frac{3}{2}\hbar\omega - \frac{1}{2}\hbar\omega = \hbar\omega, \quad (11)$$

since the photon will only be absorbed if it matches the difference in energy levels of the vibrational system. This shows up as dips in the amount of light from the sun that we observe on earth (Fig 3). Each dip is due to a harmonic oscillator of the characteristic frequency.

# UNIT 10: MORE THAN ONE ELECTRON

So far in this course, we have only considered one particle at a time in one dimension. In reality, materials are made up of many electrons and nuclei. For the purposes of this course, we will assume that the electrons do not interact with one another<sup>1</sup>. For concreteness, we will just talk about multiple electrons in this section, although the rules do apply to some other types of particles.

## After this unit, you should be able to

- Determine the ground state and excited states of a system of non-interacting electrons using energy level diagrams

## Spins

Electrons have an additional internal variable called spin, which we have not covered yet in these notes. Roughly speaking, each electron has a magnetic moment that can either point "up" ( $\uparrow$ ) or "down" ( $\downarrow$ ). The spin is very quantized, only allowing two outcomes,  $\uparrow$  or  $\downarrow$  or a superposition of the two.

## Filling levels in the non-interacting approximation

Suppose that we have solved for the energy eigenstates of a system. This means that we have a list of states,  $\Psi_n$ , and energies  $E_n$ , which correspond to solutions of the time-independent Schrödinger equation. For one electron, the ground state (lowest energy state) is given by putting the one electron in the ground state. For two electrons, the ground state is given by putting one electron of each spin  $\uparrow$  and  $\downarrow$  into the single-particle ground state. Once two electrons are in the lowest energy state, that state is "filled," and the next electron has to go in the next highest level. This procedure is called the *aufbau* principle, which means "building up."

It's easiest to understand the *aufbau* procedure using an example. In Fig 1, we put four non-interacting electrons in a harmonic oscillator such that  $\hbar\omega = 2 \text{ eV}$ . We mark the electrons with up and down arrows. The total energy of the ground state is  $2 \cdot 1 + 2 \cdot 3 = 8 \text{ eV}$ . The states with electrons in them are called occupied states, and the states without electrons in them are called unoccupied states. The lowest excited state is constructed by moving one electron from the highest occupied state to the lowest unoccupied state. The energy of this state is  $2 \cdot 1 + 3 + 5 = 10 \text{ eV}$ . That means that this oscillator, if it starts in the ground state, will absorb light at 2 eV. It will also absorb light at many other energies, corresponding to different configurations of the electrons in the states.

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<sup>1</sup>The non-interacting approximation turns out to work pretty well for a lot of materials like aluminum, silicon, diamond, gold, and so on. The reason for this is actually not very simple and is the consequence of *emergence*; the electrons **do** interact strongly but the emergent behavior is as if they don't. The study of this and the emergence of other behaviors is one of the main objectives of an entire subject of physics—condensed matter physics.

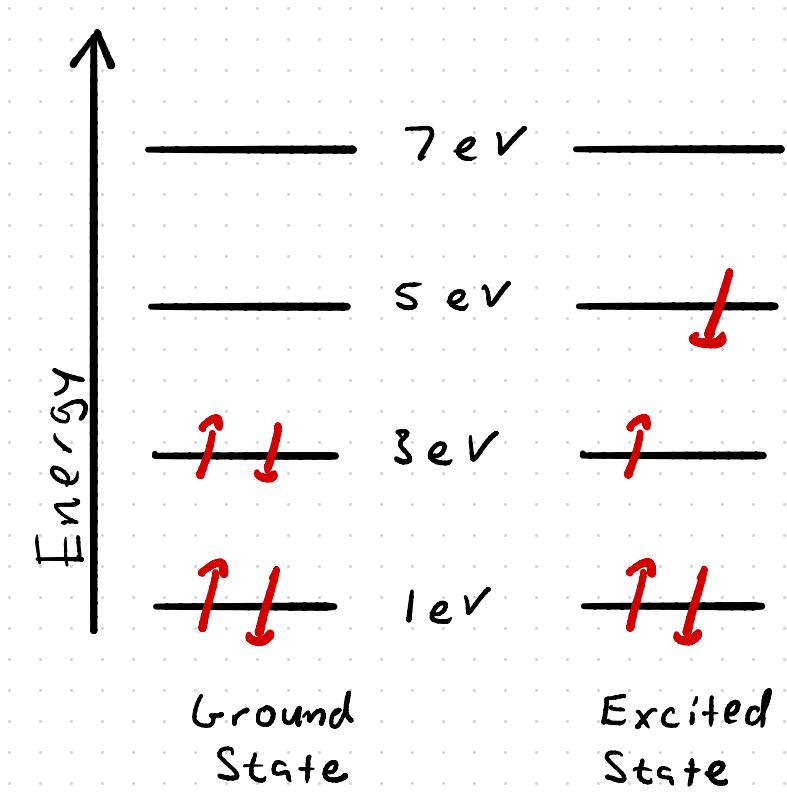


Figure 1: How to construct the ground and first excited state for four electrons in a harmonic oscillator.

