

Quantum aspects of light and matter

Notes on Quantum Mechanics

<http://quantum.bu.edu/notes/QuantumMechanics/QuantumAspectsOfLightAndMatter.pdf>

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Near the end of his life Albert Einstein wrote, "All the fifty years of conscious brooding have brought me no closer to the answer to the question: What are light quanta? Of course today every rascal thinks he knows the answer, but he is deluding himself." We are today in the same state of "learned ignorance" with respect to light as was Einstein. Arthur Zajonc, "Light Reconsidered," Optics & Photonic News, October 2003

So, chemistry is about atoms, but atoms are too small to "see" directly. The reason is that our eyes are sensitive to the visible range of light, corresponding to wavelengths from 380 nm (deep violet) to 740 nm (dark red), but even the shortest of these wavelengths is much, much larger than atoms, which are about $1 \text{ \AA} = 10^{-8} \text{ cm} = 0.1 \text{ nm}$ across.

What to do? Our only option is to explore the structure of atoms indirectly, using a fortunate feature of atoms that they do *absorb and emit light at precisely defined wavelengths*. It turns out that atoms of each element in the periodic table have a characteristic pattern of interaction with light, and this pattern, called a spectrum, serves as a fingerprint to identify the atoms of the different elements.

The simplest example is the spectrum of atomic hydrogen. Here is the absorption spectrum of hydrogen atoms in the visible wavelength range.



Absorption spectrum of gaseous hydrogen atoms at high temperature. Wavelength increases from 380 nm on the left to 740 nm on the right

The dark lines mark those wavelengths of the light that hydrogen atoms absorb. In the visible region of the spectrum there are only four such absorption lines for hydrogen atoms. Other atoms typically absorb light at many, many more different wavelengths. Absorption spectra are typically seen in light emitted from stars as it passes through clouds of atoms. In the laboratory it is more typical to see emission spectra. Here is a representation of the emission spectrum of hydrogen atoms in the visible wavelength range.



Emission spectrum of gaseous hydrogen atoms at high temperature. Wavelength increases from 380 nm on the left to 740 nm on the right

A nice display of the emission spectrum of the Sun and the atomic absorption spectra of hydrogen, helium, mercury and uranium is at <http://quantum.bu.edu/images/atomSpectra.jpeg>.

To keep things as simple as possible, let's set as our goal trying to understand the hydrogen spectrum and what this understanding can teach us about the atom.

■ Properties of waves

The very first step in using the interaction of light with atoms to sort out what is going on inside atoms is to understand what light itself is. In simplest terms, light is paired electric and magnetic field that oscillate in unison perpendicular to the direction of travel of the light. The magnetic field has a negligible effect on atoms compared to the electric field and so we'll focus our attention on the oscillations of the electrical component of light. (Because of the simultaneous presence of oscillating electric and magnetic fields, light is also called *electromagnetic radiation*. Sometime, too, the term light is used to mean just the visible range of light. We will use light to mean electromagnetic radiation, independently of whether it is visible to our eyes.)

To do this, we begin by describing the *mathematics of waves*. A *wave* is the oscillatory variation of *some property* in time and in space. If we focus on a particular point in space, the value of the changing property—the height of the wave—is seen to oscillate about some average value. If instead we focus on a particular part of the wave, such as one of its crests—a point of maximum amplitude—the wave is seen to move through space.

Examples of waves are

Wave type	Changing quantity
water	height of water
sound	density of air
chemical	concentration
light	electric and magnetic fields

A review of sines and cosines: SOH-CAH-TOA

The trigonometric functions *sine*, *cosine*, and *tangent* are used in working with waves. Hopefully these are familiar to you from high school, but here is a brief review of these functions and their values.

The sine of the angle θ (the Greek letter "theta"), $\sin(\theta)$, subtended by a right triangle with hypotenuse H and side O opposite the angle θ is O/H . The cosine of the angle θ , $\cos(\theta)$, subtended by a right triangle with hypotenuse H and side A adjacent to the angle θ is A/H . The tangent of the angle θ , $\tan(\theta)$, subtended by a right triangle side O opposite the angle θ and side A adjacent to the angle θ is O/A .

Show that a consequence of these definitions is that the tangent of an angle is the ratio of its sine and cosine, $\tan(\theta) = \sin(\theta)/\cos(\theta)$.

The so-called "American Indian chief" mnemonic SOH-CAH-TOA incorporates these definitions: SOH means Sine is Opposite over Hypotenuse; CAH means Cosine is Adjacent over Hypotenuse; and TOA means Tangent is Opposite over Adjacent.

For angles greater than 90° , the following identities can be used to express the values of the trigonometric functions in terms of those for angles in the range $0 \leq \theta \leq 90^\circ$.

$$\sin(a \pm b) = \sin(a) \cos(b) \pm \cos(a) \sin(b)$$

$$\cos(a \pm b) = \cos(a) \cos(b) \mp \sin(a) \sin(b)$$

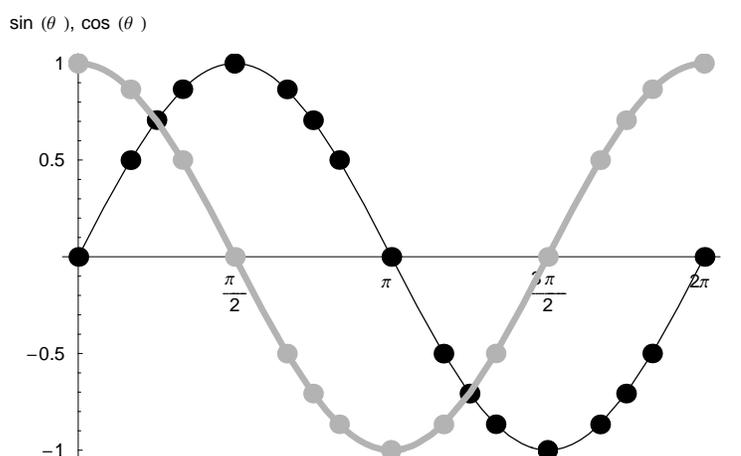
For example, at 45° the sides and hypotenuse of a right triangle are in the ratio $1/\sqrt{2} = 0.71$. This means $\sin(45^\circ) = \cos(45^\circ) = 1/\sqrt{2}$. Using the identities, we can evaluate the cosine of 135° to be

$$\begin{aligned}\cos(135^\circ) &= \cos(90^\circ + 45^\circ) \\ &= \cos(90^\circ)\cos(45^\circ) - \sin(90^\circ)\sin(45^\circ) \\ &= 0 \times 1/\sqrt{2} - 1 \times 1/\sqrt{2} \\ &= -1/\sqrt{2}\end{aligned}$$

Use the identities to show that $\sin(-45^\circ) = -1/\sqrt{2}$.

The two trigonometric identities are so useful that it is well worthwhile to memorize them.

Usually it is easiest to determine the values of sine and cosine of an angle with reference to plots of the sine and cosine and a few key values. Here are the plots, with key values marked.



Plot of the sine (black curve and points) and cosine (gray curve and points). The points on the curve are for angles 0 , $\pi/6 = 30^\circ$, $\pi/4 = 45^\circ$, $\pi/3 = 60^\circ$, $\pi/2 = 90^\circ$, etc.

Here is a table of the values of sine and cosine for key angles θ .

θ (degrees)	θ (radians)	$\sin(\theta)$	$\cos(\theta)$
0	0	0	1
30	$\pi/6$	$1/2$	$\sqrt{3}/2$
45	$\pi/4$	$1/\sqrt{2}$	$1/\sqrt{2}$
60	$\pi/3$	$\sqrt{3}/2$	$1/2$
90	$\pi/2$	1	0

Values of sine and cosine for key angles θ . Key decimal values are 0, 0.5, $1/\sqrt{2} = 0.71$, $\sqrt{3}/2 = 0.87$, and 1.

The decimal values for the key angles are 0, 0.5, $1/\sqrt{2} = 0.71$, $\sqrt{3}/2 = 0.87$, and 1. It is easy to memorize the values of sine and cosine—which you should do—since their values in the first quadrant, $0 \leq \theta \leq \pi/2$, determine the values in the other three quadrants in way that is easy to see using a sketch of the two functions. Once these values are memorized, determining the value of the sine or cosine of an angle is not hard at all.

| What is $\sin(405^\circ)$? Answer: $1/\sqrt{2} = 0.71$.

| What is $\tan(-45^\circ)$? Answer: -1 .

| What is $\sin(-30^\circ)$? Answer: $-1/2$.

| What is $\cos(-180^\circ)$? Answer: -1 .

Representing wave properties mathematically

Waves can be expressed mathematically in terms of sine or cosine curves. The value of the curve at a particular time and location represents the amplitude of the wave at that time and location. For example, to represent a sound wave with a sine curve, the value of the sine curve at a given time at each point in space corresponds to the pressure, relative to ambient pressure, at that time and location.

| What does a sine curve represent for a water wave?

| What does a sine curve represent for the electric field part of a light (electromagnetic) wave?

The most striking feature of waves is that they move through space (standing waves, which oscillate in place, are a special case). To keep things as simple as possible, let's assume we have a wave only along one direction, which we call x . If we look at a wave at a particular instant in time, it is a sine curve, say. If we look at it a moment Δt later in time, it is still a sine curve, but the whole curve has shifted by an amount Δx .

It is probably not immediately obvious, but the way such a sine wave changes with position and time can be expressed as

$$\psi(x, t) = a \sin[2\pi(x/\lambda - \nu t)].$$

The numerical value of this expression—the value of the changing property, such as the height of the water in a water wave, or the electric field in light—is called the *amplitude* (often represented by the Greek letter ψ , pronounced "psi"). To understand this expression it is helpful to analyze separately how it changes as position and time change.

Let's consider first how a wave looks for one particular time; this is like studying a photograph of the wave. To fix time, let's set the time t equal to zero. The expression for the wave when $t = 0$ is

$$\psi(x, 0) = a \sin(2\pi x/\lambda).$$

As we have seen, the value of a sine function repeats every time its argument (which is called its *phase*) changes by 2π . The phase changes because x changes. Let's see how much the phase changes if x changes by the amount λ ,

$$2\pi(x + \lambda)/\lambda - 2\pi x/\lambda = 2\pi.$$

We see that the phase changes by 2π when the position changes by the amount λ . For this reason, then length λ is called the *wavelength* (represented by the Greek letter λ , "lambda"). In a graph of the wave, the wavelength is the distance between two adjacent similar features of the wave, such as two successive crests.

Make a sketch, on the same set of axes, of the wave $\psi_1 = \sin(2\pi x/3)$ and $\psi_2 = \sin(2\pi x/6)$. Does your sketch make sense in terms of the relative wavelength of the two waves?

