

# Modern Physics Lecture Notes

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Prof. Emily Nardoni

*Department of Physics and Astronomy, Vassar College, 124 Raymond Avenue,  
Poughkeepsie, NY 12604 USA*

## Contents

<b>1</b>	<b>Part I: Special Relativity</b>	<b>3</b>
1.1	Towards Special Relativity: Galilean Relativity . . . . .	3
1.2	The Postulates of Special Relativity and their Consequences . . . . .	8
1.2.1	The Postulates . . . . .	8
1.2.2	Time Dilation: Moving Clocks Run Slow . . . . .	8
1.2.3	The Twin Paradox . . . . .	14
1.2.4	Length Contraction: Moving Rulers Contract . . . . .	15
1.2.5	Lorentz Transformations . . . . .	20
1.2.6	The Relativistic Doppler Shift . . . . .	27
1.2.7	Four-vectors and Spacetime . . . . .	30
1.3	Energy and Momentum in Special Relativity . . . . .	33
1.3.1	Relativistic Momentum . . . . .	33
1.3.2	Total Energy and Rest Mass in Special Relativity . . . . .	36
1.3.3	Relativistic Kinetic Energy . . . . .	37
1.3.4	Examples . . . . .	39
1.3.5	Beyond Special Relativity (not tested) . . . . .	42
<b>2</b>	<b>Part II: Wave-Particle Duality and Motivations for Quantum Physics</b>	<b>44</b>
2.1	The Quantum Theory of Light . . . . .	44
2.1.1	Blackbody Radiation . . . . .	44
2.1.2	The Photoelectric Effect . . . . .	52

2.1.3	Compton Scattering	55
2.2	The Particle Nature of Matter	58
2.2.1	Rutherford Scattering	58
2.2.2	Observations of Atomic Spectra	60
2.2.3	The Bohr Model of the Atom	61
2.3	The Wave Nature of Matter	67
2.3.1	de Broglie Matter Waves	67
2.3.2	What Waves in a Matter Wave?	71
2.3.3	The Uncertainty Principle & The Meaning of Observation	76
2.3.4	Matter Diffraction	79
<b>3</b>	<b>Part III: Quantum Mechanics</b>	<b>83</b>
3.1	Quantum Mechanics in 1d	83
3.1.1	Postulate: Associated to a Particle is a Wavefunction	83
3.1.2	The Schrödinger Equation: Time Evolution of the Wavefunction	88
3.1.3	Solving the Time-Independent Schrödinger Equation (TISE)	92
3.1.4	Particle in a Box	95
3.1.5	Particle in a Finite Potential Well	101
3.1.6	Superposition and Schrödinger's Cat	103
3.1.7	Quantum Harmonic Oscillator	104
3.1.8	Expectation Values of Quantum Operators	107
3.1.9	Tunneling and Reflection	112
3.2	Quantum Mechanics in 3d and Atomic Structure	113
3.2.1	The 3d Schrödinger Equation	113
3.2.2	Particle in a 3d Box	114
3.2.3	The Hydrogen Atom and the Radial Wave Equation	118
3.2.4	Angular Momentum in Hydrogen	125
3.2.5	Magnetic Dipole Moment	127
3.2.6	Spin	130
3.2.7	Pauli Exclusion and the Periodic Table	131
3.2.8	Lasers	134

# 1 Part I: Special Relativity

## 1.1 Towards Special Relativity: Galilean Relativity

Newton's classical laws of mechanics are very accurate for objects moving at not-too-fast speeds—a statement we'll make more precise later in this course. It turns out that Newton's laws obey *a* theory of relativity (known as *Galilean*, or, *Newtonian relativity*), but not Einstein's theory of special relativity. To formalize this concept, let us introduce the following frameworks for how we define our observations of physics.

**Events, Observers, and Frames of Reference:** A fundamental concept in physics is that of an *event*.

- *Event*: Something that happens somewhere at some time, specified by coordinates  $(t, x, y, z)$  in a reference frame (below). An event must have a well-defined position and a well-defined time. For example, things that are events: my watch strikes midnight; lightning strikes the tree in your backyard at 2pm EST; the start of this first PHYS 200 lecture.
- *Reference frame*: Of course, the *spacetime coordinates*  $(t, x, y, z)$  depend on what they are being measured against. A reference frame is a system for labeling the position of an event in space and time; it is defined by its choice of origin, which can be anywhere and at any time. Even though we have to specify coordinates in a particular frame, the reality of the event is independent of our labels or reference frame that we use to describe it. In particular, an important kind of reference frame is an **inertial reference frame**: a frame in which Newton's first law holds. In other words, an inertial frame of reference is one in which a body at rest remains at rest, and a body in motion moves at a constant speed in a straight line unless acted upon by an outside force. Frames moving at constant velocity with respect to an inertial system are also inertial systems. These are *non-accelerated* frames.
- *Observer*: frame of reference with a set of meter sticks and clocks with which to measure spatial coordinates and times of events—think of it as the person observing the event. These meter sticks and clocks should be compared and calibrated with other observers. Importantly, different observers will assign different space and time coordinates to the same event! Events occur independently of a given reference frame, and different observers may well describe them differently. We will see many examples of this below.

### Clicker Question: Inertial Reference frames

How many of the following are inertial reference frames?

- (a) A rocket burning its fuel.
- (b) A rocket in rotation (with no fuel burning).
- (c) A rocket with no rotation or fuel burning.

Answer: only one, (c). The third rocket has no external forces of any kind acting on it, meaning that it travels with a constant velocity. The first rocket has an external force acting on it from its fuel ejection, and is accelerating relative to our inertial frame. The second rocket exhibits a centrifugal force, and indeed Newton's first law is not upheld in this frame. (For example, suppose the nose of the rocket breaks off while I'm sitting in the cockpit of the rotating rocket. It would shoot (accelerate) away from me, due to this force.)

A consequence of this exercise is the fact that the surface of the Earth, where we do most of our physics, is *technically* not an inertial frame of reference. The Earth itself rotates about its axis, as well as around the sun. However, thankfully the accelerations due to both of these are quite small as experienced by an observer standing on the surface of the Earth, and so the Earth's surface is a fairly good approximate inertial reference frame.