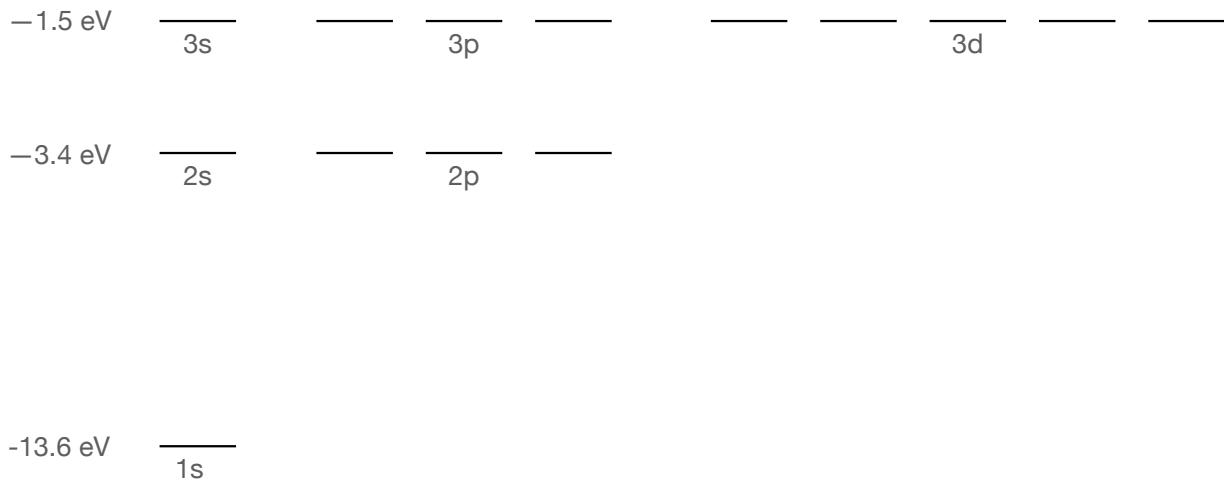


Figure 2: Energy level diagram for a hydrogen atom.

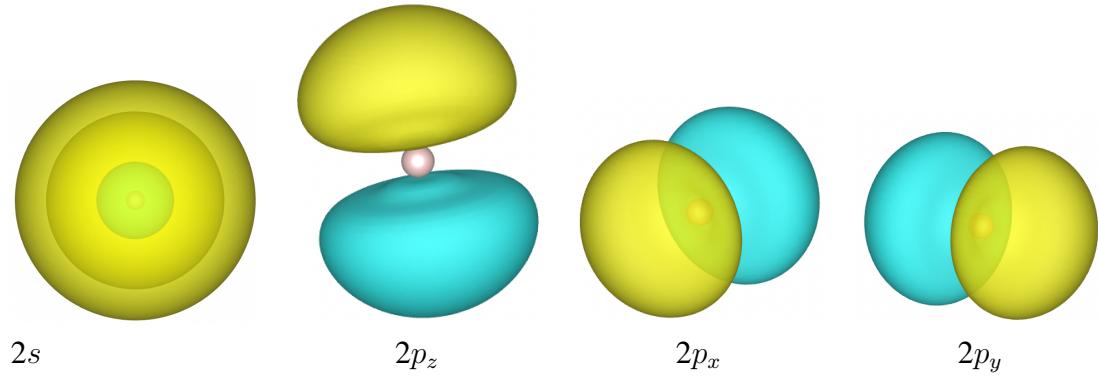


Figure 3: Images of the four states at the -3.4 eV energy level for hydrogen.

## The hydrogen atom

We now know enough to understand the periodic table and some basic chemistry, such as chemical bonds from a quantum mechanical perspective. The first three energy levels of the simplest atom, hydrogen, are shown in Fig 2. Each energy level has a different number of energy eigenstates with the same energy. For example, the energy level at -13.6 eV has only one state associated with it, while the energy level at -3.4 eV has four states. The states are labeled using terms that you may be familiar with from chemistry. The general formula for energy levels in the hydrogen atom is

$$E_n = -\frac{13.6}{n^2} \text{ eV}. \quad (1)$$

Renders of some of the energy eigenstates are presented in Fig 3. These energies and wave functions are determined by solving the Schrödinger equation in three dimensions, which one can do by hand in more advanced quantum mechanics courses.<sup>2</sup>

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<sup>2</sup>Something to look forward to!

We use the labels to indicate which state the electron is in. For example, atomic hydrogen which starts in the ground state can absorb light of the following energies, among others:

Transition	Energy (eV)
$1s \rightarrow 2p$	10.2 eV
$1s \rightarrow 3p$	12.1 eV

## The periodic table from quantum mechanics

The energy levels of multi-electron atoms are qualitatively very similar to those of hydrogen.<sup>3</sup> To find the ground state of the atom, we fill the states starting from the bottom of Fig 2, proceeding left, remembering to fill them with two electrons per *state*.