Now that we know how to identify the length of a wave, let's see the effect of changing time. The way to understand the effect of time is to see how the wave changes at a fixed point in space. We can do this by setting the position x equal to zero. The expression for the wave when $x = 0$ is

$$\psi(0, t) = a \sin(-2\pi \nu t).$$

Let's see how much the phase changes if t changes by the amount $1/\nu$.

$$-2\pi \nu \left(t + \frac{1}{\nu} \right) - (-2\pi \nu t) = -2\pi \nu t - 2\pi \nu / \nu + 2\pi \nu t = -2\pi.$$

This expression shows that when time changes by the amount $1/\nu$, the phase changes by -2π . That is, one wave cycle moves past a fixed point in time $1/\nu$. (We'll see below that the significance of the phase changing by a negative amount is the direction of travel of the wave.) The number of cycles (of spatial length λ) which pass by a fixed point per second is the reciprocal of the time required for one cycle to pass by. This is called the *frequency*,

$$\nu = 1/(1/\nu),$$

of the wave (represented by the Greek letter ν , "nu"—not to be confused with the Latin letter ν , "vee"). The frequency is commonly measured in *Hertz* (abbreviated Hz), which are inverse seconds, s^{-1} .

The speed of a wave: phase velocity

Now that we understand the separate effects of changing location and time, we can see the combined effect of changing both x and t . In this way we can study the movement of the wave.

The way we follow the motion of a wave is to identify a unique point on the wave, say a particular crest, and then to see how far it moves in a certain time. Mathematically, choosing a point on the wave means choosing a particular numerical value for the phase,

$$2\pi(x/\lambda - \nu t).$$

This is so because the value of the phase determines the value of the amplitude of the wave at a particular place x and time t .

Then, the key idea is that we can analyze the motion of a wave by realizing that the phase of our chosen point on the wave *must remain constant*, for otherwise amplitude of the wave would change. This means that if a point on the wave at position x_1 at time t_1 moves to the position x_2 at time t_2 , then the corresponding phases are equal

$$2\pi(x_1/\lambda - \nu t_1) = 2\pi(x_2/\lambda - \nu t_2).$$

This important equality is called the *stationary phase condition*. We can rearrange the stationary phase condition into the relation

$$(x_2 - x_1)/(t_2 - t_1) = \nu \lambda.$$

The left hand side of this equality is the ratio of the distance moved,

$$\Delta x = x_2 - x_1,$$

divided by the time elapsed,

$$\Delta t = t_2 - t_1.$$

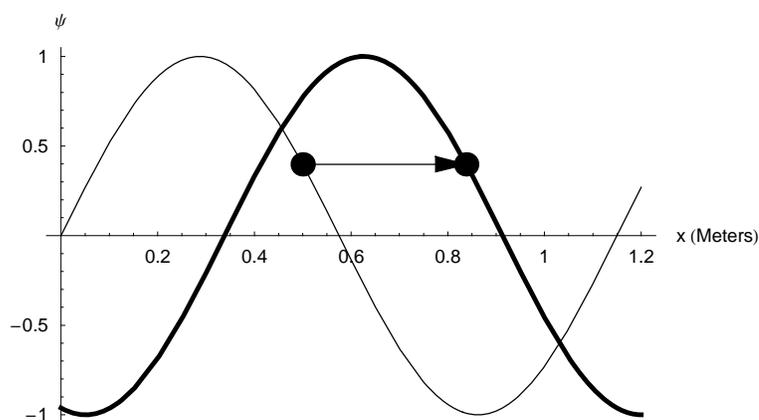
This is the *speed that the wave moves*. This speed,

$$u_\phi = \Delta x / \Delta t = v\lambda,$$

is called the *phase velocity* of the wave, where the subscript ϕ is the Greek letter "phi."

Write down an expression for a wave that travels to the left, towards smaller values of x , as time increases.

Here is an illustration of these ideas. The figure shows the movement of a sine wave that takes place in 0.025 s.



Movement of a wave. The thin curve is the wave at an initial time, t_1 . The thick curve is at a later time, t_2 . The length of the arrow is the distance, $\Delta x = x_2 - x_1$, the wave has moved in the elapsed time, $\Delta t = t_2 - t_1 = 0.025$ s. The point chosen to track the movement of the wave is arbitrary. The value of the phase, $2\pi(x_1/\lambda - \nu t_1)$, at the starting point is equal to the value of the phase, $2\pi(x_2/\lambda - \nu t_2)$, at the ending point. The equality of these phases—the stationary phase condition—determines the phase velocity of the wave, $\Delta x / \Delta t = (x_2 - x_1) / (t_2 - t_1) = v\lambda$.

Determine from the information in the figure the values of the distance traveled, wavelength, phase velocity, and frequency of this wave. You may want to start by using a ruler to measure the distance traveled. The answers are 0.34 m, 1.2 m, 12 m/s, and 10 Hz.

Calculations with waves

Phase velocity is a characteristic of each kind of wave. We are going to be concerned especially with light waves. The velocity of light is a *universal constant* of Nature and is given the special symbol c . For light traveling in a vacuum, its speed (phase velocity) by international agreement is exactly 299792458 m/s. (Note that assigning a value to the speed of light, together with a defined value for the meter, amounts to a choice of values for the second as the unit of time.)

This means that for *electromagnetic radiation of any frequency* the product of its frequency and wavelength is always equal to v_{light} . So, the next time someone asks you what's "nu", tell them "c over λ !"

A nice example of this relation is to calculate the wavelength of the radio waves from the Boston University FM radio station WBUR, which transmits on a frequency of 90.9 MHz (1 Megahertz = 10^6 Hz). Answer: $3.33 \text{ m} = 10.9 \text{ ft}$.

Compare this value to red light, which has a wavelength of $700 \text{ nm} = 7 \times 10^{-7} \text{ m}$ —ten million times smaller. This means that the frequency of red light is about ten million times higher, $\nu = 4 \times 10^{14} \text{ Hz}$.

Estimate the frequency of electromagnetic radiation with wavelength about the size of an atom. Answer: $3 \times 10^{18} \text{ Hz}$.

This corresponds to X-ray region of the electromagnetic spectrum, and in fact X-rays necessary to "see" the locations of individual atoms.

Here is an example using sound waves, Oxtoby and Nachtrieb, 2e, problem 13.7:

The speed of sound in dry air at 20°C is 340 m/s and the frequency of the sound from the middle C note on a piano is 262 Hz . Calculate the wavelength of the sound and the time it will take to travel 30 m across a concert hall. Answer: $\lambda = 1.3 \text{ m}$, $\Delta t = 0.088 \text{ s}$.

Angular frequency and angular wavenumber.

We have seen that the motion of a wave is determined by seeing how position and time need to change so that the phase

$$\phi = 2\pi(x/\lambda - \nu t)$$

remains constant—the stationary phase condition, and that the result is that a wave with this phase expression moves with phase velocity $u_\phi = \nu \lambda$. Another way to characterize the frequency and wavelength of a wave is in terms of *angular frequency* $\omega = 2\pi\nu$ and *angular wavenumber* $k = 2\pi/\lambda$. The reason these definitions are made is thereby the expression for the phase becomes

$$\phi = kx - \omega t.$$

Angular wavenumber has the units radian/meter, the increase in phase a result of a change in position by one meter; angular frequency has units radian/second, the increase in phase as a result of a change in time by one second.

The phase velocity in terms of these new quantities is $u_\phi = \omega/k$.

■ Interaction of light with matter: resonant "tugs"

The way light interacts with atoms is by exerting tugs on the positively charged nuclei and the negatively charged electrons. The tugs follow the rhythm of the oscillations in the electric field of the light. High frequency light tugs rapidly, low frequency light tugs slowly.

Here are what frequencies and wavelengths correspond to the different regions of the spectrum.

Spectral Region	Typical ν (Hz)	Typical λ (nm)
γ -ray	1×10^{19}	0.03
X-ray	1×10^{17}	3
UV	1×10^{15}	300
Violet	7.5×10^{14}	400
Blue	6.7×10^{14}	450
Green	6×10^{14}	500
Yellow	5×10^{14}	600
Red	4.3×10^{14}	700
IR	1×10^{14}	3000
Microwave	1×10^{10}	0.03 m = 1 in
FM radio	1×10^8	3 m
Short wave radio	1×10^7	30 m
AM radio	5×10^5	600 m
Long wave radio	10^4	30000 m = 20 mi

Frequencies and wavelengths correspond to the different regions of the electromagnetic spectrum.

Now, from the point of view of the charges in the atom, not all tugs are the same. In fact, most tugs have little effect on the electrons and nuclei. Rather, only if the tugs are at just the right frequency will the charges be able to follow them. Roughly speaking, the charges can follow tugs only if their frequency is near the *harmonic frequency*,

$$\nu \sim \frac{1}{2\pi} \sqrt{\frac{k}{m}},$$

where m is the mass of the charged particle experiencing the tug and the *force constant* k is a measure of how tightly the charged particle is held in the atom. This relation is called the *harmonic resonance condition*. Essentially, heavy particles (nuclei) oscillate at lower frequencies than light particles (electrons), and loosely held particles (electrons far from nuclei) oscillate at lower frequencies than tightly held particles (electrons close to nuclei).

One immediate insight we can draw from the harmonic frequency relation is that while electrons and nuclei experience comparable electrical forces (since they have charge of the same magnitude), and so have similar force constants, because nuclei are so much heavier, their resonant frequencies are much lower than those of electrons.

A proton is about 2000 times heavier than an electron. How much would this mass difference alter resonant frequencies? Answer: Frequencies due to motion of protons would be about 40 times lower than those of electrons.

Based on the answer to the last question, if electrons of a molecule absorb light in the green region of the spectrum, what region of the spectrum might you expect light to tug the nuclei of the molecule into (vibrational) motion?

We'll learn that nuclei are what is being tugged in microwave ovens, at frequencies on the order of 10^{12} Hz, whereas electrons are what are being tugged in the photoreceptor molecules of our eyes, at frequencies on the order of 10^{14} Hz.

■ Energy conservation in interaction between light and matter

A key concept in the interaction of electromagnetic radiation and matter is *energy conservation*: Energy is exchanged between the radiation and matter in such a way that the net change of energy is zero.

$$\Delta E_{\text{light}} + \Delta E_{\text{matter}} = 0 \text{ or, equivalently, } \Delta E_{\text{matter}} = -\Delta E_{\text{light}}.$$

Electrons and nuclei have mass, and so if light is tugging on them, the tugging takes energy—in the form of kinetic energy due to their motion and the potential energy due to moving away from equilibrium positions. This means energy in the light is reduced by the amount transferred to the matter. *Absorption* is the name we give for this reduction of energy of the light. When light (energy) is absorbed by matter, the energy conservation expression gives

$$\Delta E_{\text{light}} < 0, \Delta E_{\text{matter}} = -\Delta E_{\text{light}} > 0 \text{ (light absorption).}$$

The reverse process is also possible: motion of charged particles in matter can give up their energy by creating oscillating electric fields. (This is analogous to the energy required to light a bulb by turning the crank of a hand generator.) *Emission* is the name we give to this reduction (expenditure) of energy in matter to produce light. When light (energy) is emitted by matter, the energy conservation expression gives

$$\Delta E_{\text{light}} > 0, \Delta E_{\text{matter}} = -\Delta E_{\text{light}} < 0 \text{ (light emission).}$$

In either case—light absorption or emission—the total energy change is zero,

■ Amount of energy exchanged between light and matter

So, a key feature of light-matter interaction is the *exchange of energy*. A remarkable simplifying feature of this interaction is that, assuming the resonance condition between the frequency of light and matter is met, the amount of energy that can be exchanged is *determined solely by the frequency of the light*. That is, it turns out that if we know the frequency of the light—of the oscillations in its electric (and magnetic) field—then we can determine the amount of energy that can be exchanged with matter in resonance with the light at that frequency. Here is one way to do determine this energy.