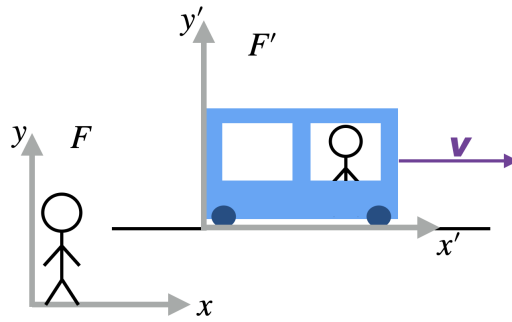


### Example Problem: An event

An observer is standing in their yard when a bee flying at a constant speed  $v$  passes by. As the bee passes immediately in front of the observer, the observer starts their timer. Denote this action as Event  $A$ . The observer then watches the bee traverse the length  $L$  of the yard in a straight line. Call Event  $B$  the moment the observer sees the bee fly past the edge of the yard, at which point they stop their timer. *Problem:* Label these events with spacetime coordinates in the reference frame of the observer.

*Solution:* We can choose the origin of spacetime to coincide with Event  $A$ , so that  $(t_A = 0, x_A = 0, y_A = 0, z_A = 0)$ . In the reference frame of the observer, the bee flies a distance  $L$  at a speed  $v$ , which therefore takes a time  $\Delta t = L/v$ , leading to  $t_B = L/v$ . We can choose the  $x$ -axis to coincide with the path of the bee, so that  $\Delta x = L$ , and  $\Delta y = \Delta z = 0$ . Then, we can label Event  $B$  as  $(t_B = L/v, x_B = L, y_B = 0, z_B = 0)$ . It would be equally correct to choose a different labeling, as long as it is consistent with  $\Delta t = L/v$ , and the total distance traversed by the bee being  $L$ .

Different observers can have different experiences of the same events. For example, an observer in frame  $F$  standing on a train platform says that a train moves by with speed  $v$  to the right. But an observer on the train would say that the train is at rest, and the person on the platform looks like they're moving to the left with velocity  $v$ .



As another example, say the passenger on the train has a ball that they throw up. Then, in their frame of reference the ball goes straight up and down. But an observer on the platform watching the ball's trajectory through the window of the train would say that the ball looks like it's moving in a parabola! If different observers can measure different coordinates for the same event, how can we possibly formulate laws of physics that all observers will agree on?

**The principle of Newtonian Relativity and Galilean transformations:** Even though things can look different in different frames of reference, the *principle of Newtonian/Galilean relativity* says that the laws of mechanics should take the *same* mathematical form in all inertial frames of reference. Put another way, physics should not depend on the physicist!<sup>1</sup> There is no one preferred frame of reference, but instead the laws of physics remain unchanged regardless of the frame.

Thus, we need a way to relate measurements made in one frame of reference with those in another—a “transformation” between frames. We call this a *Galilean transformation*. To do this, we'll start with the following “common sense” assumptions:

**“Common sense” assumption 1:** All meter sticks are the same length. In other words, length intervals are absolute and don't depend on the frame of reference.

**“Common sense” assumption 2:** All clocks tick at the same rate. In other words, time intervals are absolute and don't depend on the frame of reference.

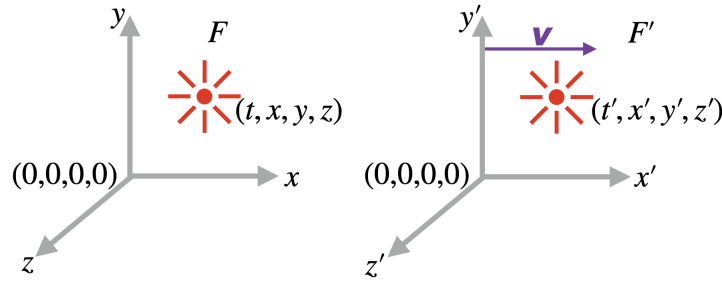
(*Note:* once we develop Einstein's theory of special relativity these “common sense” assumptions will not hold! In fact, most of the physics we'll discuss in this course does not follow common sense, so be wary of using your intuition to reason through problems.)

Based on these assumptions, we can ask how an observer on the train platform would describe an event differently from an observer on the train. For example, let's say a lightbulb flash occurs (an event!) at time  $t$  and at spatial coordinates  $x, y, z$  according to the person on the platform in frame  $F$ . *Question:* What are the coordinates of the flash according to an observer in frame  $F'$ ?

Let's say the clocks of both observers read zero as the spatial origins of  $F$  and  $F'$  coincide, i.e. at  $(x, y, z) = (x', y', z') = (0, 0, 0)$ , the clocks read  $t = t' = 0$ . For example, if we center the origin of the  $F$  coordinate system at the person standing on the platform (so they are standing at  $x = y = z = 0$  in their frame of reference), and center the origin of the  $F'$  coordinate system at the person sitting on the train (so they are sitting at  $x' = y' = z' = 0$  in the frame of reference in which they are stationary), then right as the train passes by the person on the

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<sup>1</sup>Quote by Anthony Zee, a theoretical physicist at UC Santa Barbara.



platform they both start their clocks at  $t = t' = 0$ . At coordinates  $(t, x, y, z)$  the platform observer sees the flash. But since in that time  $t$  the train has moved a distance  $vt$  to the right, in the primed coordinate system that is centered on the train, that observer sees the flash at position  $x' = x - vt$ . Since there is no relative motion between the frames in the  $y$  or  $z$  directions, the train observer would agree with those measurements in  $F$ ,  $y' = y$  and  $z' = z$ . From our assumption (2),  $t' = t$ . Thus in summary, the Galilean transformation of event coordinates between frames  $F$  and  $F'$  is

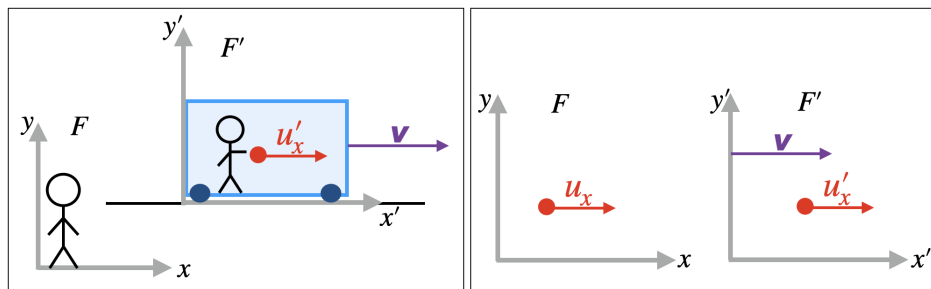
Galilean coordinate transformation:  $x' = x - vt$ ,  $y' = y$ ,  $z' = z$ ,  $t' = t$

 (1.1)

These rules say that components parallel to the direction of relative motion are measured to be different in different frames of reference, while components perpendicular to the direction of relative motion are unchanged. By our assumption (2), time is assumed to be absolute—Isaac Newton firmly believed that this must be the case, and formulated his theories of physics on it.