Atom	Number of electrons/protons	Ground state
H	1	$1s^1$
He	2	$1s^2$
Li	3	$1s^2 2s^1$
Be	4	$1s^2 2s^2$
B	5	$1s^2 2s^2 2p^1$
C	6	$1s^2 2s^2 2p^2$
N	7	$1s^2 2s^2 2p^3$
O	8	$1s^2 2s^2 2p^4$
F	9	$1s^2 2s^2 2p^5$
Ne	10	$1s^2 2s^2 2p^6$

The structure of the energy levels of atoms tells us why some atoms behave very similarly to others. For example, He and Ne are both called noble gases. Both of them have completely filled energy levels; all states at that energy are filled. This results in the non-reactivity of those atoms. On the other hand, atoms like nitrogen, oxygen, and hydrogen have unfilled levels, which leads to them forming molecules like N<sub>2</sub>, O<sub>2</sub>, and H<sub>2</sub>.

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<sup>3</sup>This is true until you get up to potassium (K), which has 19 electrons.

# UNIT 11: BAND STRUCTURE

## After this unit, you should be able to

- Determine whether a material is transparent from the energy levels and filling.
- Determine whether a material is metallic or insulating from the energy levels and filling.
- Use a semi-classical model to explain

## Introduction

In this unit, we will discuss the behavior of electrons inside materials, in a qualitative way. The quantum mechanical energy levels become partially continuous in a large system, but there are gaps. These gaps act very similarly to the gaps you've already seen in atoms, in that they can prevent materials from absorbing light of frequencies that don't correspond to energy level differences. This effect explains why for example windows are transparent while metal is not. It is also the reason for variety of colors that we see in the world around us.

We will also consider the momentum of the energy eigenstates, and we will find that the gaps in energy also create a barrier for electrons to change their momentum. To analyze the motion of electrons, we will use a semi-classical model, which is commonly used to predict the behavior of electronics. This model assumes that the dynamics of electrons are as they would be in classical mechanics, but that they can only have states that correspond to quantum states. So while a purely classical model would have continuous momentum and energy, the semiclassical description has gaps. This effect explains the existence of insulators—materials that have many electrons, but do not conduct electricity because the electrons are stuck and cannot change their momentum.

## Many particles in an infinite square well

Let's start with a very simple model of electrons in a material, let's imagine something like a copper wire. We will assume that the electrons are freely able to move, which just means that the potential energy is flat. We know how to solve this problem, the energy eigenstates are:

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad (1)$$

with energies

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

For an electron with wave function  $\Psi_n$ , the momentum has an equal probability of being

$$p_n = \pm \hbar \frac{n\pi}{L} = \pm \sqrt{2mE_n}, \quad (3)$$

because  $\sin(kx) = \frac{e^{ikx} - e^{-ikx}}{2i}$  and the momentum of  $e^{ikx}$  is  $\hbar k$ .

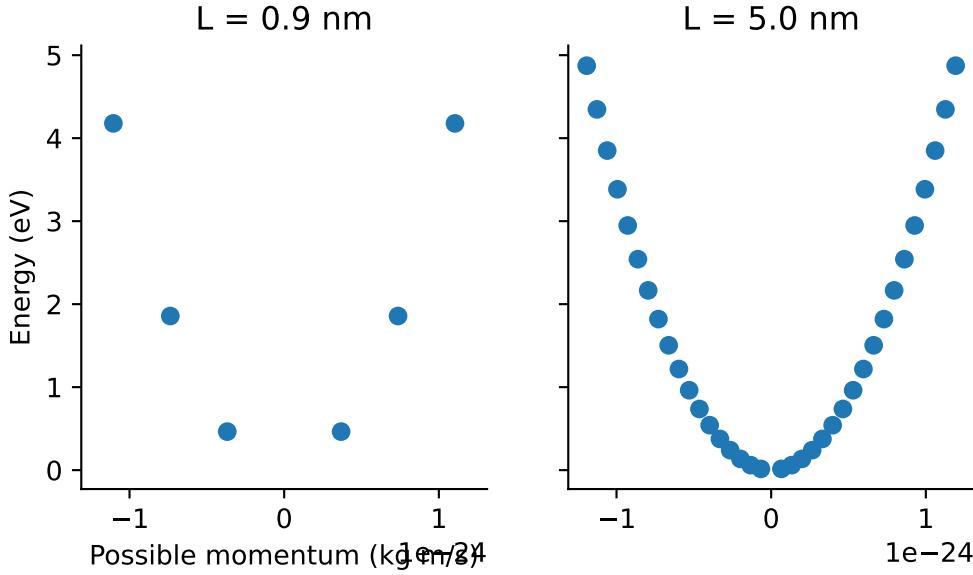


Figure 1: Energy versus momentum of the energy eigenstates for two lengths of infinite square well. As the well becomes larger, the graph fills in.

