# PHYS 214 Prelecture Readings

September 7, 2021

# CONTENTS

This booklet is a guide to the material in the PHYS 214 class at the University of Illinois. The intention of these notes is to provide succinct explanations of each of the concepts covered in the course, which will be expanded upon in the lecture of the class. It is ideal if the student reads each unit before the lecture, and again afterwards. They are divided into units, which are meant to be covered at a rate of two per week in a 7-week course.

Each unit has a section titled "After this unit, you should be able to." These are the learning goals for the chapter, and taken all together, these are the learning goals for the course. In the course, the homework, discussion, and exam questions will focus on helping you get to the point at which you have the listed skills. At the end of the course, you should have an understanding of the basics of quantum mechanics, and have some idea for what makes it so different from our comfortable classical picture of the world.

There are numerous footnotes throughout the chapters. These are meant to explain details and assumptions as they are made through the notes without interrupting the exposition. These footnotes are optional.

Finally, these notes include illustrations by the author. These are not expected to be beautiful, but they are meant to be illustrative.

One of the main features of quantum mechanics is that particles can behave like waves, so we first start with a description 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.

## 1.1  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.

## 1.2  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

$$y(x, t) = A\cos(kx - \omega t + \phi), \tag{1.1}$$

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 1.1.

For concreteness, let's consider the classical (PHYS 212) description[1] 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.

$$E_x(x, t) = E_{max}\cos(kx - \omega t + \phi) \tag{1.2}$$

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 1.2. The easiest way to read off $\phi$ is to look at the value of the electric field at $t = 0$ and $x = 0$. Then

$$\phi = \cos^{-1}(E_x(0, 0)/E_{max}). \tag{1.3}$$

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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[1]This description must be modified because light is actually *quantized*, which we will get to later in the course.

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

Table 1.1: 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 1.2 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:

$$x_{max} = \frac{\omega t - \phi}{k} \tag{1.4}$$

$$v = \frac{dx_{max}}{dt} = \frac{\omega}{k} \tag{1.5}$$

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

## 1.3 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 $I(x, t) = |y(x, t)|^2$.[2] We will average the intensity over a period $T$:

$$I_{\text{average}}(x) = \frac{1}{T}\int_0^T |A|^2|\cos(kx - \omega t + \phi)|^2 dt = \frac{|A|^2}{2}, \tag{1.6}$$

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

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[2]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.

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.

## 2.1 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.

## 2.2 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 $k$:

$$y_1(x,t) = A\cos(kx - \omega t + \phi_1) \tag{2.1}$$
$$y_2(x,t) = A\cos(kx - \omega t + \phi_2). \tag{2.2}$$

In many cases (you can always assume this in this course), the total wave is given by superposition [1], so

$$y_{\text{total}}(x,t) = y_1(x,t) + y_2(x,t). \tag{2.3}$$

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 2.1.

Using the trigonometric identity

$$\cos\alpha + \cos\beta = 2\cos\left(\frac{\alpha - \beta}{2}\right)\cos\left(\frac{\alpha + \beta}{2}\right) \tag{2.4}$$

we can find that

$$y_{\text{total}}(x,t) = 2A\cos\left(\frac{\phi_1 - \phi_2}{2}\right)\cos\left(kx - \omega t + \frac{\phi_1 + \phi_2}{2}\right) \tag{2.5}$$

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.

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[1] Waves that do this are called "linear" because they add.
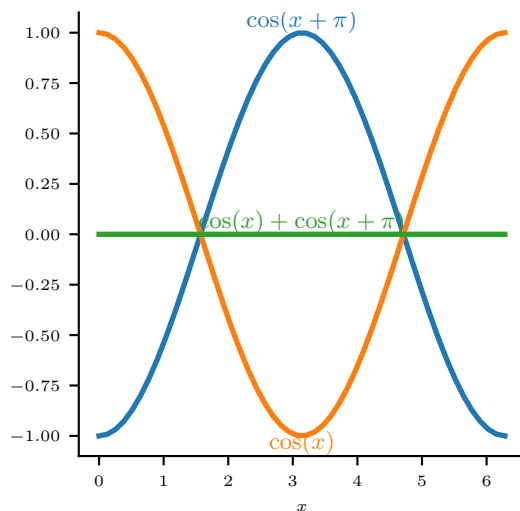
Figure 2.1: Destructive interference between two waves

## 2.3  Phasors

What if the amplitudes of the waves are different? In that case, we cannot use the trigono-metric identity in Eqn 2.4. 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 2.2) 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.

## 2.4  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 2.3) 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 percieves the sound to be. The waves that the observer experiences[2] from each source are:

$$y_1(x,t) = A\cos(kr_1 - \omega t + \phi_1) \tag{2.6}$$
$$y_2(x,t) = A\cos(kr_2 - \omega t + \phi_2). \tag{2.7}$$

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[2]This is the amplitude *at the observer's position*.

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

$t = 0$

$t = \frac{\pi}{4\omega}$

Figure 2.2: A figure that shows the relationship between phasors and harmonic waves.

Figure 2.3: An observer experiencing the intensity of waves generated from two sources in phase.

Then, using the trigonometric identity from Eqn 2.4,

$$y_1(x,t) + y_2(x,t) = 2A \cos\left(\frac{kr_1 + \phi_1 - kr_2 - \phi_2}{2}\right) \cos\left(\frac{kr_1 + \phi_1 + kr_2 + \phi_2}{2} - \omega t\right). \qquad (2.8)$$
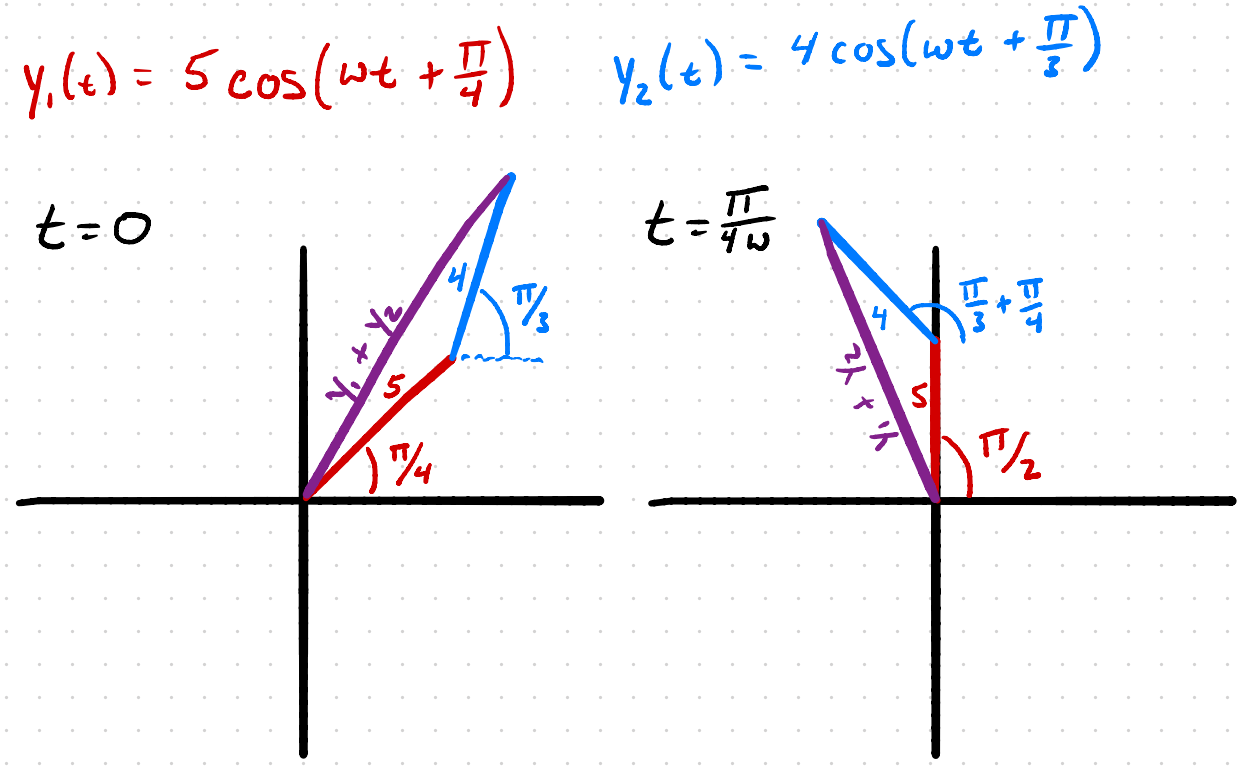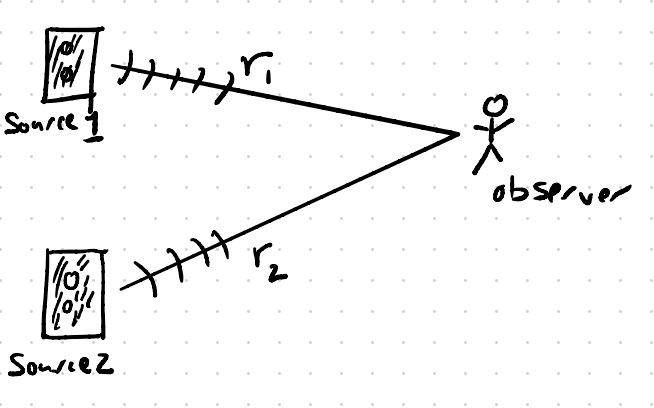
and the total average intensity for that observer is

$$I_{\text{total}} = 2A^2 \cos^2\left(\frac{kr_1 + \phi_1 - kr_2 - \phi_2}{2}\right). \qquad (2.9)$$

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

$$I_{\text{total}} = 2A^2 \cos^2\left(k\frac{r_1 - r_2}{2}\right) = 4I_1 \cos^2\left(k\frac{r_1 - r_2}{2}\right). \qquad (2.10)$$