We can transform back and forth between observations in the two frames: solving for  $x = x' + vt$ , these rules can be inverted to tell us what an observer on the platform would see given what an observer on the train sees. The result is the same law as in (1.1), but with  $v \rightarrow -v$ , which is exactly what we expected: the observer on the platform would say that the train moved a distance  $vt$  to the right.

———End Lecture 1, Sec 02.



**Galilean Addition Law for Velocities:** Next we ask: if an observer in  $F'$  sees an object going by with velocity  $u'$  in the  $x'$ -direction, what velocity  $u$  does an observer in  $F$  see the object traveling at? In other words, if the person on the train throws a ball to the right with velocity  $u'$  according to their measurements, what velocity would the observer on the platform see that the ball has?

Using the Galilean transformation, we take the differential

$$dx' = dx - vdt, \quad dt' = dt \quad \Rightarrow \quad \frac{dx'}{dt'} = \frac{dx}{dt} - v$$

or put another way, since  $dx'/dt = u'$  and  $dx/dt = u$ ,

$$\boxed{\text{Galilean velocity transformation : } u = u' + v.} \quad (1.2)$$

The ball looks like it's moving faster than  $u'$  according to an observer on the platform. This makes perfect sense with general intuition—if the train is moving to the right and the ball is thrown to the right, the platform observer would see the ball moving even faster.

Taking another derivative,

$$\frac{du'}{dt'} = \frac{du}{dt} \Rightarrow a' = a. \quad (1.3)$$

The acceleration of the ball as measured in the primed frame is the same as the acceleration as measured in the unprimed frame. Let's make a third “common sense” assumption:

**“Common sense” assumption 3:** The mass of an object is independent of the reference frame in which it's measured.

Then, these results tell us that if the force on the ball in the  $x$  direction is  $F = ma$ , then

$$F' = m'a' = F = ma. \quad (1.4)$$

We've just shown that Newton's second law takes the same form in both inertial frames of reference—a necessary and encouraging self consistency check! Our result is that in Galilean relativity, **Newton's laws of mechanics remain the same in all (inertial) frames of reference**. A physics law that takes the same form in different frames is called *covariant*.

———End Lecture 1, Sec 01.

**Electromagnetism and Galilean relativity** *Question:* Are the laws of electromagnetism invariant under a Galilean transformation?

Recall from PHYS 114 that light is an electromagnetic wave, made up of propagating electric and magnetic fields, that travels at the speed

$$\boxed{c \equiv \frac{1}{\sqrt{\mu_0 \epsilon_0}} = 2.998 \times 10^8 \text{ m/s} \approx 3 \times 10^8 \text{ m/s}} \quad (1.5)$$

We review this fact in the supplementary document *Waves Refresher*, posted to Moodle. But we just said that velocities are relative in different inertial frames of reference—in which frame of reference does this hold true? Suppose that in one inertial frame an observer measures the speed of light to be  $c$ . By our Galilean velocity transformation, this would seem to imply that an observer in a frame  $F'$  that is moving with speed  $v$  to the first frame sees light moving at speed  $c + v$ . Therefore, **the speed of light is not invariant under a Galilean transformation**.

What do the experiments say? In 1887, Albert A. Michelson and Edward Morley devised an experiment to measure the speed of light, and demonstrated that the speed of light is *always*  $c = 2.998 \times 10^8 \text{ m/s}$  regardless of the inertial frame in which you do the experiment.<sup>2</sup> In fact, every experiment that has ever been done has found that the speed of light in vacuum is always

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<sup>2</sup>Michelson won the **1907 Nobel Prize in Physics** for these precision measurements of the speed of light with the interferometer he developed.

the same. Galilean relativity simply does not hold for Maxwell's equations. So what gives—are Newton's laws and Maxwell's laws inconsistent? Do we need to change Maxwell's equations? What's going on??

It turns out that the answer to these puzzles is that a relativity principle *does* hold for both mechanics and electrodynamics, but it is not Galilean relativity. The laws of mechanics themselves need to be changed (while Maxwell's equations are perfectly fine as is). This relativity principle, *special relativity*, was formulated by Einstein in 1905, and is our next subject of study.

## 1.2 The Postulates of Special Relativity and their Consequences

Albert Einstein started from this proposition that the speed of light in vacuum should be the same in all inertial frames of reference. As we will see throughout this section, following this supposition through to its logical conclusions has amazing consequences for how observers in different frames of reference perceive time and space.

### 1.2.1 The Postulates

Einstein formulated his theory of relativity based on the following postulates. Firstly, he accepted the principle of Galilean relativity:

**Relativistic Postulate 1** : The laws of physics are the same in *all* inertial reference frames.

As we have already reviewed, this fact is essential to how we understand the universe: physics should not depend on the physicist. His second postulate perhaps seems obvious in hindsight, but at the time was a huge conceptual leap forward:

**Relativistic Postulate 2** : The speed of light in vacuum has the same value  $c = 3 \times 10^8 \text{ m/s}$  in *all* inertial reference frames, regardless of the velocity of the observer or the velocity of the source emitting the light.

The theory of relativity based on these two postulates is known as *Special Relativity*. In the following lectures, we will explore the consequences of these postulates.

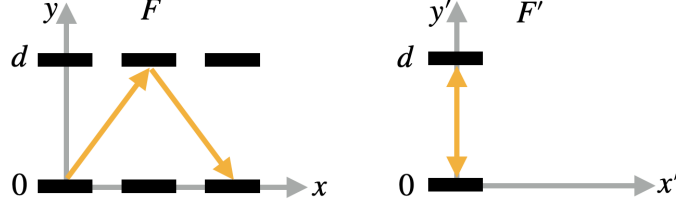
### 1.2.2 Time Dilation: Moving Clocks Run Slow

In Galilean relativity, we assumed that time was absolute,  $t' = t$  (our “Common sense” assumption 2 from earlier). The postulates of special relativity will imply that time intervals as measured by different inertial observers are *not* the same! This effect is termed **time dilation**: there is a lengthening of the time interval between two events when observed in a moving inertial frame, rather than in the rest frame of the events.

**Derivation of time dilation: Light clock on a train:** We can understand why this effect occurs with the following thought experiment. The idea is that since the speed of light is invariant in all inertial frames, it is a useful standard for measuring times and distances.



*Setup:* Consider a clock which consists of two mirrors separated by a distance  $d$ . Light bounces between them, and the clock ticks whenever light hits one of the mirrors. We put this light clock on a train, and compare how long it takes the light to pulse back and forth between the mirrors from the train's perspective (the frame  $F'$ ) versus a person on the platform's perspective (the frame  $F$ ).