Now let's consider putting  $N_e$  electrons in a wire of length  $L$ . To obtain the ground state, all states are filled up to  $n_{max} = N_e/2$ . So the energy of the highest energy electron is

$$E_{max} = \frac{\hbar^2 \pi^2}{8m} \left( \frac{N_e}{L} \right)^2, \quad (4)$$

which is called the **Fermi level**. This only depends on the fraction  $\frac{N_e}{L}$ , i.e., the number of electrons per length, which is the density of electrons. We will call the electron density  $n_e \equiv \frac{N_e}{L}$ .

Since the properties only depend on the electron density, we can take the limit as  $L \rightarrow \infty$  while keeping the electron density constant to approximate a material. This works because a piece of metal or other material is often about 1 mm in size, which is  $10^6$  times bigger than the 1 nm sizes where the individual energy levels are apparent. This is diagrammed in Fig 2, where the Fermi level is diagrammed on a continuous line (which is really made up of many states) as a function of the electron density.

## Adding a little more realism: a corrugated potential.

To add a little more realism, let's add a potential to our infinite square well. This represents (very approximately) the effect of the atoms on the electrons in the material. We will add the potential<sup>1</sup>

$$V(x) = 2U \cos(gx) \quad (5)$$

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<sup>1</sup>This model is from Andreas Wacker's band structure introduction. You can find more details here [www.teorfys.lu.se/staff/Andreas.Wacker/Scripts/](http://teorfys.lu.se/staff/Andreas.Wacker/Scripts/)

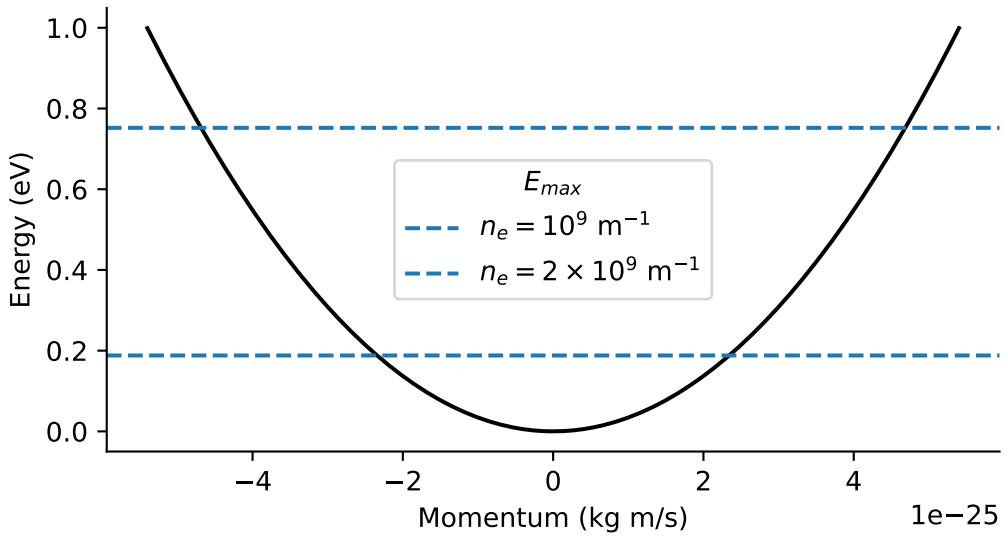


Figure 2: The energy level of the highest energy electron in the ground state depends on the number of electrons per unit volume. This energy level is called the Fermi level.

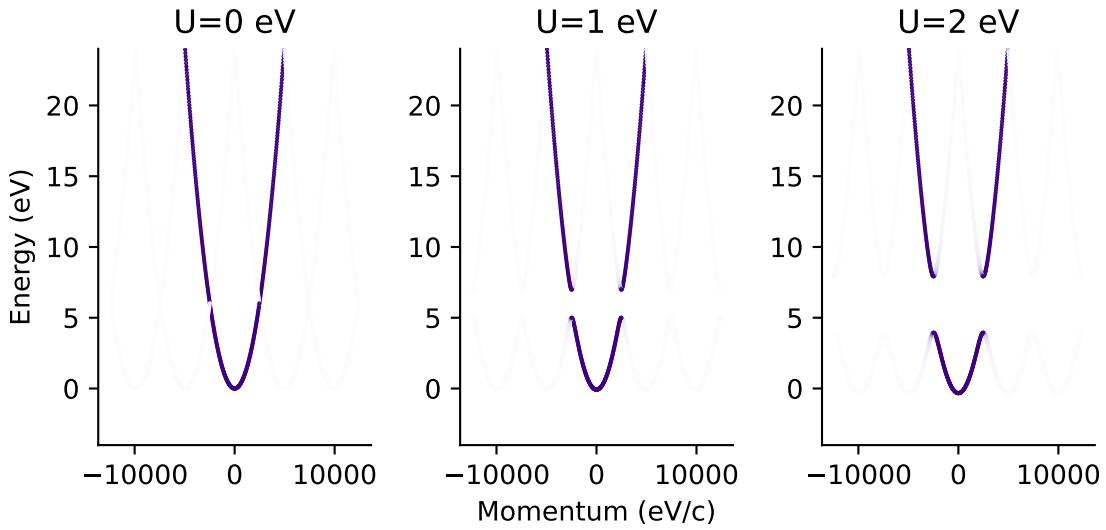


Figure 3: How the electronic states vary as we change  $U$ , which represents the strength of the interaction of atoms with the electrons. For  $U$  larger than zero, gaps in the allowed energies form. The intensity of the plot is the probability density (in momentum) that a given energy eigenstate has.