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

## 2.5   Example: Two slits

An important example of interference is the two-slit experiment, shown in Fig 2.4. 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 $\omega_1 = \omega_2)$
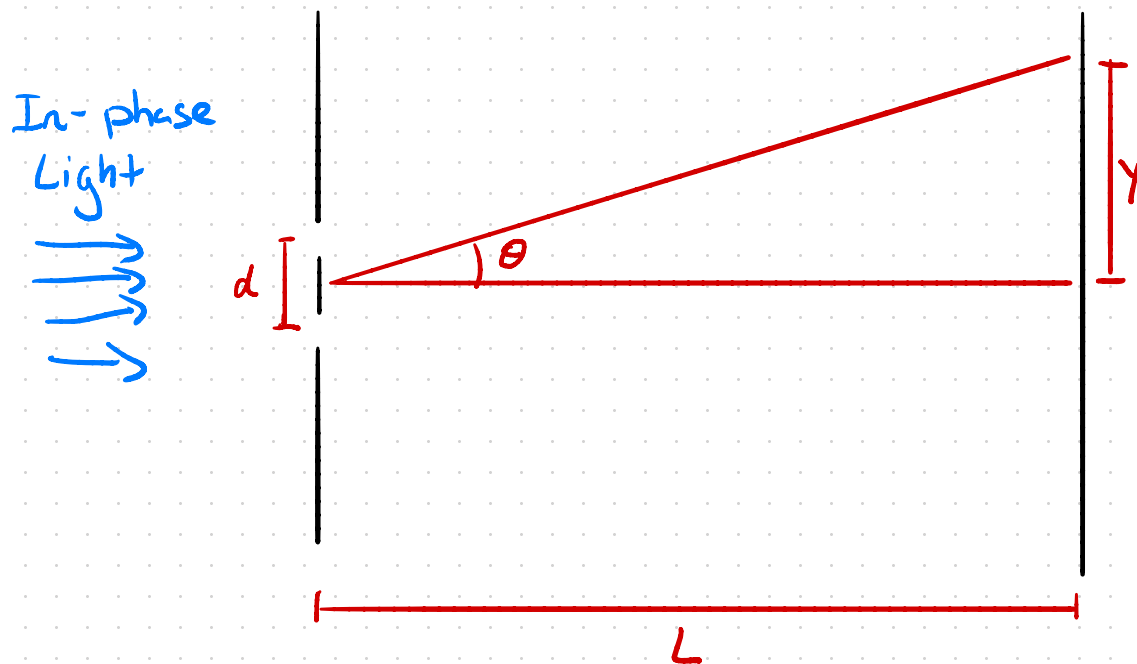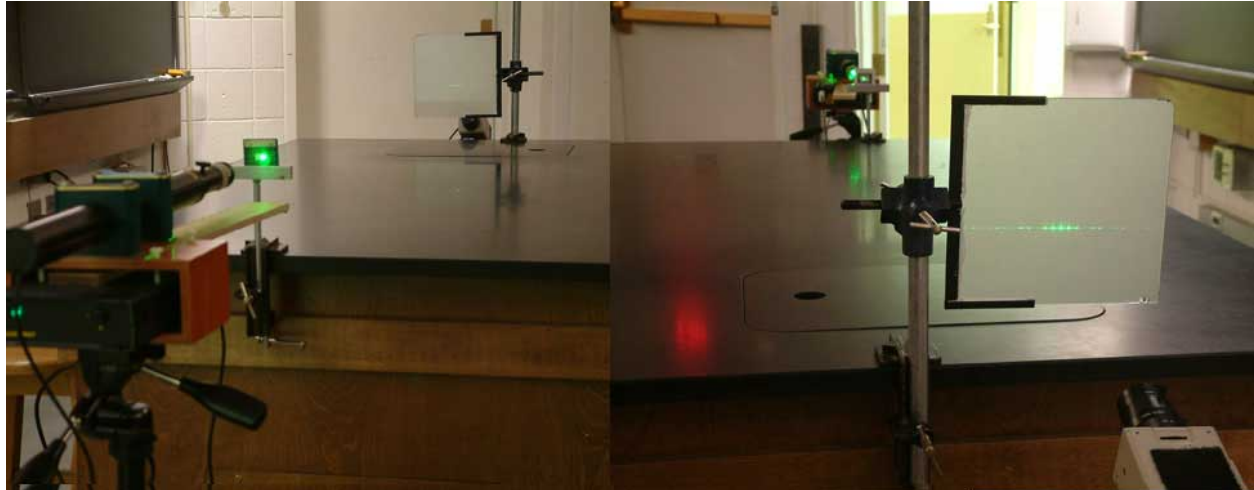
Figure 2.4: Geometric setup of a two-slit experiment. The card in the pictures has slits separated by a distance $d$ (usually a few $\mu$m). The screen is placed $L$ (a meter or two) away from the card. Then the intensity varies on the screen as we can see from a pattern of bright and dark spots. The position on the screen is $y$.
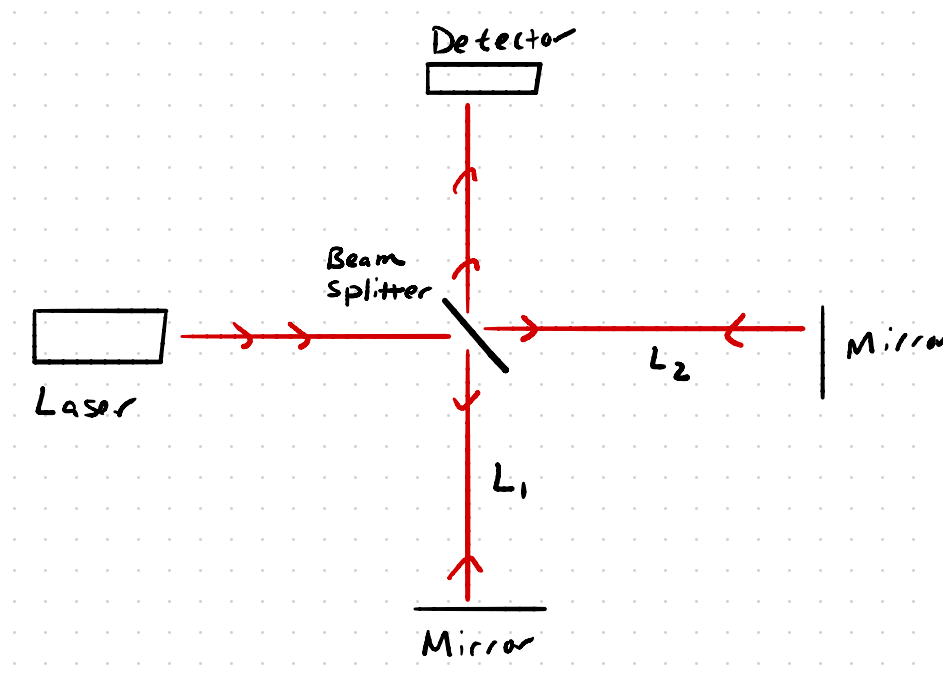
Figure 2.5: Interferometer optical setup

Because of these observations, we can use Eqn 2.10 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!

## 2.6  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 2.10, so

$$I = 4I_1 \cos^2\left(k\frac{r_1 - r_2}{2}\right). \tag{2.11}$$

$r_1$ 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:

$$r_1 - r_2 = 2(L_1 - L_2) \tag{2.12}$$

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

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.

## 3.1   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.

## 3.2   Phasors for more than two sources

Recall that the phasor diagram for two sources in constructive interference looks like $\longrightarrow\!\longrightarrow$. 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: $\longrightarrow\!\longrightarrow\!\longrightarrow$. 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[1] allows us to measure precisely what wavelengths are present in a given light source.
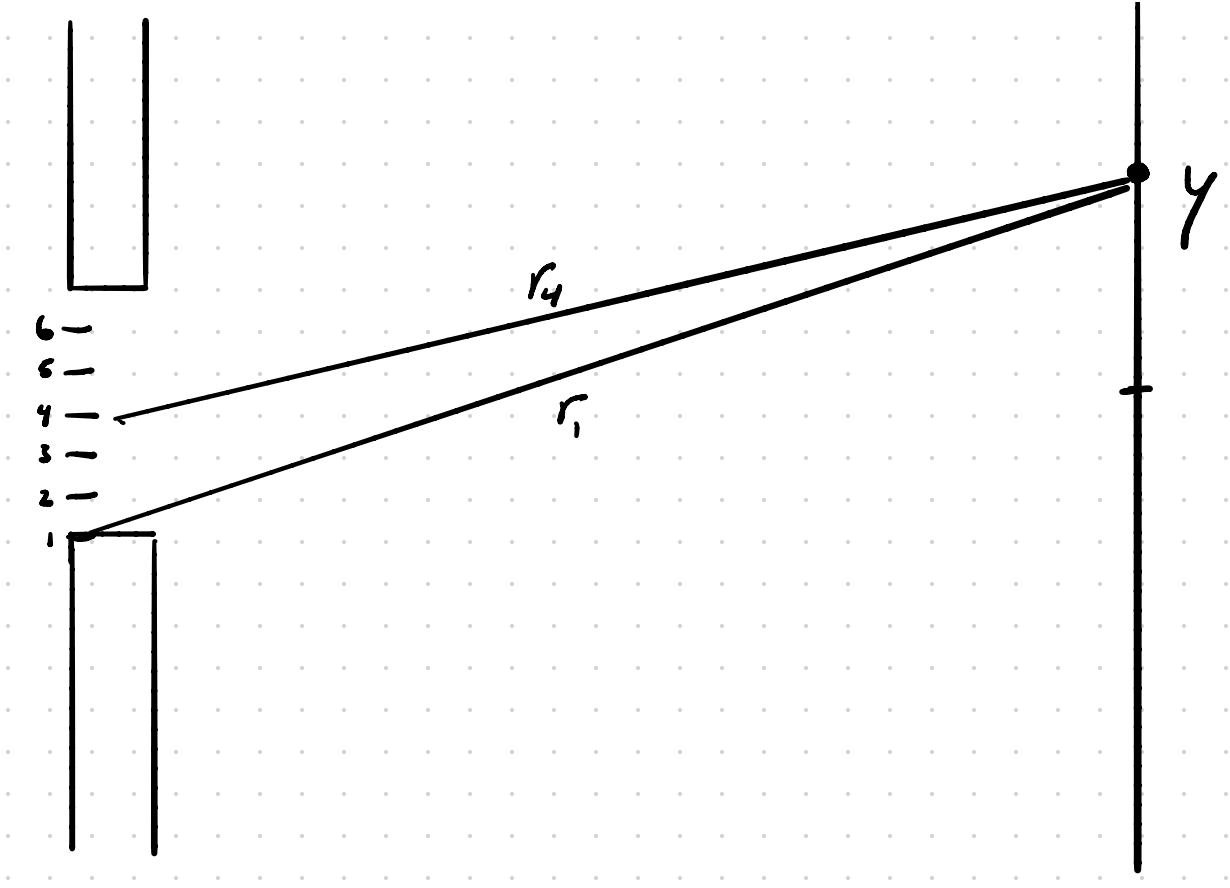
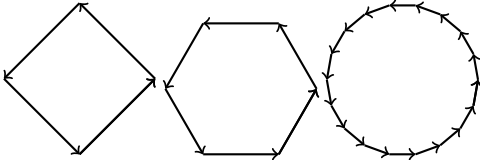Figure 3.1: The partitioning of a single slit into 6 point sources.