Call the axis along which the clock is oriented the  $y'$ -axis, which aligns with the  $y$ -axis. Let's analyze two ticks of the clock from the frame  $F'$  in which the clock is at rest, and the frame  $F$  from whose perspective frame  $F'$  is moving to the right in the  $x$ -direction at speed  $v$ , perpendicular to the clock. (Or equivalently, frame  $F$  appears to be moving to the left at speed  $-v$  from the perspective of frame  $F'$ ).

Consider Event 1 to be light leaving the lower mirror, and Event 2 to be light returning to that mirror after bouncing back from the upper mirror. We choose our coordinate system such that the origins of both  $F$  and  $F'$  overlap at Event 1, so that in each frame these events are labeled as,

$$\begin{aligned} E'_1 &= \text{light leaves lower mirror} = (0, 0, 0, 0) \\ E'_2 &= \text{light returns to lower mirror} = (t'_2, x'_2, y'_2, 0) \end{aligned} \quad (1.6)$$

and in the unprimed frame,

$$\begin{aligned} E_1 &= \text{light leaves lower mirror} = (0, 0, 0, 0) \\ E_2 &= \text{light returns to lower mirror} = (t_2, x_2, y_2, 0) \end{aligned}$$

According to our assumptions, light is observed to travel at speed  $c$  in both frames, and therefore the total time elapsed in each frame is the total distance traveled in that frame over  $c$ ,

$$ct_2 = \text{distance traveled in } F, \quad ct'_2 = \text{distance traveled in } F'.$$

Furthermore, we will continue to assume that directions perpendicular to the direction of the relative motion between the frames are unaffected (otherwise we would get all sorts of inconsistencies), thus in both frames the total distance that the light travels along the  $y$ -axis is equal to  $2d$ .

In frame  $F'$ , the total distance traveled is just  $2d$ , and so the total time elapsed in  $F'$  between Events 1 and 2 is

$$ct'_2 = 2d \quad \Rightarrow \quad d = ct'_2/2,$$

thus determining the event coordinates as follows,

$$E'_1 = (0, 0, 0, 0), \quad E'_2 = (2d/c, 0, 0, 0).$$

In frame  $F$  the light also travels along the  $x$ -direction due to the relative motion between the frames, so that the total distance traveled is given by twice the hypotenuse of the triangle

with one side equal to  $d$ , and the other equal to the distance the whole  $F'$  frame traveled to the right in time  $t_2/2$ , which is:

$$ct_2 = 2\sqrt{\left(\frac{vt_2}{2}\right)^2 + d^2}$$

Squaring both sides and solving for  $t_2$  then yields,

$$t_2 = \frac{2d}{c\sqrt{1 - \frac{v^2}{c^2}}} \quad \Leftrightarrow \quad t_2 = \frac{2d\gamma}{c}$$

where we've defined the **relativistic gamma-factor**  $\gamma$  as<sup>3</sup>

Relativistic  $\gamma$ -factor :  $\gamma \equiv \frac{1}{\sqrt{1 - \left(\frac{v}{c}\right)^2}}$

(1.7)

Substituting for  $2d/c = t'_2$  from (1.7), we have thus derived *time dilation*,

$$t_2 = \gamma t'_2. \tag{1.8}$$

Put another way, since  $t_2$  is the total time elapsed in frame  $F$  ( $t_1 = 0$ , so  $t_2 - t_1 \equiv \Delta t$ , and the total time elapsed is just  $t_2$ ), and similarly  $t'_2$  is the total time elapsed in frame  $F'$  ( $t'_2 - t'_1 \equiv \Delta t' = t'_2$ ), we can rephrase (1.8) as a relationship between the total time elapsed in the primed frame versus the unprimed frame between observed clicks of the clock,

Time dilation :  $\Delta t = \gamma \Delta t'$

(1.9)

The observers in each frame will measure a different amount of time passing between the “clicks” of our light clock.

Some comments are in order.

- We call the time between ticks as measured in the frame in which the clock is at rest the **proper time**, and typically denote the proper time by the symbol  $\tau$  rather than  $t$ . In the time dilation formula we just derived,  $\Delta t'$  was the amount of time between ticks in the clock's rest frame (frame  $F$ ), so in the way we set up this problem,  $\Delta t'$  is the proper time. From here on out when we're talking about the proper time elapsed for a clock, we'll use  $\tau$ , and so rewrite the time dilation formula as

$\Delta t = \gamma \Delta \tau, \quad \tau \equiv \text{proper time}$

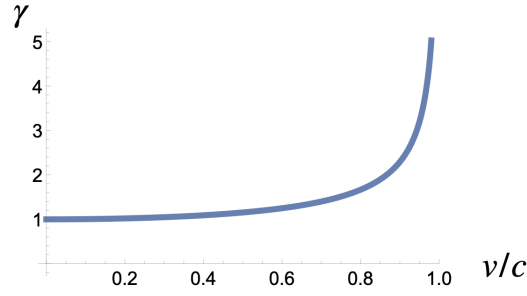
(1.10)

- The relativistic gamma factor  $\gamma$  is always  $\geq 1$ . Therefore (1.9) says that the time between clicks in the unprimed frame is *larger*, than the time between ticks as measured in the primed frame (the rest frame of the clock). In other words, **moving clocks tick slower**—the frame in which the clock appears to be moving sees the clock tick slower as compared to the rest frame of the clock.

**Exercise (1):** Show that  $\gamma \geq 1$  by plotting  $\gamma$  as a function of  $v$ . (2, harder): Prove this by showing  $\gamma(v)$  is a monotonically increasing function of  $v$  with minimum at  $v = 0$ , where  $\gamma(v = 0) \rightarrow 1$ .

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<sup>3</sup>We chose the time elapsed to be positive, picking out the positive sign when we took the square root.



- Let's understand the limiting cases of the time dilation equation. Firstly we consider the classical limit that  $v \ll c$ , the most extreme case being that  $v = 0$  so that the frame  $F'$  is at rest with respect to the frame  $F$ , then  $\gamma(v = 0) \rightarrow 1$ ,

$$\gamma(v) = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \xrightarrow{v \rightarrow 0} \frac{1}{\sqrt{1 - 0}} = 1$$

so that we simply obtain

$$v \rightarrow 0 : \quad \Delta t = \Delta t' \quad (1.11)$$

reproducing Galilean relativity. This is an important consistency check on our formalism: it should reproduce classical physics in the limit that speeds are small!