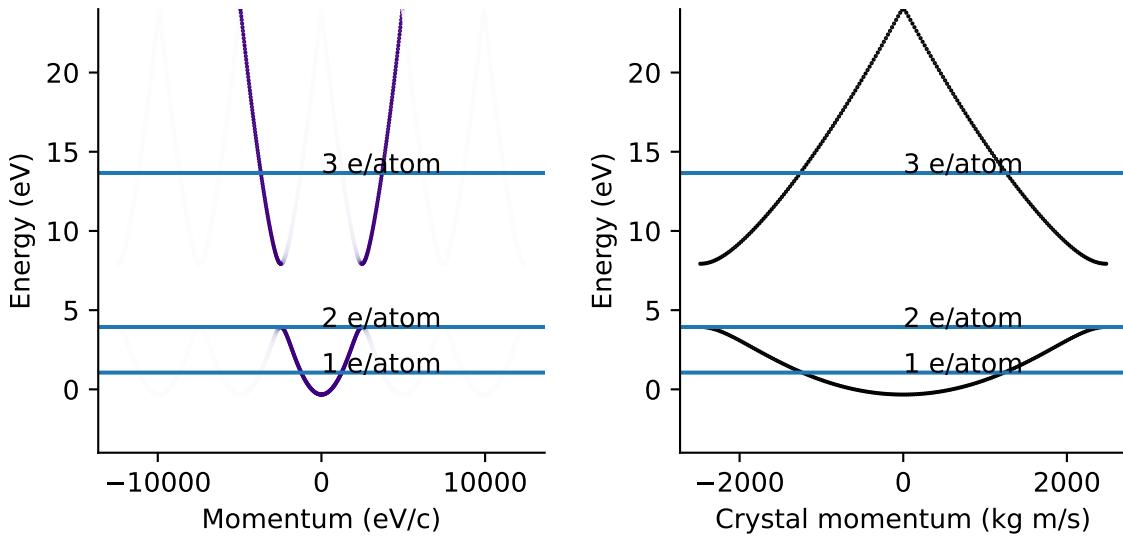


Figure 4: (left) How the filled energy levels (everything below the line is filled in the ground state) depend on the number of valence electrons per atom. The Fermi level increases as the density of electrons increases. (right) The same graph as you'll often see it for materials. Only one period of each energy band is shown, and the x-axis is now the so-called "crystal momentum."

$U$  is the strength of the potential, representing how much the atomic nuclei<sup>2</sup> affect the electrons in the material. We will not go through the solution in detail.

In Fig 3, we show the solutions of this potential. This kind of plot is called a “band structure” diagram; presumably named so because there are bands of allowed energies, rather than isolated allowed energies as in atoms. Each line is called a band. The energy gap between the bands is called the “band gap,” for hopefully obvious reasons. Note that the bands fold back on themselves so that high energy does not imply high momentum; this is an effect of the potential, and happens in more realistic models of materials.

Given the energy levels, the behavior of the material depends strongly on how the energy levels are filled, similar to the case of atoms. In Fig 4, we diagram this effect. For example, if this material were made up of sodium (Na), which has one valence electron per atom, then the first band would be half-filled. This means that there are excited states with very little extra energy above the ground state. On the other hand, if we were to make this material out of something with two valence electrons per atom, such as magnesium (Mg), then we would expect the band to be completely filled, and the first excited state is several eV higher than the ground state. Moving to three electrons per atom, now the filled levels are in the middle of a band again.

## Light absorption of metals and insulators.

For light absorption, we apply the same rules as we did for atoms. In the case of metals, ( $n_e = 1, 3$  in Fig 4) then even very low energy photons can be absorbed, since the lowest excited state is just above the ground state. In fact, the metal can absorb photons of any energy up to the difference

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<sup>2</sup>technically there are ‘free electrons’ and ‘bound electrons’, and we’re really talking about ions.

in energy between the Fermi level and the gap. Metals are reflective because they very efficiently absorb and re-emit visible light.

On the other hand, the first excited state for  $n_e = 2$  in Fig 4 requires a promotion of an electron across the gap. If the gap is large enough then the material can be transparent! For example, the reason that diamond is transparent is that it has a gap of over 6 eV, while photons in the visible range of frequencies have energies less than 4 eV. So those photons just don't have enough energy to overcome the gap, no matter how many are sent through the material. This is very similar to the photoelectric effect!