Light emitting diodes (LED's) are electronic devices that emit light of a particular color when a precise voltage, known as the *threshold voltage*, is applied. Now, voltage is energy per unit charge, and 1 Volt = 1 Joule/Coulomb. Since the colors are due to electrons oscillating in the electric field of the light, it makes sense to use the electron charge to convert threshold voltage to an energy. We can do this by multiplying the voltage by the electron charge, $e = 1.60218 \times 10^{-19}$ Coulomb. The resulting energy is known as an electron volt, eV.

▮ Show that an electron volt is 1.60218×10^{-19} Joule.

In this way we can interpret the threshold voltage as an energy.

Here are the colors of five common LED's, displayed as an emission spectrum.



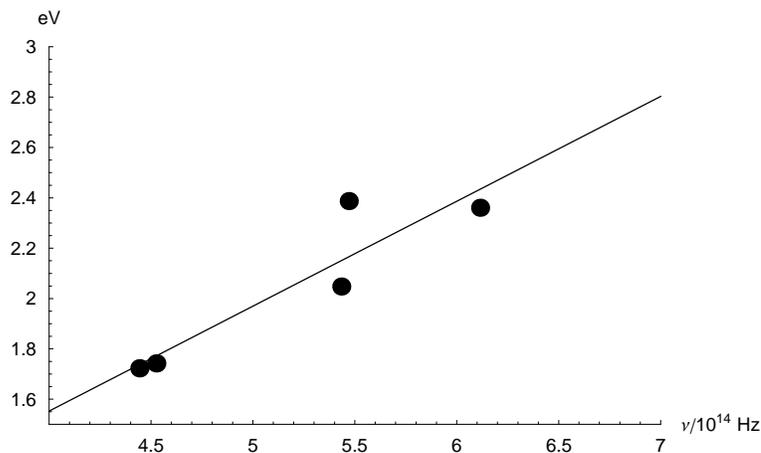
Colors of five different light emitting diodes (LED's). The horizontal axis is wavelength, increasing to the right.

Slight variations in manufacturing result in the color of a particular LED differing slightly from that of another. Typical manufacturing tolerances are ± 15 nm. Error is also introduced in the measurement of the wavelengths. Let's assume a total error in wavelength determination, due to manufacturing and measurement, of 10%. Finally, manufacturing differences and measurement error also affect the value of the threshold voltage. Let's assume a total error of 10% in the voltage determination.

Here is a table of representative wavelengths, λ , and corresponding frequencies, $\nu = c/\lambda$, for the five LED's, together with the minimum energy (in eV) determined to cause them to emit their color, taking into account a 10% error in wavelength determination and a 10% error in threshold voltage determination.

λ/nm	ν/Hz	V/eV
665	4.53×10^{14}	1.74
635	4.44×10^{14}	1.72
590	5.47×10^{14}	2.39
560	5.43×10^{14}	2.05
480	6.11×10^{14}	2.36

Here is a plot of the threshold voltage versus frequency, together with a straight line fit to the data points.



Threshold energy, in eV, versus frequency, in 10^{14} Hz, required to cause different LED's to emit light. Separate 10% errors are assumed in the determination of LED wavelength and in the determination of the threshold energy.

The plot shows that threshold energy is proportional to frequency, energy $\propto \nu$. The constant of proportionality is the slope of the line fitted to the measured points. It has the units energy/frequency, or J s. This proportionality constant is known as Planck's constant and written as h . Its value for the fit to the data shown is

$$6.6758 \times 10^{-34} \text{ Joule Second}$$

Confirm this value as follows. First, use a ruler to measure the slope of the line in the figure, in units $\text{eV}/[\nu/(10^{14} \text{ Hz})]$. Then, convert eV to Joule and use the fact that $\text{Hz} = \text{s}^{-1}$.

The currently accepted value is $h = 6.62606876 \times 10^{-34}$ J s. We could confirm this value, for example, by averaging results of repeated, more careful measurement using LED's manufactured to higher tolerance.

Calculate the percentage difference in the measured value from the actual value of Planck's constant. That is, evaluate $[(h_{\text{measured}} - h)/h] \times 100\%$. Typical percentage differences are 10%.

What we have succeeded in doing is to establish the *equivalence between the frequency and energy change of light*, namely

$$\Delta E_{\text{light}} = h\nu = hc/\lambda.$$

This relation is known as the *Einstein energy-frequency relation*, because Einstein was the first to propose the equivalence between the frequency of light and the amount of energy that light of that frequency can exchange with matter. The relation allows us to track energy flow between light and matter.

The energy unit $h\nu = hc/\lambda$ is called a *quantum of light energy*, or, more briefly, a *photon*. In terms of the energy of the photon, we can write the light-matter energy balance expressions as

$\Delta E_{\text{matter}} = -\Delta E_{\text{light}} = E_{\text{photon}} = h\nu \text{ (light absorption)}$
$\Delta E_{\text{matter}} = -\Delta E_{\text{light}} = -E_{\text{photon}} = -h\nu \text{ (light emission)}$

These expressions show that when light is absorbed by matter, a photon of light energy is removed from the light, reducing the energy of light by the amount $\Delta E_{\text{light}} = -E_{\text{photon}} = -h\nu$, and that when light is emitted by matter, a photon of light energy is added to the light, increasing the light energy by the amount $\Delta E_{\text{light}} = E_{\text{photon}} = h\nu$.

A fluorescent bulb emits light of several different wavelengths from each major region of the visible spectrum so that to our eyes its light appears white. Assume a 45 watt fluorescent bulb emits equal amounts of red, green and blue light. Assume that the blue wavelength is 450 nm. How many photons of blue light energy are emitted each second by the matter composing the fluorescent bulb. Recall that 1 watt = 1 J/s, and assume the bulb operates at 70% efficiency. Answer: $2 \times 10^{19}/\text{s}$.

The reason the number of quanta is so large is because a quantum of light is a very small unit of energy.

■ Photoelectric effect and photoionization

The idea that light exchanges energy with matter in indivisible "chunks" of size $h\nu$ was originally proposed by Einstein in 1905 to explain peculiar aspects of the *photoelectric effect* and *photoionization*. If the frequency of light is high enough, its electric field can tug on an electron in an atom so strongly that the electron is torn away from the atom. This phenomena when applied to the atoms of a metal surface is known as the *photoelectric effect*, and when it is applied to an isolated atom is known as *photoionization*.

To appreciate what is peculiar about the photoelectric effect and photoionization, let's consider, based on the wave properties of light, what we might expect to be the dependence of the ejection on the intensity and frequency of the light.

First, we might expect that no matter how low the frequency of the light, if it is intense (bright) enough, electrons will be ejected. What is observed is that if the frequency of the light is below a threshold value ν_0 , then *no electrons are ejected*, no matter how bright—no matter how intense—the light.

Second, no matter how high the frequency of the light, we might expect that if the light is not intense enough, then no electrons will be ejected. What is observed is that if the frequency of the light is above the threshold value, then *electrons are always ejected*, no matter how faint the light. Making the light weaker decreases the number of electrons ejected each second, but there are always some electrons being ejected, no matter how weak the light.

Finally, we might expect that, at a given frequency, the more intense the light, the faster the ejected electrons will be moving after they leave the metal.

It turns out that all three of these expectations are wrong. What is observed is that the kinetic energy of the ejected electrons, $m v^2 / 2$, is proportional to the amount $\nu - \nu_0$ by which the frequency of the light exceeds the threshold frequency.

These features of the photoelectric effect make no sense in terms of the wave picture of light. Einstein's proposal, which we can understand in retrospect based on our study of LED threshold voltages, is that the properties of the photoelectric effect do make sense in terms of the transfer of quanta of light energy to matter.

The minimum amount of energy needed to detach an electron can be used with the Einstein energy-frequency relation to define a *threshold energy*, and so a *threshold frequency*, ν_0 , of the light required for the detachment of the electron.

If the light has a frequency lower than the threshold frequency, $\nu < \nu_0$, then not enough energy will be available from the light—the light quanta will be too small—to detach the electron.

If the light has a frequency higher than the threshold frequency, $\nu > \nu_0$, then the remaining energy, $h \nu - h \nu_0$, of each light quantum goes into the kinetic energy of the detached electron, $\text{KE}_{\text{electron}}$. That is, if the frequency of the light is high enough so that its quanta have enough energy to detach the electron, then the energy conservation relation, $\Delta E_{\text{matter}} = -\Delta E_{\text{light}}$, can be written

$$\Delta E_{\text{matter}} = \Delta E_{\text{threshold}} + \text{KE}_{\text{electron}} = -\Delta E_{\text{light}},$$

since the energy of the light is expended in part to detach the electron, $\Delta E_{\text{threshold}} = h \nu_0$, and in part to give the electron its kinetic energy.

Einstein won the Nobel prize for this analysis of the photoelectric effect,

<http://www.nobel.se/physics/laureates/1921/einstein-bio.html>

Use the energy conservation relation to show that $\text{KE}_{\text{electron}} = h(\nu - \nu_0)$.

Different terminology is used depending in whether the electron is detached from a metal surface (photoelectric effect) or from an isolated atom (photoionization). In the photoelectric effect, the threshold energy, $\Delta E_{\text{threshold}} = h \nu_0$, is called the *work function* of the metal and it is written as the Greek letter Φ (capital "phi"). In photoionization, the threshold energy, $\Delta E_{\text{threshold}} = h \nu_0$, is called the *ionization energy* (or *ionization potential*) of the atom and it is written as *IE*.

The ionization energy of a hydrogen atom is 13.6 eV. Calculate the threshold frequency and wavelength needed to photoionize a hydrogen atom. Answer: 3.29×10^{15} Hz. To what region of the electromagnetic spectrum does this belong?

Assume a hydrogen atom is photoionized by light of frequency 1.0% greater than the hydrogen atom threshold frequency. Calculate the speed of the ejected electron, in m/s. Recall that kinetic energy is $m u^2 / 2$, where u is the speed of the electron. Answer: 219 km/s.

Assess whether your answer to the previous question is physically reasonable. For example, how long would it take an electron moving at that speed to cover the distance from Boston to Chicago? Answer: Using 1000 mi as the distance, the time to travel this distance is 7.35 s.

Electromagnetic radiation is found to eject electrons from isolated hydrogen atoms and the electrons are measure to have a speed of 0.1% of the speed of light. Calculate the wavelength of this radiation. Answer 90 nm.

Make a table of the lowest ionization energy of the hydrogen, lithium, sodium and potassium atoms. Compare the maximum possible speed of electrons ejected from these atoms by light of wavelength 205 nm. Answer: H will not be ionized; Li, 480 km/s; Na, 565 km/s; K, 775 km/s.

The work function of the chromium metal is $\Phi_{\text{Cr}} = 7.2 \times 10^{-19}$ Joule. What is the value of the work function in eV? Answer: 4.5 eV.