Next, consider what happens when the relative speed between frames approaches the speed of light,  $v \rightarrow c$ , so that the clock in frame  $F'$  is moving at a speed close to  $c = 3 \times 10^8 \text{ m/s}$  relative to the clock in frame  $F$ . In this case,  $\gamma \rightarrow \infty$ , so that the relativistic gamma factor diverges:

$$\gamma(v) = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \xrightarrow{v \rightarrow c} \frac{1}{\sqrt{1 - 1}} \rightarrow \infty$$

So in this limit, the time between ticks on the moving clock looks like it's going to infinity, so that the clock is running infinitely slowly!

Finally, what happens as we try to take  $v > c$ ? In this case  $\gamma$  evaluates to an imaginary number, since the quantity under the square root becomes negative. This is a signal that something unphysical is happening when we try to consider a frame moving at speeds larger than the speed of light. In fact, this is our first clue that  $c = 3 \times 10^8 \text{ m/s}$  is the maximum allowed speed. We will return to this point later, but for now the takeaway message is that **the universe has a speed limit, and that speed limit is the speed of light  $c$ !**

- We've been using the word "clock" liberally throughout this section, but what really is a clock? One example is your heartbeat—take  $\Delta\tau$  to be the time between beats of your heart in your own rest frame, and  $\Delta t$  to be the time according to an observer moving with velocity  $v$  with respect to your rest frame. The observer moving relative to you sees your heart beat more slowly.

### Example Problem: A flying pendulum

A pendulum is in a rocket, flying with velocity  $v = \frac{3}{5}c$  past a stationary observer. In the rest frame of the pendulum, its period is 3 seconds. What is the period  $T$  of the pendulum according to the stationary observer?

*Solution:* In this example, we're given the proper time between ticks as  $\Delta\tau = 3\text{s}$ . This

is the time as measured in the rocket's rest frame. In the frame of the stationary observer who sees the rocket pass by, the time elapsed  $T$  will be

$$T = \gamma \Delta\tau, \quad \gamma = \frac{1}{\sqrt{1 - (\frac{3}{5})^2}} = \frac{5}{4}$$

$$\Rightarrow T = \frac{5}{4} \cdot 3s = \frac{15}{4}s = 3.75s.$$

Since  $3.75s > 3s$ , the stationary observer sees the moving clock tick slower, since it takes longer to complete a period. The clock ticks *faster* in its rest frame, which in this problem is on the rocket.

### Clicker Question: Moving clocks

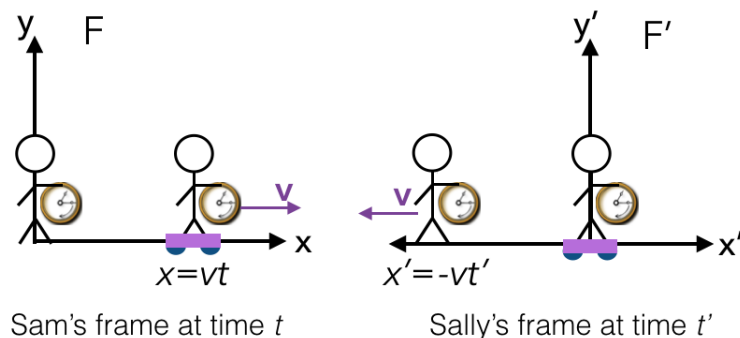
Sam measures Sally's clock ticking and concludes that Sally's clock is running slow. If Sally examines Sam's clock readings,

- (a) She would see his clock running fast.
- (b) She would see his clock running at the same rate as hers.
- (c) She would see his clock running slow.

The answer is (c), since we've just said that time runs the fastest in a clock's rest frame, and Sally is moving relative to Sam. *Both* of them see each other's clocks run slowly! Physics is the same in every inertial frame, and Sally is in an inertial frame, so should observe time dilation exactly as Sam should in his inertial frame.

But how can both frames be moving slowly when viewed from the other's? A weak analogy is that when two people who are far away from each other observe one another, each sees the other as small from their perspective.

To understand this in more detail, we can do the math! (*Note: the remainder of this box is supplementary to what we presented in lecture, but if you can understand these calculations in detail then you will be an expert on time dilation!*) Let's say that according to Sam, Sally is moving away with velocity  $v$  in the  $\hat{x}$  direction. Let Sam's rest frame be the unprimed frame, and Sally's rest frame be the primed frame. Right as Sally passes Sam, they start their clocks at the same time, at  $t = t' = 0$  as  $x = x' = 0$ . Then, Sam will see Sally's position moving at  $x = vt$ , and Sally will see Sam's position as moving at  $x' = -vt'$ . They each agree to send a light signal after a time  $T$  on their respective clocks.



1. *What is the time on Sam's clock when he receives the signal from Sally?*

Sally sends her signal at time  $T$  on her clock. But  $T$  on her clock is  $\gamma T$  on Sam's clock, by time dilation. So according to Sam, she sends the light signal at time  $\gamma T$ . According to Sam, she is a distance of  $v(\gamma T)$  away from him when the signal gets sent out, and then it needs to travel at the speed of light over that distance to get to him. Thus, on his clock, he receives the signal at

$$t_{\text{sam}} = \gamma T + \frac{v\gamma T}{c} = \gamma T \left(1 + \frac{v}{c}\right).$$

2. *Is this faster or slower than if Sally's clock were running at the same rate as Sam's?*

If Sally's clock wasn't running slow according to Sam, then she would send her light signal at time  $T$  when she is a distance  $vT$  away, and it would take a time  $vT/c$  to get to him, so Sam would've gotten the signal when his clock read

$$t_{\text{sam}}^{NR} = T + \frac{vT}{c} = T \left(1 + \frac{v}{c}\right).$$

The difference between the relativistic and nonrelativistic results is

$$t_{\text{sam}} - t_{\text{sam}}^{NR} = T \left(1 + \frac{v}{c}\right) (\gamma - 1).$$

Since  $\gamma \geq 1$ , it takes a *longer* time for the signal to reach him than if Sally's clock were running at the same rate as his, and therefore *Sam sees Sally's clock as running slow*.

3. *What is the time on Sally's clock when she receives the signal from Sam?*

First we'll calculate this in Sam's frame, and use time dilation to compute the answer in Sally's frame.