Figure 3.2: Phasor diagrams that lead to destructive interference for different numbers of point sources.

## 3.3   Diffraction from a single slit

Our goal in this section 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 $N \to \infty$.

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 3.2 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

$$k(r_2 - r_1) = \frac{2\pi}{N} \tag{3.1}$$

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

$$a\sin\theta_0 = \lambda \tag{3.2}$$

Note that this result does not depend on $N$ at all! So the limit as $N \to \infty$ 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.

## 3.4   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 $D\sin\theta_0 = 1.22\lambda$.[2]

## 3.5   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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[1]In Latin, spectrum means "image" and the -scopy relates to the study of a subject.

[2]If you want to know more, this is called the Airy disk

## 3.6 Example: diffraction and lithography

Lithography[3] is the technique used to draw tiny nanometer resolution circuits on semi-conductors 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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[3]The litho prefix means 'stone,' and the -graph suffix means to write or draw, so lithography literally means 'to draw on stone.'

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 $6.626 \times 10^{-34}$ m$^2$ 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.

## 4.1 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.

## 4.2 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 4.1 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.
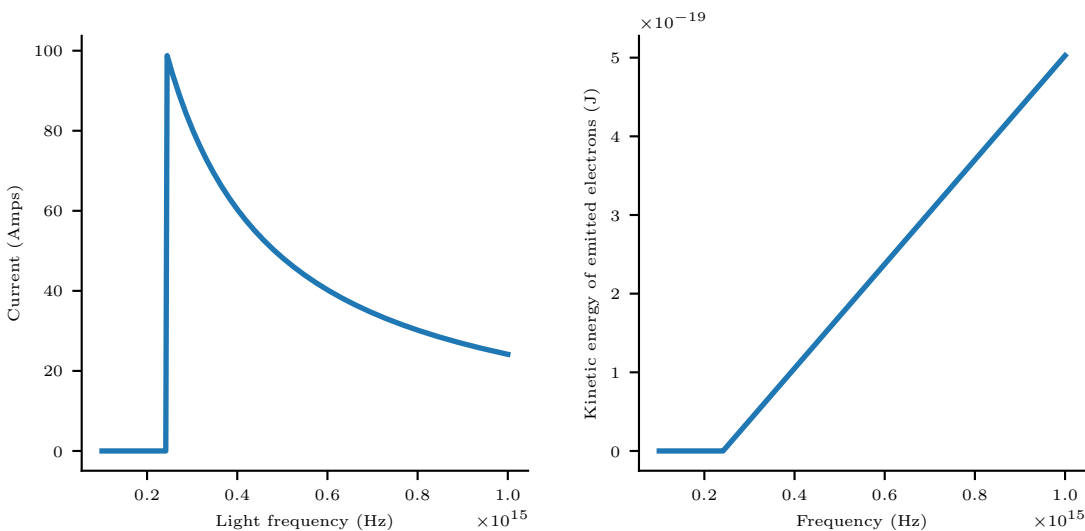
Figure 4.1: Sketches of the photoelectric effect. (left) The current observed for a fixed intensity of light of a given frequency. (right) The kinetic energy of ejected electrons as a function of the frequency of incident light.

The **threshold effect** is explained because 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

$$E_{\text{initial}} = hf - \Phi \tag{4.1}$$
$$E_{\text{final}} = KE_{\text{electron}}, \tag{4.2}$$

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 4.2. 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 4.1.

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 $hf$. [1]

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[1]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 4.1: Ways to write the momentum and energy of the photon

| | | |
|---|---|---|
| Energy | E | $hf = \hbar\omega = \frac{hc}{\lambda} = \hbar ck$ |
| Momentum | p | $h/\lambda = \hbar k = \frac{hf}{c} = \frac{\hbar\omega}{c}$ |

## 4.3   Energy and momentum of a photon

We determined that the quantum of energy for light is equal to $hf$. There is also a cor-
responding 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 mo-
mentum and energy, summarized in Table 4.1.

## 4.4   The relation between intensity and number of photons

We can use unit analysis to determine how many photons are incident on an object. Sup-
pose that light of frequency $f$ is incident on an object, with observed intensity $I$. In SI
units, $I$ is given in 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 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 mo-
mentum. 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.

# 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.

## 5.1  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.

## 5.2  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:

$$\rho(x) \geq 0 \tag{5.1}$$

and so-called normalization

$$\int_{-\infty}^{\infty} \rho(x)dx = 1. \tag{5.2}$$

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

$$P(a < x < b) = \int_{a}^{b} \rho(x)dx. \tag{5.3}$$

Because of Eqns. 5.1 and 5.2, 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.

## 5.3 Probability density examples

### 5.3.1 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

$$\int_{-\infty}^{\infty} \rho(x)dx = \int_{0}^{\infty} Ne^{-x}dx = 1. \tag{5.4}$$

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

$$\int_{0}^{\infty} e^{-x}dx = -e^{-x}|_{0}^{\infty} = 1. \tag{5.5}$$

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

### 5.3.2 Number of particles per second

Suppose that we place a detector between $x = a$ and $x = b$ $\mu$m. Suppose that the normalized probability density of a particle hitting the detector in that region is given by $\rho(x) = (0.1 + Cx)$ $\mu$m$^{-1}$ in that region, with $C = 0.05$ $\mu$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

$$P(a < x < b) = \int_{a}^{b} 0.1 + Cxdx = 0.1(b - a) + \frac{C}{2}(b^2 - a^2) \tag{5.6}$$

**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.

## 5.4 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:

- $i = \sqrt{-1}$.
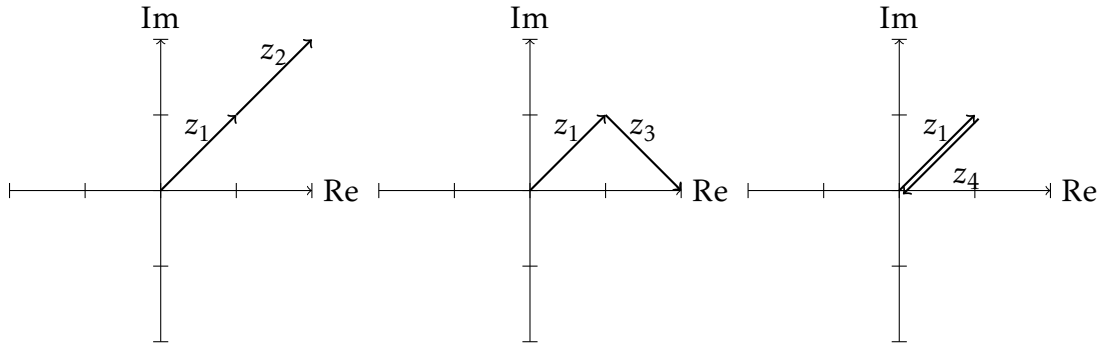
Figure 5.1: Adding complex numbers. For $z = x + iy$, the real part is $x$, labeled Re, and the imaginary part is $y$, labeled Im.

- $e^{i\theta} = \cos(\theta) + i\sin(\theta)$

- 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:

$$z_1 + z_2 = x_1 + iy_1 + x_2 + iy_2 = (x_1 + x_2) + i(y_1 + y_2) \tag{5.7}$$

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

$$z_1 \cdot z_2 = (x_1 + iy_1)(x_2 + iy_2) = x_1x_2 + iy_1x_2 + ix_1y_2 - y_1y_2 \tag{5.8}$$

## 5.5   Example: interference using complex numbers

Consider the four complex numbers:

$$z_1 = 1 + i$$
$$z_2 = 1 + i$$
$$z_3 = 1 - i$$
$$z_4 = -1 - i$$

Some sums are shown in Fig 5.1. 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,

$$|z_{12}|^2 = z_{12}z_{12}^* = (2 + 2i) * (2 - 2i) = 4 + 4 = 8, \tag{5.9}$$
$$|z_{13}|^2 = z_{13}z_{13}^* = (2) * (2) = 4, \tag{5.10}$$
$$|z_{14}|^2 = z_{14}z_{14}^* = (0) * (0) = 0. \tag{5.11}$$

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 $|v|^2 = v_x^2 + v_y^2$.

## 5.6  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

$$|z|^2 = zz^* = Re^{i\theta}Re^{-i\theta}. \tag{5.12}$$

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

$$|z|^2 = R \cdot R = R^2, \tag{5.13}$$

which is the desired relationship.

# 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, tunneling, metals and insulators, and many other physical effects.

## 6.1   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.

## 6.2   Two slit experiment for electrons

Suppose that we send electrons (one at a time) with a given momentum $p$ towards two slits. After many electrons have passed through, we count how many electrons were incident on each part of the screen. The result is shown in Fig 6.1. 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. To describe this, quantum mechanics uses a wave, called the wave function, which then is used compute probability of arrival.

## 6.3   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 $\Psi(x)$[1]. The 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

$$P(a < x < b) = \int_a^b \rho(x)dx = \int_a^b \Psi^*(x)\Psi(x)dx. \tag{6.1}$$
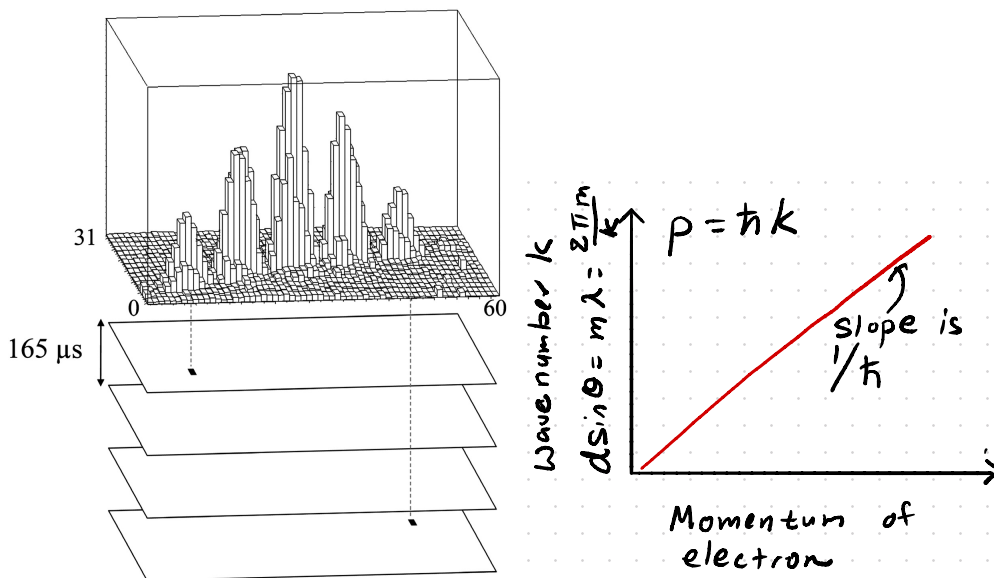
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[1]We will add time later!