What is the maximum speed an electron could be moving if it is ejected from chromium metal by light of wavelength 250 nm? (Oxtoby and Nachtrieb, 2e, problem 13.13.). Answer: 405 km/s.

Here is a question for you. Can some photoelectrons have velocity less than the maximum velocity? If so, what could cause them to have a correspondingly lowered kinetic energy?

■ Particles of light

At about the same time that Einstein made his analysis of the photoelectric effect, he also proposed his *special theory of relativity*, based on the extraordinarily puzzling experimental finding in 1887 by Michelson and Morley that light always has the same speed, *independently of the speed of the source of the light*.

This does not seem to have much to do with the quantum nature of atoms and light, but a consequence of special relativity is the prediction that quanta of light also have momentum, and so in this sense behave like particles of matter. This was the first hint of what is now known as the *wave-particle duality*.

Michelson's paper, with Edward W. Morley, "On the Relative Motion of the Earth and the Luminiferous Ether," American Journal of Science (vol. 35, 1887, p. 333-45), is available at

<http://www.aip.org/history/gap/PDF/michelson.pdf>,

and a biography and further resources are available at

<http://www.aip.org/history/gap/Michelson/Michelson.html>.

Michelson was the first American scientist to win a Nobel Prize (1907),

<http://www.nobel.se/physics/laureates/1907/michelson-lecture.html>

Einstein developed his theory of special relativity in order to account for how it could be that light always has the same speed, whether the light source is moving or not. To see how strange this behavior of light is, let's imagine instead that we fire a bullet from a gun just as Superman flies by at the speed of the bullet (being Superman, he could go faster, of course!). Since Superman has matched his speed to that of the bullet, to him the speeding bullet appears to be standing still. Now, if instead of firing a bullet, we set off a flash bulb just as Superman flies by, Superman being Superman, he'll naturally speed up to catch the light. The most amazing thing, however, is that no matter how fast Superman goes, the light recedes from him at exactly the same speed as it recedes from us. From Superman's point of view of the light from the flash bulb, it as if he is standing still, no matter how fast he is going! For some reason, light seems to disobey the rules about the speed of a projectile being relative to its source!

Perhaps the finest introduction to these ideas is Edwin F. Taylor and John Archibald Wheeler, Spacetime Physics: Introduction to Special Relativity, 2nd edition (1992) W H Freeman & Co.; ISBN: 0716723271. The extension by Einstein to reference frames accelerating with respect to one another is called general relativity, and a very accessible treatment of the key consequences of general relativity is Edwin F. Taylor and John Archibald Wheeler, Exploring Black Holes: Introduction to General Relativity, 1st edition (2000), Benjamin/Cummings; ISBN: 020138423X

The essence of Einstein's theory to account for this very strange behavior of light is the following remarkable prediction: *time proceeds at different rates* in a stationary frame of reference (us) and a moving frame of reference (Superman) in just the right amount so that light is always measured to travel the same distance in a given time. There is much more to the story (a very nice exposition is *Space and time in the modern universe*, by P. C. W. Davies), and the incredible end result is Einstein's famous relation,

$$E = m c^2,$$

expressing the equivalences between mass and energy.

The first thing to appreciate about the mass-energy relation is that the mass, m , is not the ordinary mass of an object, which we denote as m_0 , but instead it is related to it as

$$m = m_0 / \sqrt{1 - \left(\frac{u}{c}\right)^2}.$$

where u is the speed of the particle.

Calculate the ratio, m/m_0 , as a result of a 3 gram bullet moving at 600 mph. It may be helpful to use logarithms to evaluate the ratio. Answer: 1.0000000000004.

Speeds encountered in everyday experience result in a negligible increase in mass.

Calculate the ratio, m/m_0 , as a result of a 5 gram bullet moving at 95% of the speed of light. Answer: 3.2.

For particle speeds close to the speed of light, the increase in mass becomes very significant. A crucial feature of the relation is that *the mass m becomes infinite as its speed v approaches the speed of light*.

Calculate the ratio, m/m_0 , as a result of a 2 gram bullet moving at the speed of light. Answer: ∞ !

A consequence of this mass relation is that it would require an infinite amount of energy to accelerate a mass to the speed of light. This is why anything with mass may only move *slower* than the speed of light.

On the other hand, since light itself *does* move at speed c , we must conclude that *the rest mass of light is 0!*

In the limit that the speed of a mass is very much smaller than the speed of light, then we can approximate the mass as

$$m = m_0 \left\{ 1 + \frac{1}{2} \left(\frac{u}{c} \right)^2 - \dots \right\}$$

and so approximate the energy of matter as

$$E_{\text{matter}} = m_0 c^2 + \frac{1}{2} m_0 u^2 - \dots$$

That is, the energy is just the ordinary kinetic energy, $m_0 u^2 / 2$, plus an additional so-called *rest mass energy*, $m_0 c^2$. All matter has such rest mass energy. (It is rest mass energy that is released in *nuclear fusion*, in which two masses combine to form a new mass smaller than their sum, with the difference released as energy.)

You may be surprised at how large you own rest mass energy is!

I weigh about 170 lb = 77 kg. Show that my rest mass energy is 6.9×10^{18} J!

This is a huge amount of energy, by everyday measures.

I am a rower and able to achieve maximum speeds in a one-person shell (called a single scull) a bit higher than 5 m/s. Show that my kinetic energy at 5 m/s is 1000 J.

Typically, kinetic energy is a negligible fraction of a particles rest mass energy.

It turns out that light also has a mass, and so energy, even though light has no rest mass. To see this, we need to rewrite the Einstein mass-energy equation in a form that makes clear the distinction between particles with a rest mass, and light, which has no rest mass. We do this by using the relation between m and m_0 , squaring both sides of Einstein's equation and then rearranging to get

$$E^2 \left\{ 1 - \left(\frac{u}{c} \right)^2 \right\} = m_0^2 c^4,$$

or

$$E^2 = m^2 c^2 u^2 + m_0^2 c^4.$$

We can simplify this expression a little by using the symbol p for the (relativistic) momentum $m u$ (not $m_0 u$), and then taking the square root. The result is

$$E = \sqrt{p^2 c^2 + m_0^2 c^4}.$$

Carry out the steps described to obtain this expression for the energy.

Now, since light has no rest mass, this expression when applied to light becomes

$$E = p c.$$

But what is this the energy of? Einstein's proposal was that this is not the total energy of light but the energy of just one photon of light energy. That is, Einstein said that

$$E_{\text{photon}} = p c.$$

Now the extraordinary thing about this proposal by Einstein is that it amounts to saying that a photon of light energy also has a momentum $p = E_{\text{photon}}/c$! Since we have already determined that the energy of a photon is $h \nu$, this means that the momentum of a photon is

$$p_{\text{photon}} = h \nu / c = h / \lambda.$$

The two relations, $E_{\text{photon}} = h \nu$ and $p_{\text{photon}} = h / \lambda$, taken together imply a profound expansion of our conception of how light interacts with matter. While many properties of light—the way it moves through space, how it is dispersed into colors in a prism, how it is focused by lenses, etc.—are well described in terms of waves of electric and magnetic fields, Einstein proposed that the interaction of light with matter has distinctly particle-like character of exchanging fixed amounts of energy and momentum with matter. That is, while exchanging fixed amounts of energy can be taken as just the way the oscillating fields that compose light tug on matter, proposing that a photon also has momentum suggests that in some sense light must interact with matter as one billiard ball does with another. And that is quite peculiar.

Since the momentum of light is $p_{\text{photon}} = m c$, we can interpret the mass of a quantum to be $m_{\text{photon}} = h / (c \lambda)$. Calculate the "mass" of a quantum of red light ($\lambda = 700 \text{ nm}$) and of x-ray light ($\lambda = 0.1 \text{ nm}$). Answer: $3 \times 10^{-36} \text{ kg}$, $2 \times 10^{-32} \text{ kg}$.

What wavelength light has a photon mass equal to the electron mass? Answer: 0.002 nm

It is important to understand that the relation $E = p c$ is true *only* for light, that is, only when the rest mass, m_0 , is zero. That is, it is *not* true for matter, for which the rest mass is *not* equal to zero, and the velocity is always less than c .

Measuring the momentum of light: Compton scattering

So peculiar was Einstein's proposal that quanta of light carry a fixed amount of momentum, it was not accepted as so until it was verified by direct measurement. The experiment was carried out in 1923 by A. H. Compton. Compton's idea was that if light had momentum, then when it's energy is transferred to an electron, its momentum should also be transferred.

What Compton measured was the momentum imparted to an electron initially at rest by the absorption of one photon. He found that the increase in the momentum was not equal to the momentum of the photon, but only a fraction of the momentum. However, he also measured that following the absorption of the light by the electron, light of longer wavelength was emitted by the electron (due to its motion).

The emission of light of longer wavelength suggested to Compton that the amount of momentum transferred to the electron may be a measure of the momentum difference between a photon of the incident and emitted light. It turns out that if he assumed, according to Einstein's proposal, that the momentum of the photons of the absorbed light was $h/\lambda_{\text{absorbed}}$ and that of the photons of the emitted light was $h/\lambda_{\text{emitted}}$, then the increase in wavelength, $\lambda_{\text{emitted}} - \lambda_{\text{absorbed}}$, that Compton measured accounted precisely for the momentum gained by the electron.

The gist of Compton's analysis is (1) that momentum of the absorbed photon is partitioned between the emitted photon and the electron (momentum conservation)

$$\vec{p}_{\text{photon,absorbed}} = \vec{p}_{\text{photon,emitted}} + \vec{p}_{\text{electron,scattered}}$$

(since the electron is assumed initially to be at rest, its momentum is zero and so not included on the left hand side of this equation), and (2) that the combined energy of the absorbed photon and the electron before the absorption (energy conservation),

$$m_{0,e} c^2 + h c / \lambda_{\text{absorbed}} = \sqrt{m_{0,e}^2 c^4 + p_{e,\text{scattered}}^2 c^2} + h c / \lambda_{\text{emitted}}$$

He then used these two relations to show that

$$\lambda_{\text{emitted}} - \lambda_{\text{absorbed}} = \frac{2h}{m_{0,e} c} \sin^2(\theta/2)$$

where θ is the angle at which the emitted photon is detected relative to the direction of the absorbed photon's light beam. The greater the angle, the greater the transfer of momentum to the electron and so the greater the increase of the wavelength of the light as a result of the interaction.

The quantity $h/(m_{0,e} c)$ is known as the Compton wavelength. Show that its value is 0.0024263 nm.

Calculate the wavelength difference between an absorbed photon and one emitted along direction 10° and along direction 90° . Answer: 0.0000368611 nm, 0.00242631 nm.

Do the relative values of these wavelength shifts make sense physically?

Details of Compton's calculation are at

<http://scienceworld.wolfram.com/physics/ComptonEffect.html>,

and you can explore the calculations interactively at

<http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/compdat.html#c1>.

Compton's paper is "A quantum theory of the scattering to X-rays by light elements," Phys. Rev. 21, 483–502 (1923),

<http://www.aip.org/history/gap/PDF/compton.pdf>.