Sam sends the signal at time  $T$  on his clock. When he sends it, according to him she is a distance  $vT$  away from him. Then, she keeps traveling to the right as the light travels at the speed of light towards her. The time it takes the light to reach her after it is sent is

$$ct_0 = vT + vt_0 \quad \Rightarrow \quad t_0 = \frac{v}{c-v}T.$$

So according to Sam, she should get it at time  $T + t_0$ . But the time on Sally's clock passes more slowly according to Sam since it is moving with respect to him, so actually the time that she sees on her clock is related to the time on his clock that we just calculated by

$$\gamma t_{\text{sally}} = T + t_0 \quad \Rightarrow \quad t_{\text{sally}} = \frac{T}{\gamma} \left(1 + \frac{v}{c} \left(\frac{1}{1 - \frac{v}{c}}\right)\right).$$

Of course, we could have gotten this answer just by reversing the logic from Sam's calculation above. Sam sends his signal at time  $T$  on his clock, which is time  $\gamma T$  on Sally's clock by time dilation. So according to Sally, he sends the light signal at time  $\gamma T$ . The signal then has to travel a distance of  $v(\gamma T)$  to get to her at the speed of

light, so we should get  $t_{\text{sally}} = \gamma T(1 + \frac{v}{c})$ . Indeed, with some algebra we can simplify our answer above for  $t_{\text{sally}}$  to

$$t_{\text{sally}} = \frac{T}{\gamma} \left( 1 + \frac{v}{c} \left( \frac{1}{1 - \frac{v}{c}} \right) \right) = \gamma T \left( 1 + \frac{v}{c} \right).$$

4. *Is this faster or slower than if Sally's clock were running at the same rate as Sam's?*

Since we've already shown that  $t_{\text{sally}} = t_{\text{sam}}$ , the answer is exactly the same as part (2), but reversing Sam and Sally. *Sally sees Sam's clock as running slow.*

### 1.2.3 The Twin Paradox

**Statement of the paradox:** As an exploration of time dilation, let's walk through the story of twins Mateo and Maria. Mateo and Maria are 20 year old twins living on Earth. Mateo is an astronaut, and takes off in a rocket with speed  $v = 4/5c$  to a star that is 20 light years away, while Maria stays behind, watching Mateo by telescope.

We've already discussed that heart beats are a type of clock, and so if someone is moving really fast relative to me, I will see their heart beat slower according to time dilation—*i.e.*, I will see them age less. Because of this, Maria sees Mateo's heart slow down compared to hers. Explicitly, let's call the time between beats of Mateo's heart according to Maria's rest frame  $t_{\text{Mateo}}$ , and the time between beats of Maria's heart in her own rest frame (her proper time between heartbeats)  $\tau_{\text{Maria}}$ . Then,

$$\begin{aligned} \text{Maria's rest frame: } t_{\text{Mateo}} &= \gamma \tau_{\text{Maria}} = \frac{1}{\sqrt{1 - \left(\frac{4c}{5}\right)^2 \frac{1}{c^2}}} \tau_{\text{Maria}} = \frac{5}{3} \tau_{\text{Maria}} \\ &\Rightarrow t_{\text{Mateo}} > \tau_{\text{Maria}}, \end{aligned}$$

demonstrating as anticipated that Mateo's heart beats more slowly according to Maria. What this means is that for every 5 beats of Maria's heart, she only sees Mateo's heart beat 3 times, so for example after 1 year has passed according to Maria, only 3/5'th of a year will have passed for Mateo.

Since the star is 20 lightyears away in the rest frame of the Earth (Maria's rest frame), according to Maria, Mateo will reach the star after

$$\frac{20 \text{ lightyears}}{4/5c} = \frac{20 \text{ years} \cdot c}{4/5c} = 25 \text{ years}.$$

Then Mateo turns around and comes home. Thus when he returns, our calculation tells us that 50 years have passed for Maria, so that Maria is now 70 years old. However, only 30 years have passed for Mateo, and so he is only 50!

We did this analysis in the rest frame of Maria. But motion is supposed to be relative, and we should be able to analyze this situation from Mateo's point of view. From Mateo's point of view, he's at rest in a stationary space ship the whole time, and the Earth moves with speed  $4/5c$  in the opposite direction, then turns around and moves back towards Mateo until they meet. Thus, from this point of view, shouldn't Maria be the one who's only 50 when a 70 year old Jack returns? This apparent contradiction is the famous "twin paradox".

**Resolution** The resolution of this paradox lies in the fact that in the tale we just told, *Mateo is not always traveling in an inertial frame of reference*. In order to take off he has to accelerate,

and in order to get back to the Earth, he has to turn around, and therefore accelerate again (whether or not he comes to a stop and starts up again, or just turns around in a circle, both scenarios require acceleration), and as we learned, inertial frames of reference are non-accelerated frames.

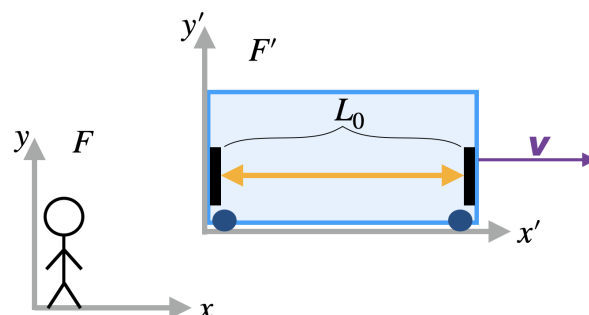
Although both twins can legitimately claim that they are at rest in their own frame of reference, only the Mateo experiences acceleration. Since Maria always remained in an inertial frame, the time dilation formula is valid for Maria's observation of Mateo, but *not* for Mateo's observation of Maria. The symmetry between observers in relative motion was broken, and so we can't rely on special relativity. Mateo is in fact the twin who will come home younger. This fact has been experimentally verified. Non-symmetric aging has been verified with atomic clocks taken on airplane trips around the world, and compared with identical clocks left behind.<sup>4</sup>

—————End Lecture 2.

### 1.2.4 Length Contraction: Moving Rulers Contract

**Derivation of length contraction: light clock on a train** We previously used the light clock experiment to conclude that starting from the two postulates of special relativity, time is in fact *not* measured the same in different inertial frames of reference. A slight modification of the same experiment can be used to likewise refute our other common sense assumption, that length is measured the same in every inertial frame. The setup is as follows.

*Setup:* Observer  $F'$  is on a train moving at velocity  $v$  relative to the platform, while an observer  $F$  stands on the train platform. There is a device that sends a light pulse from the left hand side of the box-car to the right hand side of the box-car, where it bounces off of a mirror and returns to a photosensor on the left-hand-side. The distance between the mirrors is  $L_0$  in the frame  $F'$ .