## Electrical conductivity: metals and insulators

Finally, let's think about what happens when we apply an electric field to a material. We would like to determine how the electrons respond. While in principle one can do this using quantum mechanics, typically a semi-classical approximation is used. That means that we use quantum mechanics to determine the energy and momentum of electrons, and given that, we approximate their dynamics using classical mechanics. This sort of model is used to accurately model how semiconductors behave and is used to design modern computer hardware.

Consider a single free electron with momentum  $p(0) = p_0$  and energy  $E(0) = E_0$ . We apply a constant electric field, which applies a force on the electron  $F = q\mathcal{E}$ . Let's assume that the force is in the positive direction. Newton's 3rd law tells us that  $F = \frac{dp}{dt}$ , so this force causes the momentum to increase, and therefore the energy to increase, since  $E(p) = \frac{p^2}{2m}$ . The solution is that  $p(t) = Ft$ , so the electron accelerates. This flow of electrons is electric current. For a free electron, the acceleration is allowed because there are states, and we have derived something we already know—that a free electron accelerates under an electric field.

Now let's consider the 1 electron per atom situation in Fig 4. The electron in the right-most state can increase its momentum and energy slightly due to the force on it. This leaves an empty state, which the second-to-right electron can move into, and so on, so that all electrons shift up in momentum. The entire system then has a non-zero net momentum, which results in a flow of current. This is why metals conduct electricity.

On the other hand, let's consider the 2 electron per atom situation in Fig 4. The electric field wants to increase the momentum of the right-most electron, but there are no allowed energy levels with slightly higher energy and higher momentum. So the right-most electron is stuck. This is true as well for the left-most electron; it cannot increase its momentum because there is another electron there. This is the reason that materials with electrons filled up to the gap block electrical flow, which we call insulators.

# UNIT 12: TWO-STATE SYSTEMS

## After this unit, you should be able to

- Predict the probability of a photon passing through a sequence of polarizing filters, given its initial polarization state.
- Given a spin wave function, compute the probability of transmission through a Stern-Gerlach device.

## Light polarization as a quantum state

Light can be polarized either horizontally or vertically. How do we describe that for a photon using quantum mechanics? Let's suppose that the photon is moving in the  $z$  direction, so its polarization is in the  $x, y$  plane. Let's call horizontal ( $x$ ) polarization  $\Psi_h$  and vertical ( $y$ ) polarization  $\Psi_v$ . The quantum state associated with each of them we will call  $h$  and  $v$ . A general quantum state for polarization will be  $\Psi = a\Psi_h + b\Psi_v$ , where  $a$  and  $b$  can be any complex numbers, so long as  $|a|^2 + |b|^2 = 1$ . Note that in this case, we have only discrete possibilities, as opposed to the case when we are considering the probability that a particle is at a given position ( $\Psi(x)$  from the previous section\*).

In quantum mechanics, diagonal and circular polarization are written as *superpositions* of vertical and horizontal polarization as shown in Table 1. Classically, you might expect there to be a continuum of values. Why don't we write it as  $\Psi(\theta)$ , with  $\theta$  the angle from the  $y$  axis? This is actually a very deep question which we cannot answer very rigorously in this class; you will learn this in advanced quantum mechanics. One way of looking at this is to note that in polarization, a diagonal polarization is  $\Psi_h + \Psi_v$ . On the other hand, a particle at  $x = 1$  nm is not a superposition of the particle being at  $x = 0$  nm and  $x = 2$  nm. For this course, it suffices to know that some things (position, momentum) are represented by a continuous variable while other things (polarization) are represented by discrete variables.

Table 1: Different polarizations of light written as linear combinations of horizontal( $h$ ) and vertical( $v$ ) polarization.

Polarization direction	State
Vertical	$\Psi_v$
Horizontal	$\Psi_h$
Diagonal (45 degrees)	$\frac{1}{\sqrt{2}}(\Psi_h + \Psi_v)$
Diagonal (-45 degrees)	$\frac{1}{\sqrt{2}}(\Psi_h - \Psi_v)$
Circular (right-handed)	$\frac{1}{\sqrt{2}}(\Psi_h + i\Psi_v)$
Circular (left-handed)	$\frac{1}{\sqrt{2}}(\Psi_h - i\Psi_v)$