In the paper Compton concludes that the "experimental support of the theory indicates very convincingly that a radiation quantum carries with it directed momentum as well as energy." A biography of Compton is available at

<http://www.aip.org/history/gap/Compton/Compton.html>.

In this way, the momentum of photon came to be accepted. And in this way Compton won his Nobel prize in 1927, <http://www.nobel.se/physics/laureates/1927/compton-bio.html>.

■ Waves of matter

OK, so according to Einstein's special relativity, as confirmed by the photoelectric effect and Compton scattering, evidently light interacts with matter by means of exchange of photons in such a way that both *energy and momentum* are transferred in amounts determined only by the frequency of the light,

$$\begin{aligned} E_{\text{photon}} &= h \nu_{\text{light}} \\ p_{\text{photon}} &= h / \lambda_{\text{light}} \end{aligned}$$

Einstein energy-frequency and momentum-wavelength relations.

(Note carefully that the wavelength and frequency are *not* those of the photon, but rather those of the light.)

In 1924 Louis de Broglie had the idea that perhaps these relations could be turned around,

$$\begin{aligned} \nu_{\text{matter}} &= E_{\text{matter}} / h \\ \lambda_{\text{matter}} &= h / p_{\text{matter}} \end{aligned}$$

de Broglie energy-frequency and momentum-wavelength relations.

and so interpreted as applying also to matter! Why on earth would someone have such an idea? The reason de Broglie made his proposal—at the time viewed as a bit crazy—was this: If wave properties could be associated with matter, this would provide an avenue to account for why it is that in the spectra of matter only certain wavelengths, and so energy exchanges occur.

Recall, for example, the visible portion of the emission spectrum of atomic hydrogen,



Visible portion of the emission spectrum of atomic hydrogen.

It shows that hydrogen atoms and light exchange only the following amounts of energy (in the visible range of light)

Line	λ	ΔE
1	656 . nm	1 . 89 eV
2	486 . nm	2 . 55 eV
3	434 . nm	2 . 86 eV
4	410 . nm	3 . 02 eV

Atomic hydrogen emission lines in the visible region of the spectrum.

Use the stated wavelengths to verify the stated energy change values.

de Broglie's idea was that maybe something inside matter is able to oscillate like a wave, and that the modes of oscillation somehow could account for energies at which light and matter interact.

For example, we know that a violin string, say, has a fundamental mode of vibration, with wavelength equal to twice the length of the string, but also harmonics with wavelengths equal to half the wavelength of the fundamental mode, one third the wavelength of the fundamental, and so on.

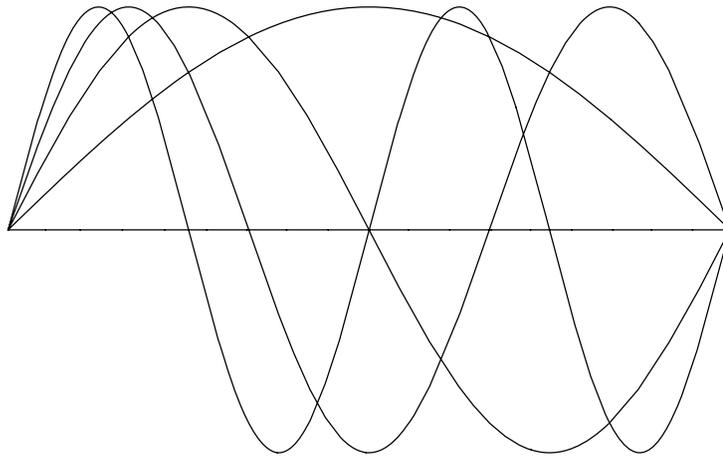


Illustration of the first four vibration modes of a violin string.

So de Broglie's hope was that by reversing the interpretation of the Einstein energy-frequency and momentum-wavelength relations, the appearance of only certain energies in matter could be understood as reflecting the appearance of only certain vibration modes.

As incredible as de Broglie's hypothesis that matter in some sense has an associated wavelength seems, it was soon confirmed experimentally. Davisson and Thomson showed, in separate experiments in 1927, that electrons passing through a crystal lattice of atoms in fact do diffract like waves, with wavelengths computed from their kinetic energy that agree precisely with those predicted by the de Broglie momentum-wavelength relation.

Details of the Davisson's experiment are at

<http://hyperphysics.phy-astr.gsu.edu/hbase/davger.html#c1>.

Davisson and Thomson shared the Nobel prize in 1936 for their work,

<http://www.nobel.se/physics/laureates/1937/index.html>.

An extraordinary side note is that Thomson's father, JJ Thomson had won the Nobel prize in 1906,

<http://www.nobel.se/physics/laureates/1906/thomson-bio.html>,

for showing that electrons behave like particles!

As a result the experimental verification of his hypothesis, de Broglie was awarded the Nobel prize in 1929 for his reinterpretation of the Einstein relations,

<http://www.nobel.se/physics/laureates/1929/broglie-bio.html>.

■ Electron in a box

The two de Broglie relations,

$$\begin{aligned} \nu_{\text{matter}} &= E_{\text{matter}}/h \\ \lambda_{\text{matter}} &= h/p_{\text{matter}} \end{aligned}$$

relate energy to frequency and momentum to wavelength. To explore the consequences of these relations, we need independent information about one of the two quantities in each relation.

If we assume we have a particle of mass m confined to a one-dimensional region of width L , and if we assume further that the particle is able to move freely in that region, then its energy is just the kinetic energy due to its motion,

$$E_{\text{matter}} = \frac{1}{2} m u_{\text{matter}}^2 = \frac{p_{\text{matter}}^2}{2m}.$$

If we assume further that the "matter wave" associated with the particle must vanish at each edge of the region, then this means an integer number of half-wavelengths must span the width of the box,

$$n \frac{\lambda_{\text{matter}}}{2} = L, \quad n = 1, 2, \dots$$

analogous to the violin string example above. These two relations, together with the two de Broglie relations are what we need to find those values of energy corresponding to each matter wave.

From the de Broglie relation, the momentum of the particle is restricted to those values corresponding to the possible matter wave wavelengths that can be accommodated in the box,

$$p_{\text{matter},n} = h / \lambda_{\text{matter},n} = \frac{h n}{2L}.$$

This means that the kinetic energy that a particle can have is proportional to the square of the number of half-wavelengths in the matter wave,

$$E_{\text{matter},n} = \frac{p_{\text{matter},n}^2}{2m} = \frac{h^2 n^2}{8mL^2}, \quad n = 1, 2, \dots$$

This last expression shows that the particle can have only certain energies. This seems to get us close to the goal of accounting for the property of matter to interact with light at only certain energies.

Absorption spectrum of an electron in a box

Now, the frequencies corresponding to the possible energies,

$$\nu_{\text{matter},n} = E_{\text{matter},n} / h = \frac{h n^2}{8mL^2}, \quad n = 1, 2, \dots,$$

do *not* agree with those that we would measure for a particle confined in a one dimensional box.

Here is an example. The frequency of lowest energy absorption line of an electron confined to a 1.00 nm region is 2.73×10^{14} Hz. But as the following question shows, this frequency does *not* agree with any of the frequencies of the matter waves of the electron.

Show that the frequencies of the first three matter waves, namely those for $n = 1, 2,$ and $3,$ matter wave of such an electron are 0.909×10^{14} Hz, 3.64×10^{14} Hz, and 8.18×10^{14} Hz

Energy balance in the spectra of an electron in a box

Actually, the previous question is a bit of a trap: Should the frequencies corresponding to the possible energies of an electron in a box agree with the absorption frequencies? The answer is No!

Here is why. Recall that the guiding principle of our analysis of the interaction of light with matter is conservation of energy. If the electron absorbs energy $h\nu$, then this means (1) the light has lost this amount of energy and so (2) the electron has gained this amount of energy,

$$\Delta E_{\text{matter}} = -\Delta E_{\text{light}} = E_{\text{photon}} = h\nu \text{ (light absorption).}$$

That is, to account for the absorption frequency we need to calculate the frequency corresponding to the *change in energy* of the electron,

$$\Delta E_{\text{matter}} = E_{\text{matter},n_f} - E_{\text{matter},n_i} = \frac{h^2}{8mL^2} (n_f^2 - n_i^2)$$

namely

$$\Delta E_{\text{matter}}/h = \frac{h}{8mL^2} (n_f^2 - n_i^2) = \nu_{\text{matter},n_f} - \nu_{\text{matter},n_i}$$

Show that the frequency of the frequency of lowest energy absorption line of an electron confined to a 1.00 nm one-dimensional region, 2.73×10^{14} Hz, is indeed equal to $\nu_{\text{matter},2} - \nu_{\text{matter},1}$.

It is crucial to understand that while de Broglie's relations allow us to associate a frequency and energy in matter, this de Broglie frequency does *not* correspond to any frequency seen in the spectrum of the matter. The frequencies we *do* see in spectra are *always* determined by the *energy change* in the matter, and so by *differences of de Broglie frequencies*.

Calculate the frequencies of the next two absorption lines of an electron confined to a 1.00 nm one-dimensional region. Answer: 7.27×10^{14} Hz, 1.36×10^{15} Hz.

Calculate the de Broglie frequencies of the $n = 3$ and $n = 4$ energies of the electron. Answer: 8.18×10^{14} Hz, 1.45×10^{15} Hz.

Show that the difference of the de Broglie frequencies of the $n = 3$ and $n = 4$ energies from the de Broglie frequency for the $n = 1$ energy is the frequencies of the next two absorption lines.

■ Taking stock

We can summarize everything we have learned so far as follows. The de Broglie relations,

$$\begin{aligned} \nu_{\text{matter}} &= E_{\text{matter}}/h \\ \lambda_{\text{matter}} &= h/p_{\text{matter}} \end{aligned}$$

de Broglie relations.

together with the fundamental energy-balance relations of the light-matter interaction,

$$\begin{aligned} E_{\text{matter},f} - E_{\text{matter},i} &= -\Delta E_{\text{light}} = E_{\text{photon}} = h\nu \text{ (light absorption)} \\ E_{\text{matter},f} - E_{\text{matter},i} &= -\Delta E_{\text{light}} = -E_{\text{photon}} = -h\nu \text{ (light emission)} \end{aligned}$$

Light-matter interaction energy balance.

account for the lines in the spectra of the matter.

However, there are three very significant and quite puzzling conceptual consequences of getting to this point. First, de Broglie's relations introduce the idea of a *matter wave*. But what on earth is it that is waving? Second, and following from the first, how can a particle, which we think of as something being in a particular region of space ("here, and not there"), be represented by a wave, which is by definition spread throughout space (else its wavelength—the distance from peak to peak—has no meaning). Third, we seem to have lost touch with the physical picture of light interacting with matter by means of electrical charge in matter oscillating in synchrony with the electric field of light. Is there a way to regain it?

Exploring these questions will profoundly deepen our understanding of the quantum aspects of matter. Be warned, however, the new ideas we are about explore will almost certainly pose many new questions in your mind. That's ok, though—that's the way science is!

■ What's waving in a matter wave?