This thought experiment essentially turns the clock in from our derivation of time dilation on its side. We'd like to time the round trip of the light pulse between the mirrors, and use this measured time to infer the length of the train car. In particular, our strategy will be to solve for the time elapsed between ticks in the primed frame as a function of  $L_0$ , the time elapsed between ticks in the unprimed frame as a function of the length of the clock measured in that frame (which we'll call  $L$ ), and then use the time dilation formula to relate the two.

On the train (the rest frame of the clock), the light pulse travels a distance:

$$\text{distance traveled according to } F' = 2L_0 = c\Delta\tau,$$

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<sup>4</sup>In order to understand exactly how Mateo's calculation of their ages agrees with Maria's and understand how his acceleration changes the naive calculation, we would need the broad theory of *General Relativity*, which is a whole other course entirely.

where we have denoted the time elapsed between the light leaving the photodetector on the left and back to the photodetector as  $\Delta\tau$ , since this is the proper time between ticks (the time elapsed between ticks in the clock's own rest frame). Therefore, the time elapsed in this frame is,

$$\Delta\tau = \frac{2L_0}{c} \quad (1.12)$$

Meanwhile, on the platform, the time the light takes to travel from emission to the right-side mirror is different from the time to travel back from the right-side mirror to the photodetector on the left, because the train is moving to the right during the light's travel time. Let the length of the light clock as measured in the frame  $F$  be denoted as  $L$ . Then, the time  $\Delta t_{L \rightarrow R}$  that it takes the light to travel from the left mirror to the right mirror in this frame is,

$$\Delta t_{L \rightarrow R} = \frac{(L + v\Delta t_{L \rightarrow R})}{c} \Rightarrow \Delta t_{L \rightarrow R} = \frac{L}{c - v},$$

while similarly, the time it takes to travel from the right mirror to the left mirror is,

$$\Delta t_{R \rightarrow L} = \frac{(L - v\Delta t_{R \rightarrow L})}{c} \Rightarrow \Delta t_{R \rightarrow L} = \frac{L}{c + v}.$$

Putting these together, the total time  $\Delta t$  is,

$$\Delta t \equiv \Delta t_{L \rightarrow R} + \Delta t_{R \rightarrow L} = \frac{2}{c} \frac{L}{1 - \frac{v^2}{c^2}} = \frac{2L\gamma^2}{c} \quad (1.13)$$

From our time dilation thought experiment, we know that  $\Delta t = \gamma\Delta\tau$ , since  $\Delta t$  is the moving frame from the perspective of the observer on the train with the light clock, and  $\Delta\tau$  is the proper time that elapses according to that clock. Substituting for (1.12) and (1.13), we find

$$\begin{aligned} \Delta t &= \gamma\Delta\tau \\ \frac{2L\gamma^2}{c} &= \gamma \cdot \frac{2L_0}{c} \Rightarrow L = \frac{L_0}{\gamma} \end{aligned}$$

We have thus derived the formula for length contraction,

Length contraction:  $L = \frac{L_0}{\gamma}$

(1.14)

Since the relativistic gamma factor is always greater than or equal to one ( $\gamma \geq 1$ ), this says that the length *along the direction of motion* as measured in the frame which sees the object moving is *less* than the length as measured in the objects rest frame. **Moving rods contract in the direction of relative motion!**<sup>5</sup> The length of an object is maximal in the frame in which the object is at rest. The length of an object as measured in its rest frame is called the **proper length**, so in this formula,  $L_0$  is the proper length of the clock, and indeed  $L_0$  is always greater than or equal to  $L$ .

Much as we did for the time dilation formula, we should examine how this formula reduces in the classical limit that  $v \ll c$ , so that  $\frac{v}{c} \rightarrow 0$ . In this case,  $\gamma \rightarrow 1$ , and indeed we find that both reference frames measure the same length of the object. This is again an important consistency check on our theory.

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<sup>5</sup>Importantly, objects do **not** contract in directions perpendicular to the line of motion—while we have not proven this fact here, it would cause all sorts of inconsistencies.



### Example Problem: Precision measurement

Suppose you have a meter stick, and you can measure lengths up to  $1\text{mm}$  precision. Determine the speed  $v$  at which relativistic effects become measurable for this ruler.

If the meter stick is moving relative to the laboratory frame, we will measure its length as

$$L = \frac{L_0}{\gamma} = \frac{1\text{m}}{1/\sqrt{1 - \frac{v^2}{c^2}}}$$

When the meter stick is at rest, we measure it as  $L = 1\text{m}$ . If we can measure only with the precision of  $1\text{mm} = 0.001\text{m}$ , then we will be able to measure a change in the length of the meter stick when  $L = (1 - 0.001)\text{m} = 0.999\text{m}$ . Therefore, we can solve for

$$0.999\text{m} = \frac{1\text{m}}{1/\sqrt{1 - \frac{v^2}{c^2}}} \Rightarrow \frac{v}{c} = 0.045.$$

So for speeds  $v \gtrsim 0.045c = 1.35 \times 10^7\text{m/s}$ , length contraction will result in an effect that is measurable down to  $1\text{mm}$ .

To compare, the fastest jet on Earth can fly at approximately  $3.3 \times 10^3\text{m/s}$ , which is still four orders of magnitude away from being able to see this effect!

### Example Problem: The fast and the cubical

A cube with sides of length  $a$  is sent moving at a constant speed  $v = (3/5)c$ . What is the volume of the cube in this frame?

Only one side of the cube will appear length contracted, the side which is parallel to the relative motion between the frames, while the other sides remain unchanged. In this problem,  $\gamma = \frac{5}{4}$ . Therefore, the volume is product of the lengths of the three sides,

$$V = a \cdot a \cdot \frac{a}{\gamma} = \frac{a^3}{\gamma} = \frac{4}{5}a^3. \quad (1.15)$$

*Aside:* For this problem, we have assumed that the motion is parallel to one side of the cube to make our lives easier. But, even if we didn't make this assumption we would get the same answer, the math would just be more difficult! For example, consider your Homework Problem 3, where you are asked to consider a rectangle moving to the right at an angle. Once you finish that problem, compare the area of the rectangle in its rest frame,  $A_0 = ab$ , with the area of the shape in the frame in which it appears to be moving,  $A$ . You should get that  $A = A_0/\gamma$ , consistent with this example.

### Clicker Question: The Pole-vaulter paradox

A Vassar student who attends Physics 200 lecture (but doesn't do their homework...) is working with the Poughkeepsie farm project. They befriend a farmer who is reading about Special Relativity as a hobby.