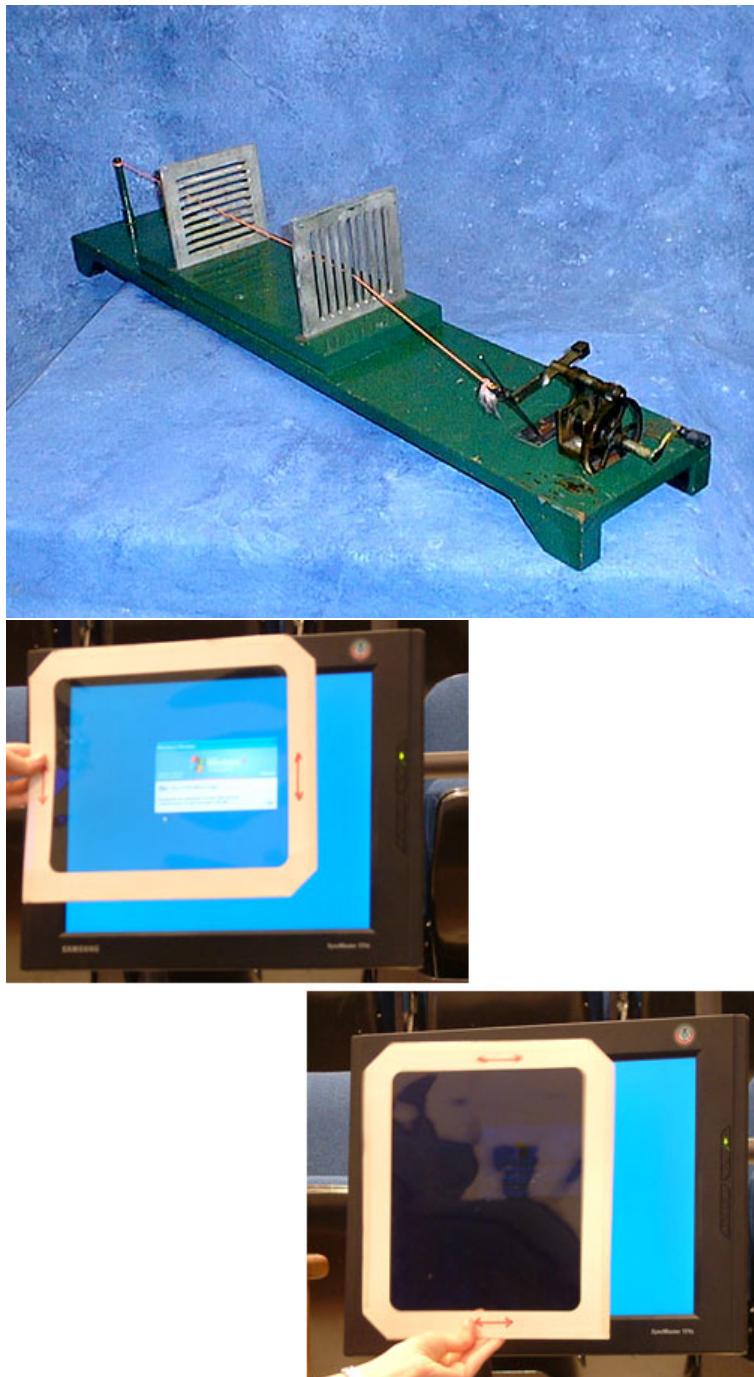


Figure 1: (top) A model of how polarization filters work. If the lines are arranged in opposite ways, the electric field cannot oscillate in either direction, and the light is blocked. (bottom) Light from LCD screens is polarized. If the filter is held one way, you can see the screen, if it's held the other way, it's blocked.

Table 2: States with definite spin in different directions for systems with two spin possibilities.

Spin direction	State
$\hat{z}$	$\uparrow$
$-\hat{z}$	$\downarrow$
$\hat{x}$	$\frac{1}{\sqrt{2}}(\uparrow + \downarrow)$
$-\hat{x}$	$\frac{1}{\sqrt{2}}(\uparrow - \downarrow)$
$\hat{y}$	$\frac{1}{\sqrt{2}}(\uparrow + i\downarrow)$
$-\hat{y}$	$\frac{1}{\sqrt{2}}(\uparrow - i\downarrow)$

## Measurement of polarization

Now let's suppose what happens when a photon encounters a filter that only lets vertically polarized light through it. What do you suppose will happen? Surely, if the photon is vertically polarized, it will simply pass through the filter. On the other hand, if the light is horizontally polarized, it will not pass through the filter.

What about when the light has a diagonal polarization, so that its polarization is given by  $\frac{1}{\sqrt{2}}(\Psi_h + \Psi_v)$ ? It turns out that the photon has a **50% probability** of passing through a vertical filter. And after the photon passes through the filter, its polarization is  $\Psi_v$ . Why has it changed? Well, we said before that only vertically polarized light passes through the filter, so if the photon passed through the filter, it must be vertically polarized.

The polarization  $\Psi$  is telling us the *probability* that the photon will pass through a filter. If the polarization is given by  $a\Psi_v + b\Psi_h$  (with  $|a|^2 + |b|^2 = 1$ ), then the probability of the photon passing through the vertical filter is given by  $|a|^2$ , and of passing through the horizontal filter is given by  $|b|^2$ .

## Electron and atom spin

The spin of an electron or some atoms is described very similarly to the polarization of light (remember, matter and light are very similar in quantum mechanics!). In these systems, there is an internal quantity called *spin*<sup>1</sup> that can either point up or down (or left or right, or forward or backward). This results in a magnetic moment either pointing up or down. This applies to several different types of systems: electrons, neutrons, protons, deuterium (hydrogen with a proton and a neutron), silver atoms (Ag), and other atoms. The states are given as in Table 2, where  $\uparrow$  means that the magnetic moment is pointed in the  $+\hat{z}$  direction and  $\downarrow$  means that the magnetic moment is pointed in the  $-\hat{z}$  direction.