Figure 6.1:   (left) Diffraction of electrons through two slits.  The z axis is the count of electrons, which arrive at random roughly every 165 $\mu$s. From Frabboni et al. Ultramicroscopy **116**, 73 (2012). (right) The relationship between the incident momentum of the electron and the wave number $k$ inferred from the spacing of the peaks.

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.

## 6.4   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[2] 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

$$\Psi(x) = A(e^{ikr_1} + e^{ikr_2}),\tag{6.2}$$

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[2]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.

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:

$$\Psi(x) = Ae^{ikr_1}(1 + e^{ik(r_2 - r_1)}) \tag{6.3}$$

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

$$\rho(x) = \Psi^*(x)\Psi(x) \tag{6.4}$$

$$= \left[A^* e^{-ikr_1}(1 + e^{-ik(r_2 - r_1)})\right]\left[Ae^{ikr_1}(1 + e^{ik(r_2 - r_1)})\right] \tag{6.5}$$

$$= |A|^2(2 + e^{-ik(r_1 - r_2)} + e^{ik(r_1 - r_2)}) \tag{6.6}$$

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

$$\rho(x) = |A|^2(2 + 2\cos(k(r_2 - r_1))), \tag{6.7}$$

which can be simplified using a trigonometric identity to give

$$\rho(x) = 4|A|^2\cos^2\left(\frac{k(r_2 - r_1)}{2}\right). \tag{6.8}$$

This should look very familiar; in fact it is the same as Eqn 2.10. We know that the peaks in probability will occur at angles such that

$$d\sin\theta = m\lambda, \tag{6.9}$$

where $d$ is the distance between the slits.

## 6.5 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 6.1, 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.

## 6.6   Normalization of wave functions

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

$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x)dx = 1 \tag{6.10}$$

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

$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x)dx = 1 \tag{6.11}$$

$$A^2 \int_0^L e^{ikx}e^{-ikx} = A^2 L. \tag{6.12}$$

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

$$\int_a^b \frac{1}{L}dx = \frac{b-a}{L}, \tag{6.13}$$

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 $L$.

## 7.1 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.

## 7.2 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:

$$\Psi(x,t) = Ae^{i(kx-\omega t)}, \tag{7.1}$$

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

$$\Psi(x) = Ae^{ikx}. \tag{7.2}$$

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 7.2, 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

$$\rho(x) = \Psi(x)\Psi^*(x) = |A|^2. \tag{7.3}$$

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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[1]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 $F = \frac{dp}{dt}$.

## 7.3   Eigenstates

The wave function in Eqn 7.2 is called an *eigenstate*[2] 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,[3] so we will not cover this. In later units, we will learn how to find *energy eigenstates*, which are very important in quantum mechanics.

## 7.4   Superposition of wave functions

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

$$\Psi(x) = A\left(e^{ik_1 x} + e^{ik_2 x}\right) \tag{7.4}$$

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

$$\Psi(x) = A\left(ae^{ik_1 x} + be^{ik_2 x}\right), \tag{7.5}$$

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 7.1, 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.

## 7.5   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:

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \tag{7.6}$$

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[2]"Eigen" is from German, where it means 'same.'
[3]Dirac delta functions
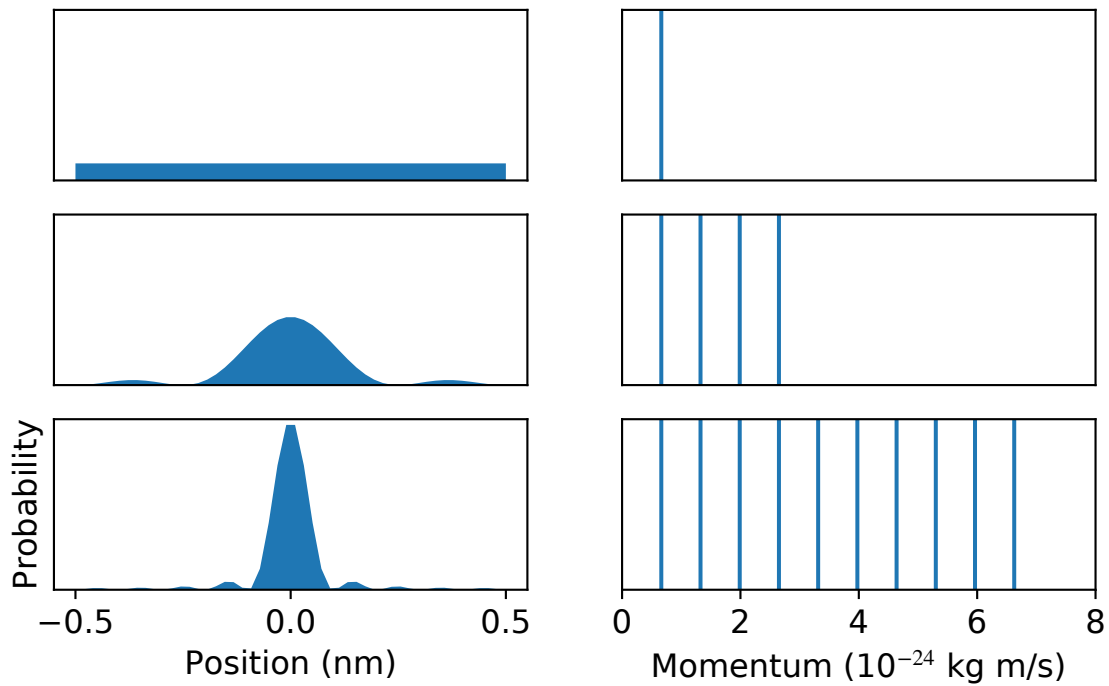
Figure 7.1: Making a localized wave function using a sum of momentum eigenstates. Each row is one wave function; the left is the probability density for position, while the right is the probability density for momentum. The momentum probability density is a bunch of spikes because it is a sum of momentum eigenstates. To make a wave function with high probability to be in one position, it's necessary to include many possible momenta.
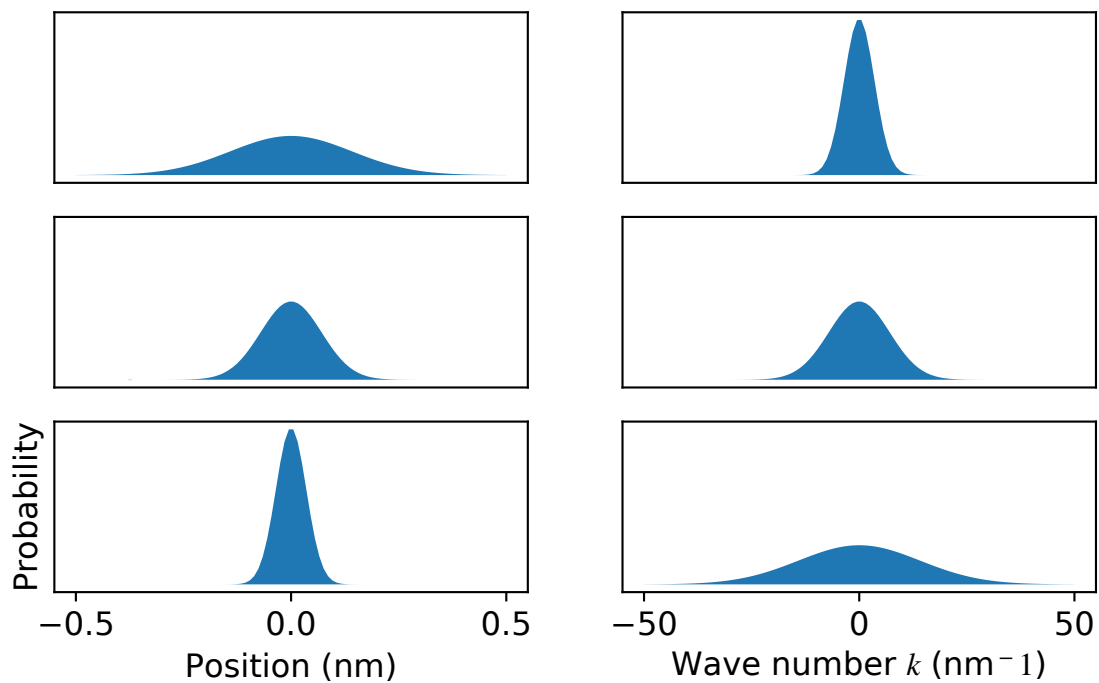
Figure 7.2: The position and momentum probabilities for various wave functions. Each row corresponds to one wave function with form proportional to $\exp(-x^2/2\sigma^2)$, and the probability of measuring position and momentum is given in each column.

This relationship puts fundamental physical limits on how well we can predict the outcome of an experiment.[4]

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[4]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.

# 8 Time independent Schrödinger equation

To summarize the last few sections, 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!

## 8.1 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 $x = b$.

## 8.2 The equation

The time-independent Schrödinger equation tells us which wave functions are energy eigenstates. This will in turn allow us to determine what energies a system can take on.

For this section, we will just consider a wave function at a given time, which we will write $\Psi(x)$. For a particle of mass $m$ in one dimension, the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + U(x)\Psi(x) = E\Psi(x). \tag{8.1}$$

In this equation, $U(x)$ is the external potential energy.

There are several important things to note about this equation:

- Only certain wave functions satisfy Eqn 8.1. 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 satifies Eqn 8.1.

- Energy eigenstates are also called **stationary states**. We will show this in the time dependence sections.

## 8.3 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:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} = E\Psi(x). \tag{8.2}$$

The most common solution method is to guess a wave function and check whether it satisfies Eqn 8.2. Let's guess $\Psi_k(x) = Ae^{ikx}$ as the wave function. Then

$$-\frac{\hbar^2}{2m}\frac{d^2Ae^{ikx}}{dx^2} = -\frac{\hbar^2}{2m}(ik)^2Ae^{ikx} = \frac{\hbar^2k^2}{2m}\Psi_k(x). \tag{8.3}$$

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

$$\frac{1}{2}mv^2 = \frac{p^2}{2m} = \frac{\hbar^2k^2}{2m}. \tag{8.4}$$

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

## 8.4 Example: 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,

$$U(x) = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{otherwise} \end{cases} \tag{8.5}$$

Given this, let's look back at Eqn 8.1 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

$$\Psi(x) = \begin{cases} A\sin(\frac{n\pi x}{L}) & \text{if } 0 < x < L \\ 0 & \text{otherwise,} \end{cases} \tag{8.6}$$

where $n$ is an integer.