The first step in answering this question is to see what the mathematical expression is for the matter wave. The first thing to try is to rewrite the general expression for a wave that we have discussed,

$$\psi(x, t) = a \sin[2\pi(x/\lambda - \nu t)].$$

using the de Broglie relations. The result is

$$\psi(x, t) = a \sin[2\pi(x/\lambda_{\text{matter}} - \nu_{\text{matter}} t)] = a \sin[(p_{\text{matter}} x - E_{\text{matter}} t)/\hbar],$$

where \hbar , pronounced "h bar," is the standard abbreviation for $h/(2\pi)$. We can interpret this expression as meaning that the matter wave is moving, with phase velocity

$$u_{\phi} = \nu_{\text{matter}} \lambda_{\text{matter}}.$$

For example, for a particle confined to a one-dimensional region of width L , in which it moves freely, the phase velocity is

$$u_{\phi} = \frac{h n}{4 m L}.$$

Use the expressions we have found for the energy and wavelength of such a particle to show that this expression for the phase velocity is correct.

Calculate the phase velocity of an electron confined to a one-dimensional 1.00 nm region when it has the lowest possible energy. Answer: 1.82×10^5 m/s.

It turns out that this form of the matter wave is not quite right. One of the requirements of the quantum description of matter that has a definite energy is that the time variation of its matter wave be

$$e^{-i E_{\text{matter}} t/\hbar} \text{ (time variation of matter wave with energy } E_{\text{matter}} \text{)}.$$

In this expression, e is the base of the natural logarithm, $i = \sqrt{-1}$ (and so $i^2 = -1$). The factor $e^{-i E_{\text{matter}} t/\hbar}$ is an example of what is known as a *complex exponential*. A general complex exponential $e^{i x}$ is a special combination of sine and cosine known as the *Euler relation*,

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

and so $e^{-i E_{\text{matter}} t/\hbar} = \cos(E_{\text{matter}} t/\hbar) - i \sin(E_{\text{matter}} t/\hbar)$.

|| Show that $e^{i\pi/2} = i$, $e^{i\pi} = -1$, $e^{i3\pi/2} = -i$, and $e^{i2\pi} = e^0 = 1$.

In terms of the exponential time dependence, the matter wave for a particle in a box with energy E_{matter} is

$$\psi(x, t) = a \sin(p_{\text{matter}} x) e^{-i E_{\text{matter}} t/\hbar}.$$

To emphasize the particular form of the time dependence in matter waves, let's write a general matter wave (in one dimension) as

$$\psi(x, t) = \psi(x) e^{-i E_{\text{matter}} t/\hbar},$$

with the understanding that $\psi(x)$, the spatial part of the matter wave, is different for different kinds of systems; for example, $\psi(x) = a \sin(p_{\text{matter}} x/\hbar)$. As we will now see, there are two very good reasons why time needs to appear in a matter wave of definite energy, E_{matter} , in terms of the complex exponential $e^{-i E_{\text{matter}} t/\hbar}$.

The first reason is that then matter in its lowest energy state will be stable, in the sense that it cannot drop to a still lower energy state by emission of light energy.

The second reason is that then interaction of light with charged particles makes them oscillate at frequencies determined by *differences* of de Broglie frequencies (and so, particle energies).

■ Born interpretation: What's waving is *probability amplitude*

It was Max Born who provided the answer that we use today. Born postulated that matter waves, or *wavefunctions* as they are more commonly known today, are oscillations of *probability amplitudes*. Probability amplitudes have physical meaning according to the following *recipe* (or rule):

The product of a wavefunction corresponding to time increasing (flowing forward) and the same wavefunction corresponding to time decreasing (flowing backward) is the *probability density* of the particle.

This is a real mouthful, so let's digest it a bit at a time.

The formulation of Born's recipe in terms of a time-symmetric prescription is due to John Cramer, Transactional interpretation of quantum mechanics, Reviews of Modern Physics, Volume 58, 1986, pages 647–687. A very nice, qualitative discussion of this interpretation is given in John Gribbin, Schrodinger's Kittens and the Search for Reality (Little Brown & Company, 1995, ISBN 0316328383), pages 223–247.

First, about probability density: The terminology probability density is used because in three dimensions, the product has the dimensions probability *per unit volume*. To know the *probability* of a particle being within a small volume dV centered at a particular point in space, we need to multiply the probability density there by the small enclosing volume.

If we are working in just one dimension, the probability density has the dimensions probability *per unit length*. To know the *probability* of a particle being within a small distance dx centered at a particular point in one dimension, we need to multiply the probability density there by the small enclosing length.

How would you use probability density to determine probability working in two dimensions?

It is because of this connection between the wavefunction and probability that wavefunctions are sometime referred to as probability *amplitudes*.

Second, about the direction of time: A neat device to change the direction of time in a wavefunction is to replace everywhere i by $-i$; this replacement is called *complex conjugation*, and a function $f(x, t)$ to which complex conjugation has been applied is written $f(x, t)^*$. So we can write the probability of a particle represented by a wavefunction $\psi(x, t)$ being within dx of a particular place, say x' , as

$$\psi(x', t)^* \psi(x', t) dx = \psi(x')^* e^{i E_{\text{matter}} t/\hbar} \psi(x') e^{-i E_{\text{matter}} t/\hbar} dx = \psi(x')^* \psi(x') dx = |\psi(x')|^2 dx.$$

Here we have introduced the standard notation $|f(x)|^2$ for the product of a function and its complex conjugate. The crucial feature of Born's recipe is that whenever the wavefunction has a definite energy, then probabilities computed from it *are independent of time*, since the complex exponentials cancel,

$$e^{i E_{\text{matter}} t/\hbar} e^{-i E_{\text{matter}} t/\hbar} = e^0 = 1.$$

For this reason, we say a particle with a well defined energy is in a *stationary state*, in that its probability density not change over time.

In three dimensions, the probability of the electron being within a volume $d\mathbf{r}$ centered at a particular place, say $\mathbf{r}' = (x', y', z')$, is

$$\psi(\mathbf{r}', t) \psi(\mathbf{r}', -t) d\mathbf{r} = \psi(\mathbf{r}', t) \psi(\mathbf{r}', t)^* d\mathbf{r} = |\psi(\mathbf{r}')|^2 d\mathbf{r}.$$

The probability of finding the particle within a larger region, say (for one dimension) between $x = a$ and $x = b$, is

$$\int_a^b |\psi(x)|^2 dx.$$

Since a particle must be found *somewhere*, the Born recipe requires that the probability of finding it anywhere at all must be one,

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

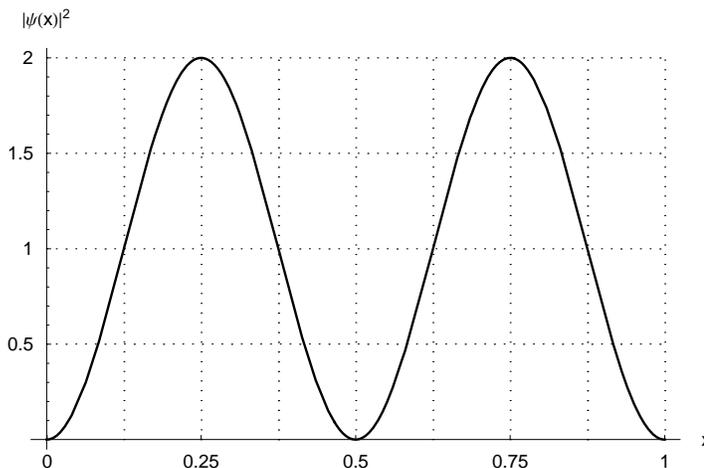
This relation is known as the *normalization condition* and wavefunctions that satisfy this condition are said to be *normalized*.

Calculating probability densities

To get familiar with calculating probabilities from wavefunctions, let's use as example a wavefunction of a particle confined in the region $0 \leq x \leq 1$,

$$\psi(x) = \sqrt{2} \sin(2\pi x).$$

Here is the corresponding probability density,



Probability density of a particle confined to the region $0 \leq x \leq 1$.

The essence of computing probabilities of a particle being within a region Δx of a particular place x_0 is to multiply the probability density at x_0 by the width of region, $|\psi(x_0)|^2 \Delta x$.

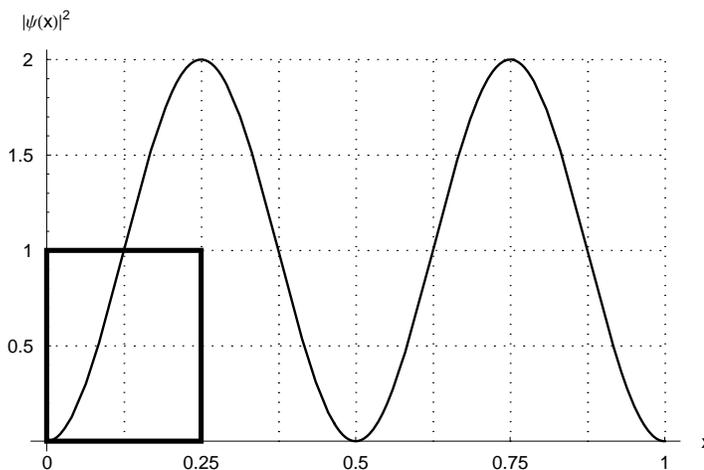
What is the probability of finding the particle within $\Delta x = 0.01$ of $x_0 = 0.25$? Answer: 0.02.

What is the probability of finding the particle within $\Delta x = 0.01$ of $x_0 = 0.125$? Answer: 0.01.

What is the probability of finding the particle within $\Delta x = 0.01$ of $x_0 = 0.50$? Answer: 0.

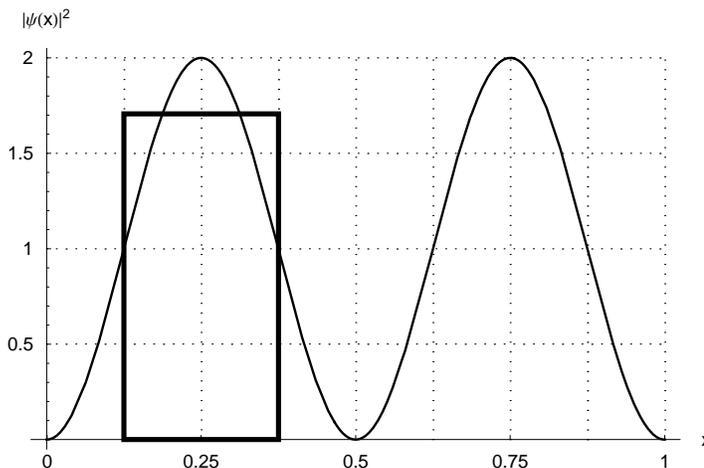
Computing probabilities using $|\psi(x_0)|^2 \Delta x$ assumes that $\psi(x)$ changes negligibly over the region Δx . If the region is so large that this is not the case, we can still easily approximate probabilities by using rectangular areas.

For example, we can estimate the probability of the particle being somewhere in the region $0 \leq x \leq 0.25$ by evaluating the area of the rectangle of width equal to $\Delta x = 0.25$ and height equal to the value of the probability density, $|\psi(x = 0.125)|^2 \approx 1$, evaluated at the midpoint of the region, $x = 0.125$. This is illustrated in the following figure.