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<sup>1</sup>It is called spin because the particle acts as if it's spinning, which gives rise to angular momentum and a magnetic field. However, this is angular momentum *without* classical rotation. Yep.



Figure 2: Stern-Gerlach experimental setup. The changing magnetic field separates randomly oriented atoms into two streams.

### Measurement of spin and a generalized rule for measurement

Let's suppose that we have an arbitrary spin state given by  $a \uparrow + b \downarrow$ . Then we can compute the probability of measuring a spin pointing up by using the same rule as we had before:

$$P(\hat{z}) = \frac{|a|^2}{|a|^2 + |b|^2}, \quad (1)$$

and a similar rule for  $P(\hat{z})$ . Remember the collapse rule: if we do measure spin in the  $\hat{z}$  direction, then afterwards the wave function is  $\uparrow$ , even if it was something else before.

To find the probability of observing the spin in the  $\hat{x}$  direction, we have to use a slightly more generalized version of the same rule, which is very similar to the dot product you may have seen in vector math. Assume that  $|a|^2 + |b|^2 = 1$ ; then,

$$P(\hat{x}) = \left| \frac{1}{\sqrt{2}} (\uparrow + \downarrow)^* \cdot (a \uparrow + b \downarrow) \right|^2 = \left| \frac{1}{\sqrt{2}} (a + b) \right|^2. \quad (2)$$

Note the complex conjugate for the state that we're measuring. Similarly,

$$P(\hat{y}) = \left| \frac{1}{\sqrt{2}} (\uparrow + i \downarrow)^* \cdot (a \uparrow + b \downarrow) \right|^2 = \left| \frac{1}{\sqrt{2}} (a - ib) \right|^2. \quad (3)$$

You can verify for yourself that this rule has some sensible properties: a state with definite spin direction will, with probability 1, be observed in that direction. In general, the measurement rule for a particle with wave function  $\Psi$  and a state with definite direction  $S$  is:  $P(S) = |S^* \cdot \Psi|^2$ . Make sure to normalize your wave function to use this rule. You can also use this rule for polarization! A strange fact of this rule is that if the spin is definite in  $\hat{z}$ , then it is maximally indefinite in  $\hat{x}$  and  $\hat{y}$ ; a measurement in each of these directions has a 50/50 chance of being positive or negative.

### Stern-Gerlach experiment

The Stern-Gerlach experiment is one of the experiments that really show that we have to use the description of spin. The rules presented in this chapter are the simplest ones that have been come

up with that also predict the output of this experiment. A measurement of the spin direction is performed by sending the particle through a changing magnetic field. The particle will be deflected an amount proportional to the alignment of the particle's magnetic moment with the magnetic field. Classically, one would expect to see a range of deflections, depending on which direction the magnetic moment happened to be pointing. However, in reality, we only see **two** deflections; one up and one down. This already is evidence for the quantum nature of spins; when we measure the spin, we only get one of two values.

Things get very interesting when we perform multiple experiments in a row on the same atoms. Let's consider adding a second measurement in the  $\hat{z}$  direction after the one in Fig 2, but so that it only intercepts the  $+z$  atoms. Since we already measured the  $z$  direction and found it to be  $+z$ , the wave function is simply  $\uparrow$ . With probability 1, the atoms pass through the upper path. This is similar to the polarization behavior!

Now suppose we measure in the  $x$  direction and choose the  $+x$  atoms. Their wave function is now  $\frac{1}{\sqrt{2}}(\uparrow + \downarrow)$ . If we then measure the  $z$  direction, then the atoms will go up and down with equal probability, since it is an equal superposition of  $\uparrow$  and  $\downarrow$ . And so on, there are many fun games one can play with this. The behavior of spins is another instance of an uncertainty principle, similar to what we saw with momentum and position. If the spin direction in the  $z$ -axis is definite, then the  $x$  and  $y$  directions are uncertain, and vice versa.

## Philosophical interlude

This is again a place where you might reasonably ask why is it this way, so that the  $x$ -direction of spin can never be definite when the  $y$  direction of spin is definite. A similar motif appears in the uncertainty principle between momentum and position. There are actually several levels of understanding this. The first, and most important is that it works. This math predicts the outcome extremely precisely not just the experiments we have presented here, but also a number of other, even stranger experiments in which multiple spins interact with each other. At its core, physics is about making precise models of reality and so if our mathematical model represents the experiments accurately, then to some extent we have done our job, and this does it.

One might also ask whether "this is it;" that is, are there deeper principles that have this behavior as a result? The answer is yes, there are, although they are a bit beyond this class. Actually there are a number of principles that you've already seen which are the result of deeper principles, for example, the constant speed of light(special relativity, which is in reach for many of you), conservation of energy (Noether's theorem, which takes a little while), and spin (the combination of special relativity and quantum mechanics). Keep asking why, and you'll eventually get to an unknown, though. You can take the principles we've learned in this class and perfectly successfully apply them to many physical problems of relevance, or you can choose to explore the deeper principles. Either path is valid!