We can find $A$ by enforcing normalization:

$$\int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right)dx = 1. \tag{8.7}$$

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:

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \tag{8.8}$$

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.

## 8.5   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.

## 8.6   Example: 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:

$$f_1 = \frac{10.2 \text{ eV}}{4.135667 \times 10^{-15} \text{eV} \cdot \text{s}} = 2.466 \times 10^{15} \text{s}^{-1} \tag{8.9}$$

and similarly for $f_2$. Those are the frequencies of light that can be absorbed by a hydrogen atom in the ground state.[1] 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 - (-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.

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[1]In reality, this is broadened a little bit by temperature effects.

## 9.1 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.

## 9.2 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:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + \frac{1}{2}kx^2\Psi(x) = E\Psi(x). \tag{9.1}$$

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

$$\frac{\hbar^2 b^2}{2m}A\sin(bx) + \frac{1}{2}kx^2A\sin(bx) = EA\sin(bx) \tag{9.2}$$

$$\frac{\hbar^2 b^2}{2m} + \frac{1}{2}kx^2 = E \tag{9.3}$$

$$\tag{9.4}$$

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[1]: $\Psi(x) = Ae^{-\alpha x^2}$. We take the derivative on the left-hand side

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[1] The guess and check method is a long-standing and useful tool in physics!

and find:

$$-\frac{\hbar^2}{2m}A(4\alpha^2 x^2 - 2\alpha)e^{-\alpha x^2} + \frac{1}{2}kx^2 Ae^{-\alpha x^2} = EAe^{-\alpha x^2} \tag{9.5}$$

$$x^2\left(\frac{1}{2}k - \frac{4\hbar^2\alpha^2}{2m}\right) + \left(\frac{\hbar^2\alpha}{m} - E\right) = 0 \tag{9.6}$$

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

$$\alpha = \frac{1}{2\hbar}\sqrt{mk} \tag{9.7}$$

$$E = \frac{\hbar^2\alpha}{m} = \frac{\hbar}{2m}\sqrt{mk}. \tag{9.8}$$

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.


## 9.3   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. 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: $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$, where $n = 0, 1, 2, \ldots$. 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 $n = 1, 2, \ldots$. 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.


## 9.4   Using energy levels to determine the potential

A common way of understanding the vibrations in molecules is to send infrared light through a gas or suspension of them, 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.
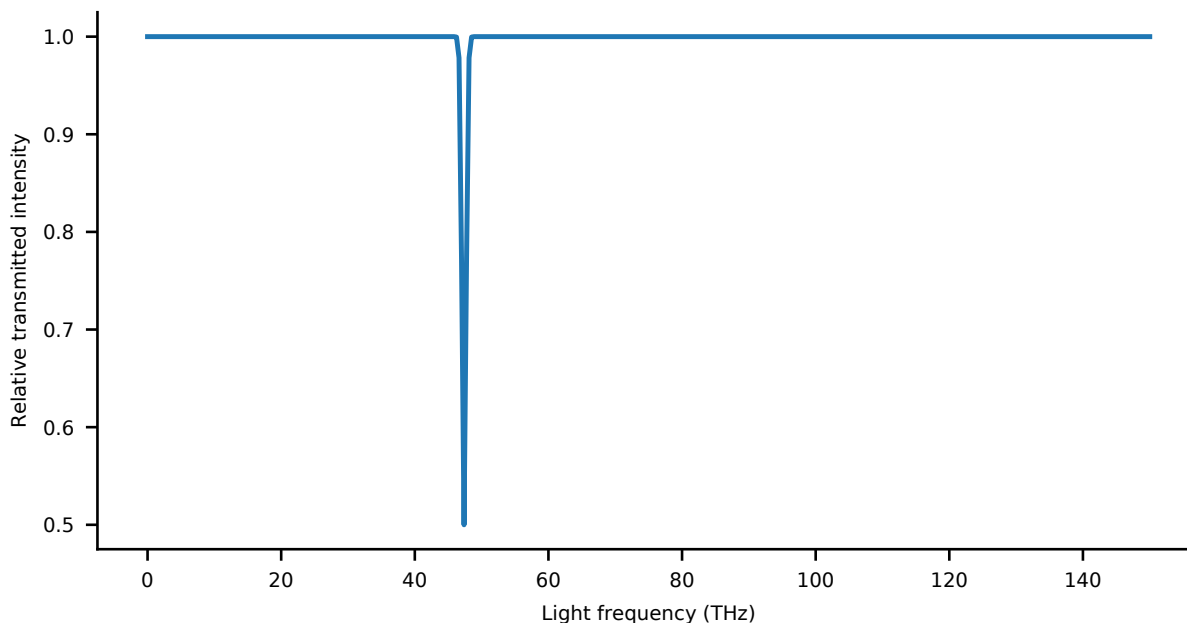
Figure 9.1: Simulated transmission of light through a gas of $O_2$ molecules. There is a dip in transmission of light which corresponds to the vibration of the two oxygen atoms.

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 tell $\omega$ by using

$$E_{\text{photon}} = hf \tag{9.9}$$

$$E_{\text{photon}} = \frac{3}{2}\hbar\omega - \frac{1}{2}\hbar\omega = \hbar\omega, \tag{9.10}$$

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 9.1). Each dip represents one vibrational state.

# 10 Time dependence in quantum mechanics

So far we have focused on wave functions at a given time. In reality, wave functions change with time. In this section, we will see that:

1. If a particle's wave function begins in an energy eigenstate, its probability density will not change with time.

2. If a particle's wave function is a superposition of energy eigenstates, then the probability density will oscillate with a frequency proportional to the difference between the energy of the different states.

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

- Find the oscillation frequency of a superposition of two eigenstates, if the energy difference is given.

- Verify whether a wave function given as a function of $x$ and $t$ satisfies the time-dependent Schrödinger equation.

## 10.2   Time dependent Schrödinger equation

The time dependent Schrödinger equation was not derived from anything; it's an equation that, as it turns out, satisfies a few things that we already know about quantum particles, along with a few physical principles. It is given as follows:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) \tag{10.1}$$

Some things to note about this equation:

- This is a partial differential equation. $\partial f(x,y)/\partial y$ means to keep x constant and take the derivative with respect to $y$.

- The right hand side is very similar to part of the time independent Schrödinger equation.

- There is the imaginary number $i$ in the equation, multiplying the time derivative. The solutions will be complex.

## 10.3   Energy eigenstates are stationary

In this section, we will prove that energy eigenstates have a probability density that does not depend on time. First, let's consider what that statement means. The probability

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density is $\rho(x,t) = |\Psi(x,t)|^2$. That means that $\Psi$ itself might depend on time, but as long as the magnitude squared does not depend on time, this statement will be true.

Assume that at time $t = 0$ $\Psi(x,0)$ is an energy eigenstate with energy $E$. Now let's guess a time dependence an energy eigenfunction: $\Psi(x,t) = e^{-i\omega t}\Psi(x,0)$. We don't know $\omega$ yet; we will find it later by using the time dependent Schrödinger equation. This guess satisfies the time-independent Schrödinger equation, Eqn 8.1 at all times:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) = E\Psi(x,t). \tag{10.2}$$

The factor $e^{-i\omega t}$ does not change this because it doesn't depend on $x$, so it just cancels on both sides. Therefore, we can write the time-dependent Schrödinger equation as:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = E\Psi(x,t) \tag{10.3}$$

Now we only need to compute the time derivative on the left hand side:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = i\hbar\Psi(x,0)(-i\omega)e^{-i\omega t} = \hbar\omega\Psi(x,t), \tag{10.4}$$

where we have used the fact that $(-i)i = 1$. Combining these two equations, we get:

$$\hbar\omega\Psi(x,t) = E\Psi(x,t). \tag{10.5}$$

So, this guess will work if $\hbar\omega = E$.

Now let's show that the probability density $\rho(x,t) = |\Psi(x,t)|^2$ is not dependent on time:

$$\rho(x,t) = \Psi^*(x,t)\Psi(x,t) = e^{i\omega t}\Psi^*(x,0)e^{-i\omega t}\Psi(x,0) = \Psi^*(x,0)\Psi(x,0), \tag{10.6}$$

which is independent of time. The $e^{-i\omega t}$ is called a **phase** of the wave function, but that doesn't change the probability of what we observe.

## 10.4   Superposition

Now suppose that a particle starts out **not** in an energy eigenstate, but in a equal superposition of two energy eigenstates. This is written as $\Psi(x,0) = \frac{1}{\sqrt{2}}(\Psi_1(x,0) + \Psi_2(x,0))$ Let's guess a functional dependence:

$$\Psi(x,t) = \frac{1}{\sqrt{2}}(e^{-i\omega_1 t}\Psi_1(x,0) + e^{-i\omega_2 t}\Psi_2(x,0)), \tag{10.7}$$

where $\omega_1 = E_1/\hbar$ and $\omega_2 = E_2/\hbar$. If you plug this into the time dependent Schrödinger equation, you will find that the equation is satisfied, after doing some algebra. The time dependent Schrödinger equation satisfies superposition–if two functions satisfy the equation, then any sum of those functions will also satisfy the Schrödinger equation.

## 10.5  Beat frequencies

In the previous section, we showed that if the wave function at $t = 0$ is a superposition of two energy eigenstates (specifically $\Psi_1 + \Psi_2$), then its time dependence is

$$\Psi(x,t) = \frac{1}{\sqrt{2}}(e^{-i\omega_1 t}\Psi_1(x,0) + e^{-i\omega_2 t}\Psi_2(x,0)). \tag{10.8}$$

Pulling out a factor of $e^{-i\omega_1 t}$,

$$\Psi(x,t) = \frac{1}{\sqrt{2}}e^{-i\omega_1 t}(\Psi_1(x,0) + e^{-i(\omega_2-\omega_1)t}\Psi_2(x,0)). \tag{10.9}$$

Now, let's check the time dependence of the probability density of the $\Psi(x,t)$ in Eqn 10.9.

$$\rho(x,t) = \Psi^*(x,t)\Psi(x,t) \tag{10.10}$$

$$= \frac{1}{2}\left(\Psi_1^*(x,0) + e^{i(\omega_2-\omega_1)t}\Psi_2^*(x,0)\right)\left(\Psi_1(x,0) + e^{-i(\omega_2-\omega_1)t}\Psi_2(x,0)\right) \tag{10.11}$$

$$= \frac{1}{2}\left(|\Psi_1(x,0)|^2 + |\Psi_2(x,0)|^2 + e^{-i(\omega_2-\omega_1)t}\Psi_1^*(x,0)\Psi_2(x,0) + e^{i(\omega_2-\omega_1)t}\Psi_1(x,0)\Psi_2^*(x,0)\right). \tag{10.12}$$

This might look like an intimidating formula, and it is not really necessary to memorize it. The important thing to realize about this is that the only time dependence in it is in terms like $e^{i(\omega_2-\omega_1)t}$, which we know from Euler's formula to equal $\cos((\omega_2 - \omega_1)t) + i\sin((\omega_2 - \omega_1)t)$. These are *oscillatory* functions, which repeat every with a period $T = 2\pi/(\omega_1 - \omega_2)$. Since $\omega_n = E_n/\hbar$, we can also compute the period of oscillation as $T = \frac{2\pi\hbar}{E_2-E_1}$. So the **period of oscillation depends on the difference between the energies of the states.** If the states are very close in energy, the oscillation is very slow, and if the states are very different in energy, the oscillation is fast.