The result is $|\psi(x = 0.125)|^2 \Delta x = 1 \times 0.25 = 0.25$.

Use the rectangle illustrated in the following figure to estimate the probability of finding the particle within $\Delta x = 0.25$ of $x_0 = 0.25$? Answer: 0.4.



Such estimates can be made as exact as we wish by spanning the region with increasing numbers of adjacent small rectangles. Of course, in the limit of infinitesimally narrow rectangles we have the result from calculus that the calculation reduces to an integral. For the example wavefunction here, the general expression for the probability of finding the particle somewhere in the region $a \leq x \leq b$ is

$$\int_a^b \psi(x)^2 dx = 2 \int_a^b \sin^2(2\pi x) dx = b - a + \frac{\sin(4\pi a) - \sin(4\pi b)}{4\pi}.$$

Using this expression, we can evaluate the exact value of the previous problem to be 0.41. In practice, however, we can make quite reasonable estimates by careful choice of a single rectangle, or at most just a few.

Use the calculus result given above to show that the probability of finding the particle somewhere between $x = 0$ and $x = 1$ is 1. That is, show that the wavefunction is normalized.

Use the result of the previous problem, but without using the calculus result quoted above and without using any rectangles, to show that the probability of the particle being in the region $0 \leq x \leq 1/2$ is exactly 1/2.

Are wavefunctions real?

It is crucial to understand that the Born recipe gives only *indirect* physical meaning to the wavefunction, as a means to compute probabilities. In particular, as far as we know today, the wavefunction itself does not appear to be directly accessible. Indeed, so far as I am aware we do not have any experimental evidence of the physical reality of wavefunctions; that is, wavefunctions are abstract quantities rather than physical objects, and so in this sense they may simply be calculational tools.

■ How does light make electrons jiggle?

The Born interpretation tells us how matter waves relate to physical reality. With this insight, let's return to the question of how interaction of light with charged particles makes them oscillate at frequencies determined by *differences* of de Broglie frequencies (and so, particle energies).

The key is to recall that light interacts with matter by causing its charged particles to oscillate in synchrony with the oscillation of the electric field of the light. So, we need to understand how light can make an electron jiggle.

Heisenberg's first paper on quantum mechanics addressed this question.

W. Heisenberg, "Quantum-theoretical re-interpretation of kinematic and mechanical relations," Z. Phys. 33 (1925) 879-893. A translation of this paper into English, and also of most of the other key works on the creation of quantum mechanics is in B. L. van der Waerden, "Sources of Quantum Mechanics," (Dover, 1968, ISBN 0-486-61881-1).

The challenge (and what Heisenberg set himself to) is to identify something in matter that (1) has the needed frequency of oscillation, proportional to a *difference* of atom energies, but (2) that at the same time does not lead to motion of charges in matter in the absence of light. The reason for requiring no motion of charges in the atom in the absence of light is that such motion would cause atoms to emit light when no light is present (which they do not) and quickly collapse (which they do not) due to the loss of energy to light. That is, the question is how to account for oscillation in the atom in the presence of light, but to have no oscillation—and so no radiative collapse—if no light is present?

Heisenberg won the Nobel prize for his answer.

Heisenberg knew he had to associate something with each possible energy value of the electron that, when connected to another energy value, would result in a frequency proportional to the *difference* of the energy values.

The essence of Heisenberg's approach amounts to the following three steps (Heisenberg did not lay them out separately, however). First is the idea we have already introduced, to associate with the spatial matter wave, $\psi_{\text{atom},j}(x)$, corresponding to each possible energy value, E_j , of the electron, the complex exponential $e^{-i2\pi E_{\text{atom},j}t/h} = e^{-i\omega_{\text{atom},j}t}$; that is, to express the matter wave of the j -th energy level as

$$\Psi_j(x, t) = \psi_j(x) e^{-i\omega_{\text{atom},j}t}.$$

Next, is the idea that the effect of the light on the atom was to produce a *mixture of two matter waves*, say,

$$\psi_j(x) e^{-i\omega_{\text{atom},j}t} + \psi_k(x) e^{-i\omega_{\text{atom},k}t}.$$

Finally, Heisenberg postulated that interaction with light results in a spatial distribution of electron charge given by Born recipe (which he anticipated), the product of the mixture of matter waves and their time reversed mixture, for the two energy levels,

$$\begin{aligned} & |\psi_j(x) e^{-i\omega_{\text{atom},j}t} + \psi_k(x) e^{-i\omega_{\text{atom},k}t}|^2 = \\ & \psi_j(x)^2 + \psi_k(x)^2 + 2\psi_j(x)\psi_k(x)\cos[(\omega_{\text{atom},k} - \omega_{\text{atom},j})t]. \end{aligned}$$

Here, for simplicity, we assume the spatial parts of the wavefunctions are real and so that complex conjugation is moot for them.

Show that this expression is correct, using the consequence of the Euler relation that $e^{ix} + e^{-ix} = 2\cos(x)$.

The key feature of this result is that the distribution of the electron probability density, and so the electron charge distribution, oscillates with the required frequency, given by the *difference of the de Broglie frequencies*.

Let's see how Heisenberg's approach works for an electron in a one-dimensional box and an electron in a hydrogen atom.

Example: Electron in a one-dimensional box

We know that for an electron in a one-dimensional box to interact with light, it must oscillate at the frequency of the light. The matter wave of such an electron with energy E_n is

$$\psi_n(x, t) = \sqrt{2/L} \sin(k_n x) e^{-i\omega_n t},$$

where the factor $\sqrt{2/L}$ insures the wavefunction is normalized.

If you have had calculus, you can confirm that the wavefunction is normalized by verifying that $\int_0^L [\sqrt{2/L} \sin(k_n x)]^2 dx = 1$.

Such an electron with fixed energy *cannot oscillate*, since its probability density is independent of time,

$$\psi_n(x, t)^* \psi_n(x, t) = (\sqrt{2/L} \sin(k_n x) e^{-i\omega_n t})^* (\sqrt{2/L} \sin(k_n x) e^{-i\omega_n t}) = \frac{2}{L} \sin^2(k_n x).$$

For there to be oscillation at a particular frequency, the matter wave of the electron must be a mixture of matter waves for different energies. The simplest such mixed matter wave is

$$\Psi(x, t) = \frac{1}{\sqrt{2}} \{\psi_1(x, t) + \psi_2(x, t)\} = \frac{1}{\sqrt{2}} \{\sin(k_1 x) e^{-i\omega_1 t} + \sin(k_2 x) e^{-i\omega_2 t}\},$$

where the factor $1/\sqrt{2}$ insures the mixture is normalized.

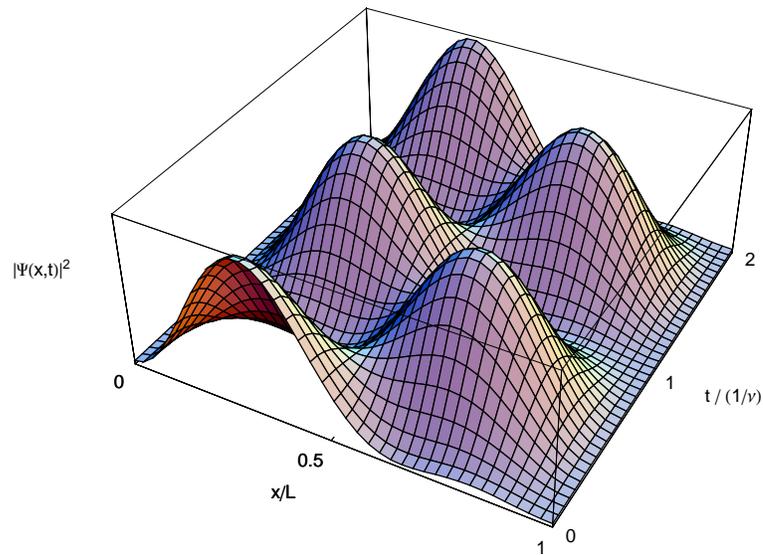
Show that if ψ_1 and ψ_2 are normalized, then this mixture of them is normalized.

The probability density corresponding to this mixed matter wave,

$$\Psi(x, t)^* \Psi(x, t) = \frac{1}{L} \{\sin^2(k_1 x) + \sin^2(k_2 x) + 2 \sin(k_1 x) \sin(k_2 x) \cos[(\omega_2 - \omega_1) t]\}$$

does oscillate, at frequency $\omega = \omega_2 - \omega_1$, just as required by the Einstein energy-frequency relation.

Here is a visualization of the oscillation of the probability density.

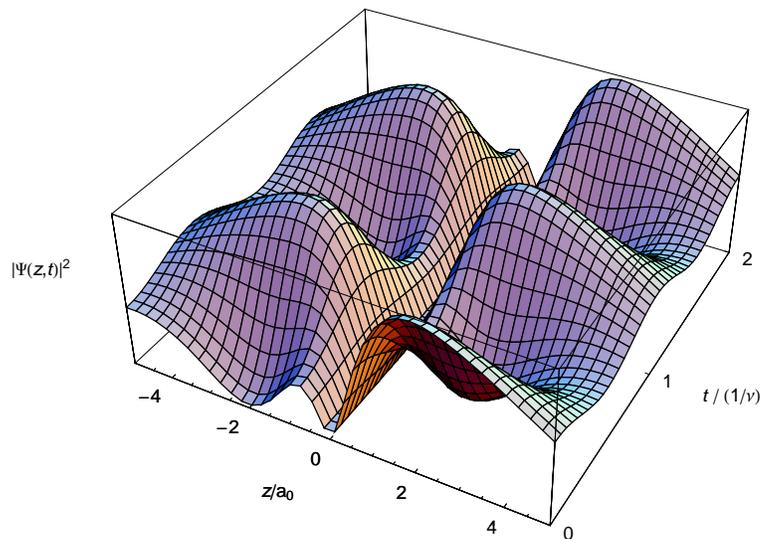


Probability density on an electron in a one-dimensional box of width L interacting with light of angular frequency ω equal to the difference in angular frequency of the lowest and next lowest energy of the electron in the box. This frequency corresponds to the fundamental absorption line of the electron in the box.

The figure shows two frequency cycles of time. In this time the electron probability density is seen to shift back and forth across the box twice, matching the oscillation of the electric field of the light of the same frequency.

Example: Electron in hydrogen atom

Here is a visualization of the analogous probability density oscillation corresponding to the hydrogen atom Lyman α ($n = 1 \rightarrow n = 2$) absorption.



Probability density on the electron in hydrogen atom interacting with light of angular frequency ω equal to the difference in angular frequency of the lowest ($n = 1$) and next lowest ($n = 2$) energy of the electron. This frequency corresponds to the Lyman α absorption line of atomic hydrogen. Oscillation is along the axis, z , of the electric field of the light. The hydrogen atom nucleus is at $z = 0$.

As before, the figure shows two frequency cycles of time. The electron probability density is seen to shift back and forth from one side of the nucleus (at $z = 0$) to the other twice, matching the oscillation of the electric field of the light of the same frequency.

■ Representing a "particle" with waves: wavepackets

At this point we know a little about what a matter wave—a wavefunction—is and how the combination of matter waves of two different energies account for the frequency of spectral lines being determined by *differences* of matter wave de Broglie frequencies.