## 10.6  Summary

Our picture of quantum mechanics is now complete. A quantum mechanical object is described using a wave function, $\Psi(x,t)$. $|\Psi(x,t)|^2$ gives the probability density of finding the particle at any position $x$ at a time $t$. The time evolution of $\Psi(x,t)$ is given by the time-dependent Schrödinger equation.

In classical mechanics, all quantities about a particle are definite at the same time. In quantum mechanics, this is not the case; as we saw in the Heisenberg Uncertainty Principle, the more definite the position, the less definite the momentum, and vice versa. A similar thing occurs with energy and position. For all the situations we considered in this class, the wave functions with definite energy were spread out over many positions. That means that a wave function with more definite position will by necessity be a superposition of many energy eigenstates, and so its energy will be indefinite (when observed, many energies have non-zero probability).

In classical mechanics, since position and energy are both definite, energy conservation implies that if a particle starts with total energy $E$ and moves in a conservative potential energy $U$, it will never end up in a position where $U(x) > E$. In quantum mechanics, if we start a particle with definite total energy $E$, that implies that it is in an energy eigenstate. That eigenstate may have a non-zero probability density at a point where $U(x) > E$. So if we observe its position, we might see it at such a position. Conservation of energy gets saved through the measurement process; the only events that occur are the ones in which the total energy of the external world and the particle is conserved.

In this section, we will see that in quantum mechanics this means that the particle can pass through barriers that would not be passable in classical mechanics, which is called "tunneling." In quantum mechanics, there are no impassable barriers, but the probability of tunneling decreases exponentially with the height and width of the barrier and the mass of the particle.

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 this section, we will just provide you with the energy eigenstates for a given potential, and discuss what they mean.

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

- Estimate the energy difference between the ground and first excited state of a double well as a function of the height and width, given the energy difference at a known height and width.

- Compute the rate of a particle tunneling between two wells

- Identify the 'forbidden zones,' in which a particle would never be found classically. Compute the wave function decay when the potential is constant, given the energy of the eigenstate.
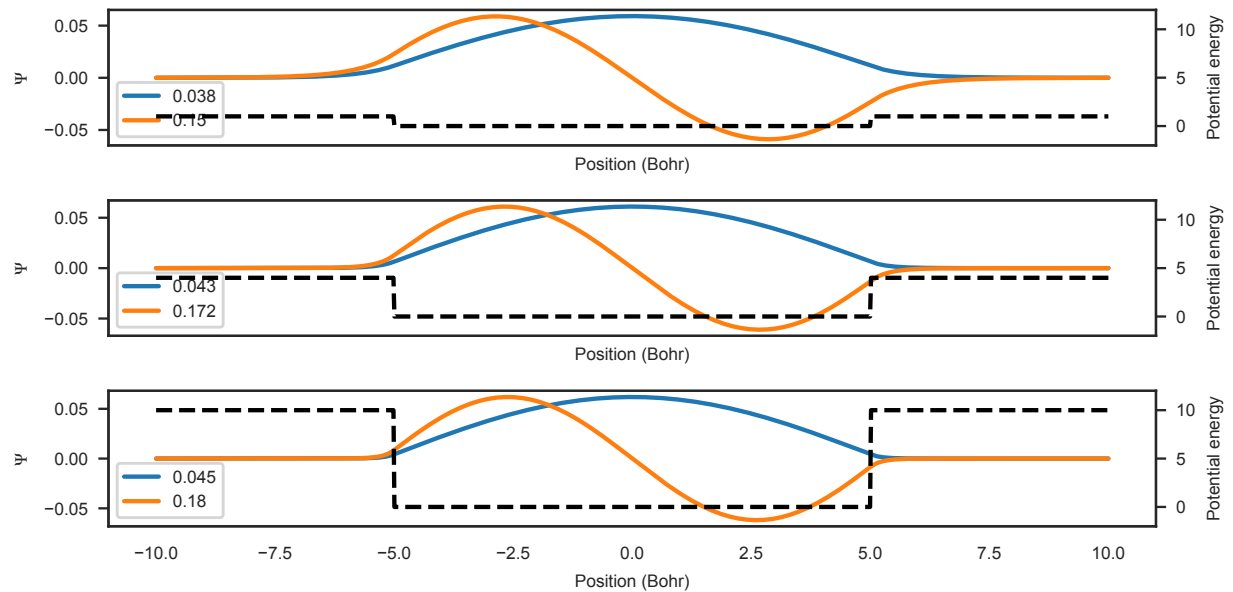
Figure 11.1: First two energy eigenstates for an electron in a finite well.

## 11.2 Finite square well

A finite square well is an approximate model of a quantum dot, which is a very small feature in a semiconductor, or a nanoparticle $\sim 1$ nm wide. Because of the interactions of an electron with the nuclei and other electrons in the dot, the electron has a slightly lower potential energy within the dot than outside it. Depending on the material, the attraction can be stronger or weaker. The finite square well can also be thought of as a model of the cross-section of a very narrow wire. In modern computing technology, the wires are only a few nm across, and surrounded by material that prevents the electron from escaping the wire.

Fig 11.1 shows the first two energy eigenstates for an electron in a finite square well as we change the depth, where we have used so-called atomic units, where energy is 27.2114 eV and position is 0.529 Å. This thus represents a quantum dot which is around 0.5 nm across.

You may notice that when the well is very deep, the solutions look quite similar to the infinite square well, with sinusoidal functions. As the well becomes more shallow, the probability for the particles to be found outside the well increases. Note that despite the way these are plotted, the energy of the eigenstates is still quite a bit smaller than the depth of the well, so classically these particles would never be found outside the well, but in quantum mechanics this is possible. The ground state energy also decreases as the well depth decreases.
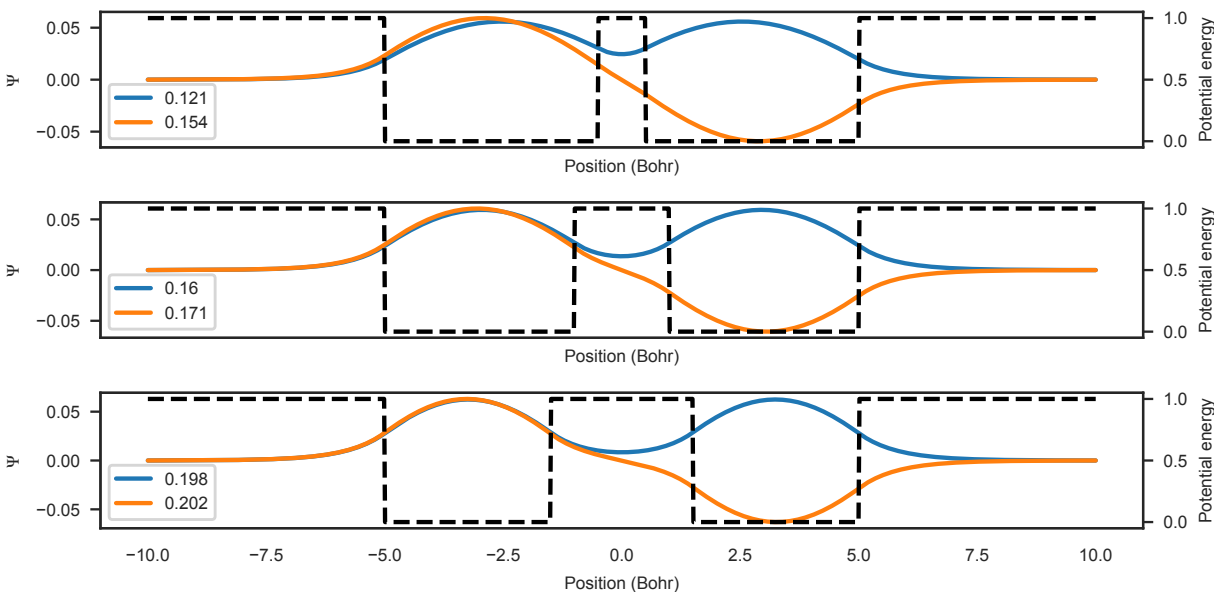
Figure 11.2:

## 11.3   Two wells

Things get particularly interesting if we now consider two wires or two dots that are very close to one another. This is diagrammed in Fig 11.2, where the lowest two energy eigenstates are again plotted. Even though the energy of the particle is below the energy of the well, the wave functions are non-zero even in the barrier, and connect in the middle. The larger the barrier, the less they connect and the closer they get in energy.

The difference between the first two energies will be important later. In general, there is an exponential dependence:

$$\Delta E = Ce^{-\kappa\sqrt{mV}L}, \tag{11.1}$$

where $V$ is the height of the barrier, $m$ is the mass of the particle, $L$ is the thickness of the barrier, and $C$ and $\kappa$ depend on specifics of the system, such as the exact shape of the barrier.

## 11.4   Example: Time dependence of a superposition of the ground and excited state of two wells

Since we now have the capability to explore dynamics in quantum mechanics, let's ask a dynamics question. Suppose the electron at $t = 0$ has a very high probability to be in the left well. One wave function that satisfies this initial condition is $\Psi = \frac{1}{\sqrt{2}}(\Psi_1 + \Psi_2)$. This occurs because $\Psi_1$ and $\Psi_2$ are both positive in the left hand well, so when we add the functions, they constructively interfere. In the right hand well, on the other hand, $\Psi_1$ is positive while $\Psi_2$ is negative, so they destructively interfere.
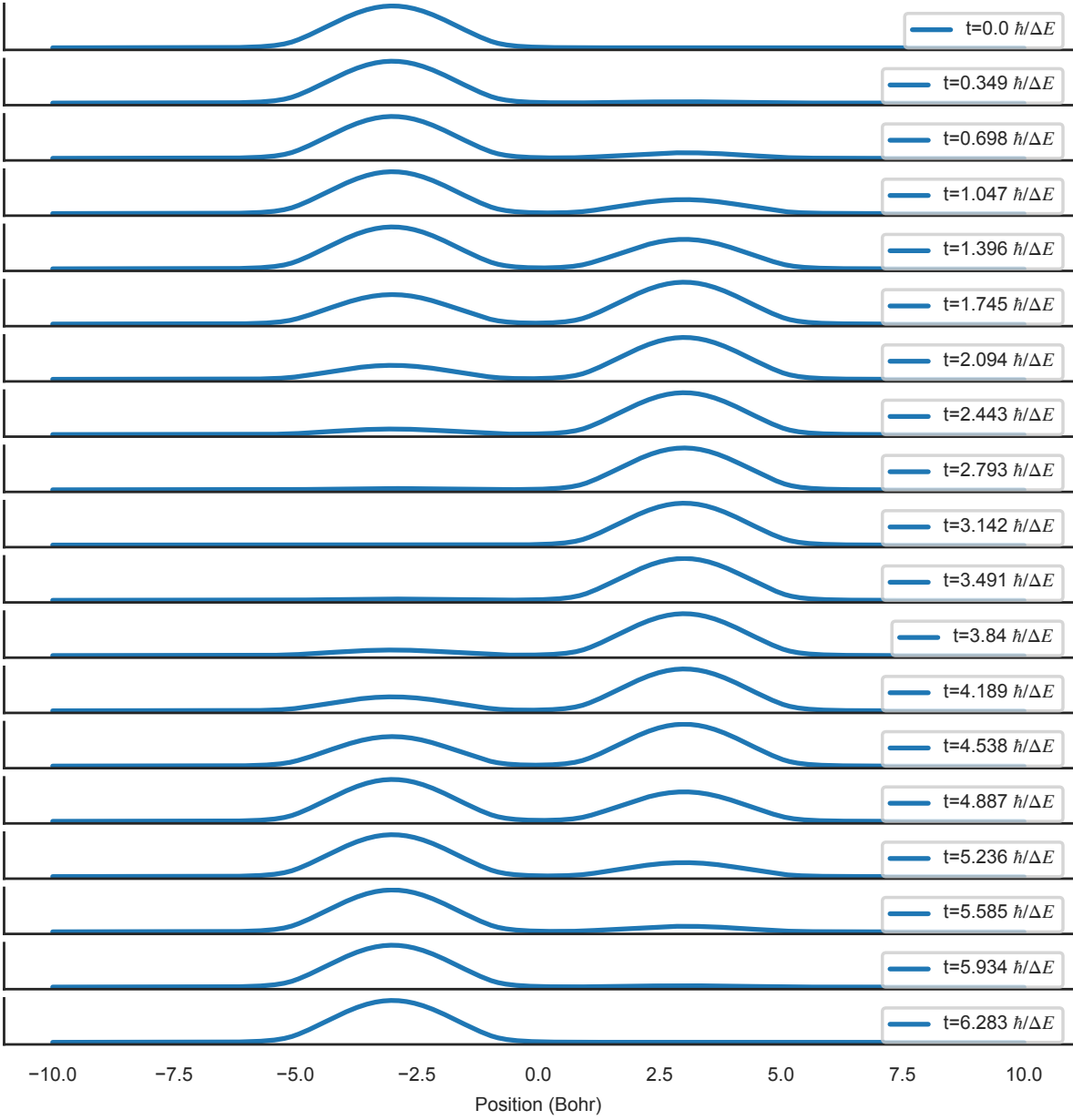
Figure 11.3: The time dependence of a particle that starts in one well of a double well potential.

The probability density of this superposition is given by the $t = 0$ line in Fig 11.3. The time dependence of the wave function is computed by

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left(e^{-iE_1t/\hbar}\Psi_1(x) + e^{-iE_2t/\hbar}\Psi_2(x)\right). \tag{11.2}$$

The probability density $|\Psi(x,t)|^2$ is plotted in Fig 11.3.

One can see that when $t = \pi\hbar/\Delta E$, where $\Delta E$ is the energy difference between the two energy eigenstate energies, the particle is very likely to be found in the second well. This happens despite the fact that the energy of the particle, were we to measure it, is much lower than the barrier between the wells. This *does not happen in classical mechanics*; if water is flowing in a channel, it does not suddenly hop out into an adjacent channel. However, for very small things, this can be a large effect.

## 11.5   Example: Rate of tunneling between wires

One of the limiting factors for modern computers is the tunneling between adjacent wires. One can roughly model this as two wells separated by a barrier. The electrons start in one wire, and occasionally will tunnel to the other one. The time it takes for an electron to tunnel across the barrier between wires is roughly $t = \pi\hbar/\Delta E$. So, if the wires are $L$ long, and there are $n_e$ electrons per unit distance in the wire, the current is

$$n_eL/t = n_eL\Delta E/\pi\hbar \tag{11.3}$$

electrons per second. This effect limits how small the circuit components can be in electronics; if there is too much leakage between wires, the circuits will not function correctly.

## 11.6   The wave function in the classically forbidden region

If we know the energy of an energy eigenstate, and if the potential energy is constant in the barrier, we can determine the form of the wave function in the classically forbidden region. The time independent Schrödinger equation in this region is

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V\Psi(x) = E\Psi(x) \tag{11.4}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} = (E - V)\Psi(x) \tag{11.5}$$

In the classically forbidden region, $E - V$ is negative. A guess wave function that works is $Ae^{-Kx}$. This is exponential instead of sinusoidal because of the negative right hand side of the equation. Taking two derivatives, we obtain

$$\frac{\hbar^2K^2}{2m} = V - E \tag{11.6}$$

$$K = \sqrt{\frac{2m(V - E)}{\hbar^2}}. \tag{11.7}$$

The decay constant is larger for larger mass particles, which means that these particles penetrate less into the classically forbidden zone. This is one reason why we don't see this behavior at human scales; the masses are large enough that it is very unlikely to find a macroscopic object in the classically forbidden region.

## 11.7 "Negative" kinetic energy (discussion)

It may be tempting to think that in the classically forbidden region, the particle has negative kinetic energy, since its potential energy is apparently higher than its total energy "in that region." However, this reasoning doesn't work in quantum mechanics; the kinetic energy is not defined at a given position; the momentum is determined by the expansion in momentum eigenstates, as we did in earlier units. Kinetic energy depends on the *entire* wave function. One has to specify what is being measured, and the wave function will give the probability of that measurement.

For example, suppose we wish to determine the outcome of a kinetic energy measurement on a particle in a finite well. Measuring kinetic energy means measuring momentum and then computing $p^2/2m$. To compute the probability of a given momentum, we must first expand the wave function in terms of momentum eigenstates:

$$\Psi(x) = \sum_k c_k e^{ikx} \tag{11.8}$$

where $k$ is the wave number. The probability of obtaining momentum $p = \hbar k$ is $|c_k|^2$. Suppose that we measure some momentum $p = \hbar k$. Then the wave function afterwards is $Ae^{ikx}$, where $A$ is some constant amplitude. That wave function is not confined to the well any more (it has probability of being anywhere), and will always have positive kinetic energy. We would then have to measure the position and would have a probability to measure it anywhere in space. If we try to measure position first, we would encounter a similar situation.

Energy is still conserved in the act of measurement. For example, one way we could measure the momentum of the electron is to have it absorb a photon of a given frequency (which has a known momentum) and then measure the momentum of the ejected electron by having it pass through a magnetic field and seeing how it curves. This method is called angle-resolved photoemission (ARPES), and is used in research labs. Since the collision is elastic, both total momentum and energy are conserved, as has been verified experimentally. We never end up with a total energy less than the energy of the electron plus the energy of the photon, unless something else took it.

# 12 Many electrons and band structure

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[1]. For concreteness, we will just talk about multiple electrons in this section, although the rules do apply to some other types of particles.

## 12.1 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

- Be able to determine whether a material is transparent from the energy levels and filling.

- Be able to determine whether a material is metallic from the energy levels and filling.

## 12.2 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.

## 12.3 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 12.1, we put four non-interacting electrons in a harmonic oscillator such that $\hbar\omega = 2$ eV. We mark the