What you may be wondering, however, is: How can a particle, which we think of as something being in a particular region of space ("here, and not there"), be represented by a wave, which is by definition spread throughout space (else its length—the distance from peak to peak—has no meaning)? That is, how can we reconcile our image of a particle as a localized object with our image of a wave as oscillating over an extended region?

A caution on the use of language:

*We will show now one way to reconcile the wave aspect of electrons with the image of an electron as being a localized object—a "particle." But at a more fundamental level, whether quantum objects appear as waves or particles has meaning **only** in terms of the kinds of measurements we make on them. That is, as far as anyone knows, the so-called wave-particle duality is an inescapable aspect of every quantum object.*

*This duality can trap us in a thicket of fantasy that can be avoided only by being careful to **not** to ascribe to quantum objects a **preexisting** particle or wave character, but instead to do so only in terms of the **behavior** exhibited in measurements we make upon them. That is, if in a measurement a quantum object appears as a particle, that does **not** mean that the object behaved as a particle **before** we measured it. In particular, quantum mechanics tells us **nothing** about what quantum objects are before we make measurements on them.*

For example, if you find yourself visualizing an electron, say, either as a particle or as a wave, then you are indulging in fantasy as far as quantum mechanics is concerned. Please keep this in mind when we speak of something as behaving as a wave or as a particle.

In particular, we are now going to see how to represent quantum objects as being localized in space. This is quite different than to say (incorrectly) that we are now going to see how to represent localized quantum objects, for quantum objects have no such characteristic except in terms of measurements made on them

We might agree that perhaps an electron does behave as a wave inside an atom. But surely it behaves as a particle as it traces out images on the insides of the cathode rays tubes of our televisions and CRT computer monitors. (Remember, as noted above, such language is unjustified by quantum mechanics, but seems reasonable to us because objects in our everyday world can be talked about as *either* waves or particles.)

In fact it *is* possible to reconcile a wave picture and a localized particle picture, by using the property of waves that they oscillate between *positive and negative values*, for this means waves can cancel each other out (*destructive interference*) or reinforce one another (*constructive interference*), depending on their relative wavelengths and phases. We can use wave interference to construct combinations of wavefunctions—a so-called *wavepacket*—that can have any degree of localization that we choose. Highly localized particles, in particular, are wavepackets composed of wavefunctions with so many different wavelengths that the wavefunctions interfere destructively everywhere except in a small region of space. This small region where the resulting probability amplitude is large is "where the particle is."

Wavepacket example

The equal mixture of $\psi_1(x, t)$ and $\psi_2(x, t)$ that we used to understand how light makes an electron jiggle is a simple example of a *wavepacket*—a combination of waves of different energies and so different wavelengths. That example illustrated two key aspects of all wavepackets. The first, which we have focused on earlier, is that, because they are composed of wavefunctions with different energies, wavepackets *move*. The second, which we investigate now, is that the wavepacket has a different shape than its parts, owing to wavefunction interference. It is this second aspect that allows us to tailor a wavepacket to be localized over a narrow region.

Remember, the key idea is that the more different wavelengths we combine in a wavepacket, the more localized is the resulting wavepacket and so probability density. We have already seen how mixing wavefunctions of different energies results in motion, so here we focus instead on the effect, for a given time, of the number of wavefunctions we add to the mixture.

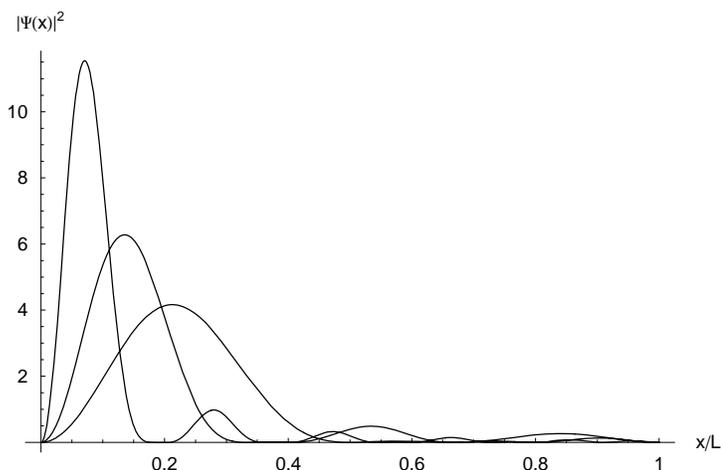
For convenience, let's set the value of time to be $t = 0$. Then a simple extension of the two-wavefunction mixture is a mixture

$$\Psi(x) = \frac{1}{\sqrt{N}} \{ \psi_1(x, 0) + \psi_2(x, 0) + \psi_3(x, 0) \dots + \psi_N(x, 0) \}$$

of N lowest energy wavefunctions $\psi_j(x, 0) = \sqrt{2/L} \sin(j \pi x / L)$ of a particle confined to the region $0 \leq x \leq L$ but free to move within that region. (The factor $1/\sqrt{N}$ makes the total probability computed from the wave packet equal to one.) For example, here is the wavepacket consisting of equal amounts of the three lowest-energy wavefunctions

$$\Psi(x) = \sqrt{\frac{2}{3}} \{ \sin(\pi x / L) + \sin(2 \pi x / L) + \sin(3 \pi x / L) \}.$$

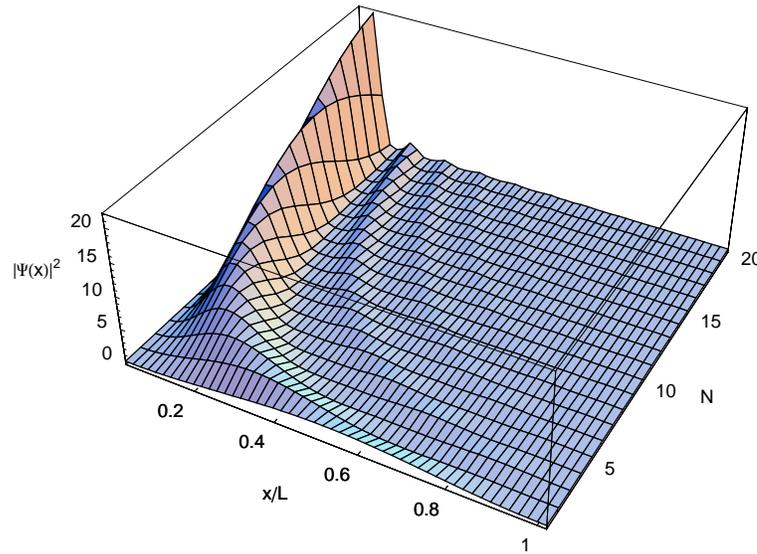
To illustrate the effect of increasing the number of different wavefunctions in the wavepacket, here are the probability densities corresponding to this wavepacket, and to the wavepackets consisting of equal amounts of the five and ten lowest-energy wavefunctions.



Probability density of wavepackets consisting of equal amounts of the three (lowest leftmost peak), five, and ten (highest leftmost peak) lowest-energy wavefunctions of a particle confined to the one dimensional region of $0 \leq x \leq L$.

We see that as the number of different wavelengths increases, the wavepacket becomes increasingly peaked and so localized near the left edge of the region.

We can illustrate the effect of the number of different wavefunctions in the wavepacket on its localization more strikingly with a surface plot of probability density versus number of wavefunctions.



Probability density of wavepackets consisting of equal amounts of the N lowest-energy wavefunctions of a particle confined to the one dimensional region of $0 \leq x \leq L$.

Heisenberg uncertainty principle

The surface shows that the peaks in the probability density becomes sharper and sharper as more and more different wavelength wavefunctions are combined. In the extreme, to represent a highly localized particle, very many different wavelengths need to be combined. But this in turns means, by the de Broglie relation, $p = h/\lambda$, that very many different momenta, p , need to be combined. That is, the price we pay to localize a particle to a within a small region is to lose knowledge of the momentum of the particle. That is, the uncertainty in where the particle is, δx , is inversely proportional to the uncertainty in the momentum, $\delta p = h/\delta\lambda$, of the particle.

The precise relation, known the *Heisenberg uncertainty principle*, is

$$\delta x \delta p \geq \frac{h}{2\pi}.$$

It means that there is a fundamental limitation on how precisely we can localize a particle. If we are very precise, then there is a very large uncertainty in the momentum (and so speed and direction) of the particle, so that a short time later we will not know where the particle will be. Conversely, if we specify the momentum of a particle very precisely, then its wavepacket will contain only a few different wavelengths and so be very spread out, so that we will not know where the particle is.

For these reasons, it is not meaningful to ask what is the de Broglie wavelength of a localized particle, for such a particle is composed of many different wavelengths. Similarly, it is not meaningful to ask where a particle is that has a precisely defined energy and so just a single de Broglie wavelength.

It is in this way that we see that wave and particle viewpoints a *mutually incompatible descriptions of reality* at the quantum level. This is the profound consequence of the wave nature of matter (and so also of the particle nature of light).

Root-mean-squared (rms) deviation

The quantities δx and δp that appear in Heisenberg's indeterminacy relation are *root-mean-squared* (rms) deviations. Here is how to compute an rms deviation: Take the square *root* of the *mean* (or average) of the *squared* deviations, where a deviation is the difference between a particular value and the mean of all of the values.

Here is an example to illustrate how this works. Say thirteen students took an exam, and the scores were

`scores = {78, 51, 43, 56, 63, 49, 61, 91, 33, 87, 44, 67, 59};`

out of a possible 100.

Confirm that the mean score is 60.2.

Here are the deviations from the mean and the squared deviations with the corresponding exam scores,

x	$\langle x \rangle - x$	$(\langle x \rangle - x)^2$
78.0	-17.8	318.5
51.0	9.2	83.8
43.0	17.2	294.3
56.0	4.2	17.3
63.0	-2.8	8.1
49.0	11.2	124.4
61.0	-0.8	0.7
91.0	-30.8	951.5
33.0	27.2	737.3
87.0	-26.8	720.7
44.0	16.2	260.9
67.0	-6.8	46.9
59.0	1.2	1.3

Verify the values in this table for exam score 63.0 and exam score 33.0.

Confirm that the mean of the squared deviations is 274.3 and so that the rms deviation is 16.6.

Alternative way to compute rms deviation

There is an equivalent way to compute the rms deviation, namely, as

$$\delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2},$$

where $\langle \dots \rangle$ denotes the mean of the enclosed quantity, that is, as the square root of difference between the mean of the squared scores and the square of the mean of the scores.

Show that this equivalence is correct in general.

Show that this equivalence is correct for the example above.

A particle's position is measured in four separate experiments, and the values obtained along the x axis were -0.4 , 1.1 , 0.3 , and 0.7 , all in meters. Calculate the rms deviation, δx , including units, of the particle position corresponding to this data.

The same particle's velocity is measured in four separate experiments, and the values obtained along the x axis were 1.3 , 0.9 , -1.6 , and 0.1 , all in meters per second. The mass of the particle is 1.00 kg. Calculate the rms deviation of the particle momentum, δp , including units, corresponding to this data.

Calculate the uncertainty product, $\delta x \delta p$, including units, of the particle.