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[1]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.
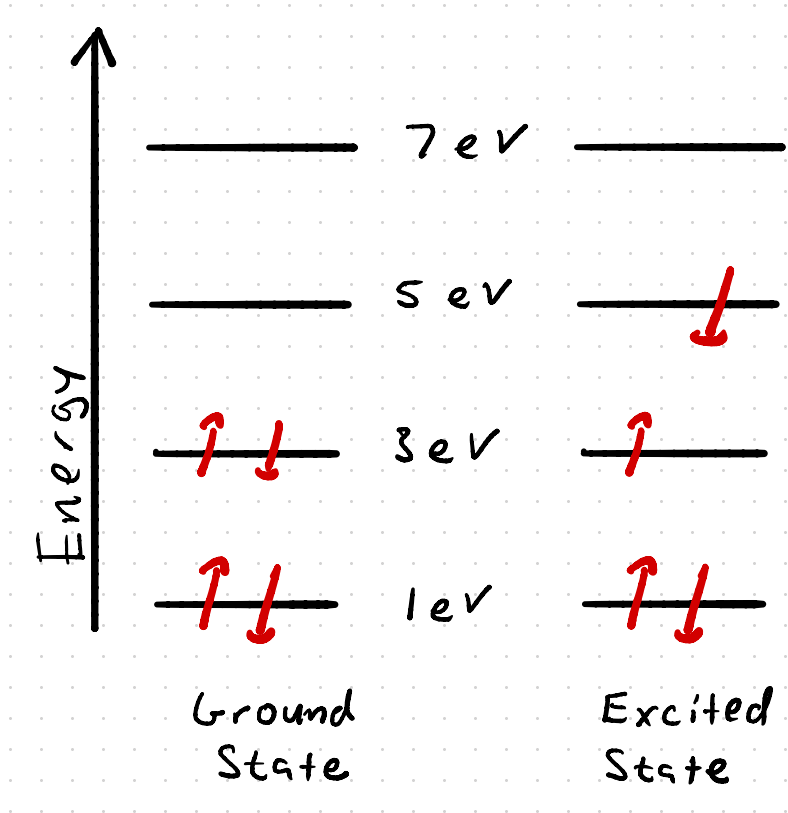
Figure 12.1: How to construct the ground and first excited state for four electrons in a harmonic oscillator.
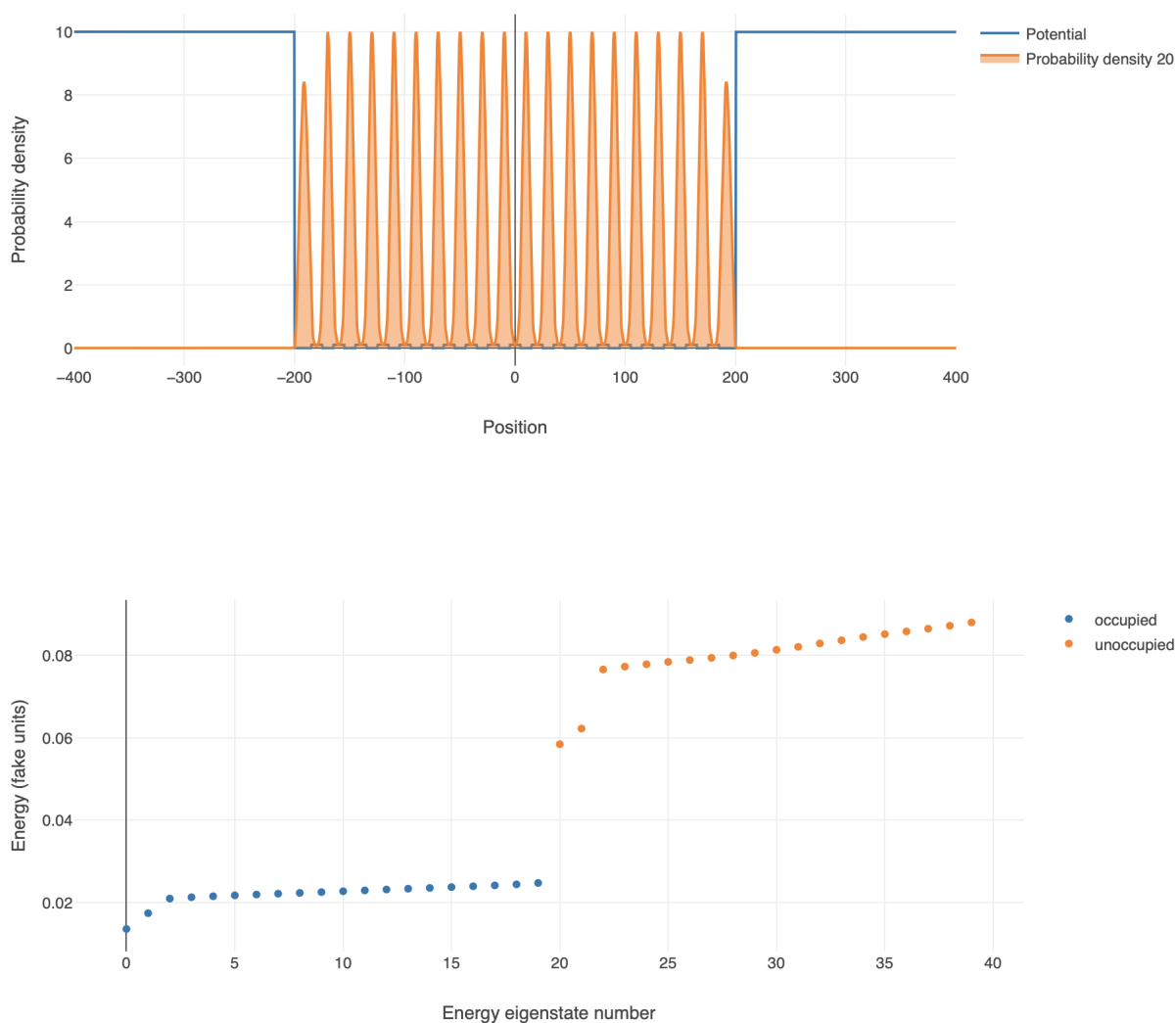
Figure 12.2: An approximation to a solid of 20 atoms, with 20 wells and 40 electrons

electrons with up and down arrows. The total energy of the ground state is $2 \cdot 1 + 2 \cdot 3 = 8$ 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 $2 \cdot 1 + 3 + 5 = 10$ 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.

## 12.4   Two wells, four wells, $\infty$ wells

We are going to use our coupled wells from Unit 11 to approximate solids. Consider the image in Fig 12.2. We have 20 wells and 40 electrons, so the first 20 states are occupied.

In the energy units used here, one can read off the graph that creating an excited state would require a little under 0.04 fake units. Suppose we removed two electrons from this system, so that the highest state is unoccupied. In that case, it would take only a very small amount of energy to create an excited state. We call the smallest energy that it takes to create an excited state the gap. In summary,

| Number of electrons | Gap |
|---|---|
| 20 | $\sim 0.04$ |
| 18 | $\sim 0.00$ |

The gap of a material determines what light it can absorb and emit, just like in the simpler cases we saw earlier in quantum mechanics. This is determined by what energy levels are available in the quantum system and how many electrons are present. While it may be difficult to determine the energy levels from first principles, once those are known either from experiment or calculation, once that is done, we can predict the interaction of matter with light using these levels.

Some examples:

- **Silicon dioxide glass**, which is used in windows, has a large gap of almost 9 eV for the electrons. The smallest wavelength we can see has photons of around 3.1 eV, so glass cannot absorb them.[2]

- **Aluminum** metal has zero gap, which means that it absorbs and emits light very well. It is so effective at this that it is used for mirrors.

- **Silicon** transistors have their gap modified by adding and removing *dopants*, such as boron and nitrogen, which have more or less electrons than the silicon atom. This is the effect that allows transistors to work.

## Metals, insulators, and semiconductors

The gap of materials also has to do with conductivity. One way of looking at this is that in order for a material to conduct electricity, it must be easy to add and remove electrons from the material.

To help visualize this, imagine two pieces of aluminum which are placed next to one another, and we would like to move an electron from one piece to another. This is an excited state, but the energy of that excited state is very close to the energy of the ground state, since there are many unoccupied and occupied states in the same energy range.

On the other hand, consider two pieces of glass (with a gap of 9 eV) next to one another. Removing an electron from one piece and adding it to another results in a state with energy around 9 eV higher than the ground state. That means that a fairly large barrier must be overcome for every electron that is to be moved. Glass therefore does not conduct electricity very well, unless a huge electric field is put on it, and is called an insulator.

Finally, let's consider silicon, which has a gap of only $\sim 1$ eV. The energy barrier to moving electrons is quite a bit smaller than in glass, but much larger than in aluminum.

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[2]Silicon dioxide glass does absorb in the infrared due to vibrations, but not due to the electrons.

It is small enough that temperature can push the electrons over the barrier and so silicon is called a semiconductor. When we apply an electric field some electrons move due to the temperature, but not nearly as many as metals.

## Physical constants

| | | |
|---|---|---|
| speed of light | $c$ | $2.998 \times 10^8$ m/s |
| Planck constant | $h$ | $6.626 \times 10^{-34}$ J s |
| | | $4.135 \times 10^{-15}$ eV s |
| | $\hbar$ | $1.054 \times 10^{-34}$ J s |
| | | $0.658 \times 10^{-15}$ eV s |
| electron volt | eV | $1.602 \times 10^{-19}$ J |
| electron charge | $e$ | $1.602 \times 10^{-19}$ C |
| Bohr radius | $a_0$ | $0.05292$ nm |
| electron mass | $m_e$ | $9.109 \times 10^{-31}$ kg |
| | | $0.511$ MeV/$c^2$ |
| proton mass | $m_p$ | $1.673 \times 10^{-27}$ kg |
| | | $938.3$ MeV/$c^2$ |
| neutron mass | $m_n$ | $1.675 \times 10^{-27}$ kg |
| | | $939.6$ MeV/$c^2$ |
| hydrogen mass | $m_H$ | $1.674 \times 10^{-27}$ kg |

## Waves

| Symbol | Name | SI units |
|---|---|---|
| $k$ | Wave number | m$^{-1}$ |
| $\lambda$ | Wavelength | m |
| $\omega$ | Angular frequency | rad/s |
| $\phi$ | Phase | radians |
| $T$ | Period | s |
| $f$ | Frequency | s$^{-1}$ |
| $I$ | Intensity | W/m$^2$ |
| $A$ | Amplitude | $\sqrt{\text{W/m}^2}$ |

$$f = \omega/2\pi = 1/T$$
$$k = 2\pi/\lambda$$
$$I_{avg} = \frac{|A|^2}{2}$$

## Trigonometric identities

$$\cos\alpha + \cos\beta = 2\cos\left(\frac{\alpha-\beta}{2}\right)\cos\left(\frac{\alpha+\beta}{2}\right)$$
$$\cos^2\alpha + \sin^2\alpha = 1$$
$$A^2 + B^2 + 2AB\cos\phi = C^2$$

Intensity of superposition of two waves of equal magnitude

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

## Diffraction

$$a\sin\theta_0 = \lambda$$
$$D\sin\theta_0 = 1.22\lambda$$

## Complex numbers

$$i = \sqrt{-1}$$
$$e^{i\theta} = \cos(\theta) + i\sin(\theta)$$
$$z = x + iy$$
$$z^* = x - iy$$
$$|z|^2 = zz^* = x^2 + y^2$$

## Photons

$$p = \hbar k = h/\lambda$$
$$E = hf = \hbar\omega$$

# Wave functions

$$\rho(x,t) = \Psi(x,t)\Psi^*(x,t)$$

$$P(a < x < b) = \int_a^b \rho(x,t)dx$$

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

Measurement rule

$$\Psi = a\Psi_1 + b\Psi_2$$

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

# Quantum matter

Wave function of momentum $p$

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

$$p = \hbar k$$

Heisenberg Uncertainty Principle

$$\Delta x \Delta p \geq \hbar/2$$

# Schrödinger equation

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

Infinite square well eigenstates

$$\Psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L}) & \text{if } 0 < x < L \\ 0 & \text{otherwise,} \end{cases}$$

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

# Harmonic oscillator

Ground state

$$\Psi_0(x) = Ae^{-\alpha x^2}$$

$$\alpha = \frac{1}{2\hbar}\sqrt{mk}$$

$$E = \frac{\hbar^2 \alpha}{m} = \frac{\hbar}{2m}\sqrt{mk}$$

Spectrum

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, n = 0, 1, 2, \ldots$$

# Time dependent Schrödinger equation

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

Time dependence of energy eigenstates

$$\Psi(x,t) = e^{-i\omega_n t}\Psi_n(x)$$

$$E_n = \hbar\omega_n$$

# Double wells

$$\Delta E = Ce^{-\kappa\sqrt{mV}L},$$