On the farm there is a barn with 2 doors 4 meters apart. There is a pole with proper length 5 meters. The farmer goads the student to run very fast and therefore fit the 5 meter pole in the 4 meter barn. As the farmer learned from their readings, if the student runs at speed  $v = (3/5)c$ , the pole would appear to be length contracted relative to its proper length of  $L_{\text{pole},0} = 5m$ , to a length  $L_{\text{pole}} = 4m$ ,

$$L_{\text{pole}} = L_{\text{pole},0}/\gamma = 5m \cdot \sqrt{1 - \left(\frac{3}{5}\right)^2} = 4m.$$

But the student tells the farmer “You are nuts! There is no way that the pole can fit”. Who is right, and why?

- (a) The farmer is right and the student fits the entire pole in the barn. The student is wrong!
- (b) The student is right and the pole does not fit in the barn. The farmer is wrong!
- (c) Each person’s observations confirm that they are right.

In this problem, the relative speed between the barn and the pole yields  $\gamma = 5/4$ . From the perspective of the farmer standing at rest next to the barn, the pole appears contracted relative to its proper length, so

$$L_{\text{pole}} = L_{\text{pole},0}/\gamma = 5m \cdot \sqrt{1 - \left(\frac{3}{5}\right)^2} = 4m.$$

In this frame the barn is its proper length,  $L_{\text{barn},0} = 4m$ . If the front of the pole crosses the front of the barn at time  $t = 0$ , then a time

$$\Delta t = \frac{L_{\text{barn},0}}{v} = \frac{4m}{3/5c} = \frac{20m}{3c} \approx 2.2 \times 10^{-8} s$$

later, the front of the pole will be at the back of the barn and the back of the pole will be at the front of the barn. So in the rest frame of the barn, indeed it looks like the pole does fit!

However, from the perspective of the runner with the pole (call this the primed frame), the pole is its proper length of  $5m$ , and it is the barn that appears length contracted relative to its proper length  $L_{\text{barn}}$ ,

$$L'_{\text{barn}} = L_{\text{barn},0}/\gamma = \frac{4m}{5/4} = 3.2m.$$

So what’s going on?

In this frame, the ends of the pole do not coincide with the walls of the barn at one instant in time; instead, the event of the front of the pole reaching the back of the barn occurs *before* the back of the pole reaches the back of the barn. **Events which are simultaneous in one rest frame are not simultaneous in another!** There is no contradiction, the observers really do each see observations that confirm that they are right. The correct answer is (c).

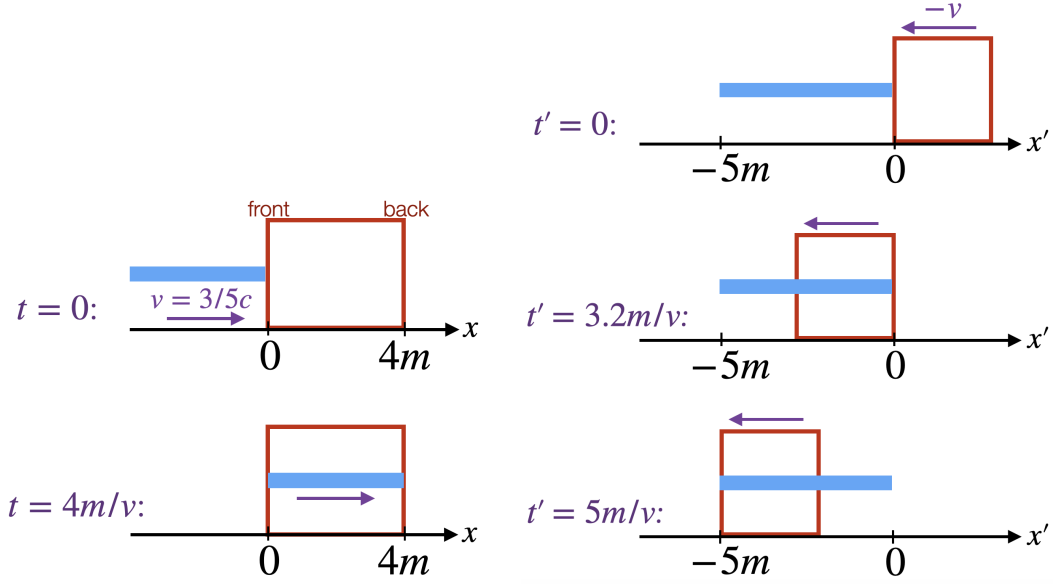


Figure 1: Different events viewed in the at-rest reference frame of the barn (left) versus the at-rest reference frame of the pole (right), resolving the pole-vaulter paradox.

Let's dive into the solution to this question a little further. Let us consider the following events:

- Event 1 = front of pole is at front of barn
- Event 2 = front of pole is at back of barn
- Event 3 = back of pole is at front of barn

In the rest frame of the barn, the pole which appears to be of length  $L_{\text{pole}} = 4m$  is moving to the right with speed  $v = (3/5)c$  towards the barn of length  $L_{\text{barn},0} = 4m$ , so that the coordinates  $(t, x, y, z)$  of these events are as follows:

$$\begin{aligned}
 E_1 &= (t_1, x_1, y_1, z_1) = (0, 0, 0, 0) \\
 E_2 &= (t_2, x_2, y_2, z_2) = (L_{\text{barn},0}/v = 2.2 \times 10^{-8} \text{ s}, L_{\text{barn},0} = 4m, 0, 0) \\
 E_3 &= (t_3, x_3, y_3, z_3) = (L_{\text{pole}}/v = 2.2 \times 10^{-8} \text{ s}, 0, 0, 0)
 \end{aligned} \tag{1.16}$$

(The  $y$  and  $z$  directions will play no role in this discussion.) In particular, Events 2 and 3 are *simultaneous*, so that the pole does indeed appear to fit into the barn at one instant in time.

On the other hand, in the rest frame of the pole (of proper length  $L_{\text{pole},0} = 5m$ , the barn of apparent length  $L'_{\text{barn}} = 3.2m$  is moving to the left with speed  $v = -(3/5)c$ , so that the Events have the following coordinates:

$$\begin{aligned}
 E'_1 &= (t'_1, x'_1, y'_1, z'_1) = (0, 0, 0, 0) \\
 E'_2 &= (t'_2, x'_2, y'_2, z'_2) = (L'_{\text{barn}}/v = 1.8 \times 10^{-8} \text{ s}, 0, 0, 0) \\
 E'_3 &= (t'_3, x'_3, y'_3, z'_3) = (L_{\text{pole},0}/v = 2.8 \times 10^{-8} \text{ s}, -L_{\text{pole},0} = -5m, 0, 0)
 \end{aligned} \tag{1.17}$$

In this frame, Events 2 and 3 do *not* occur at the same time, so indeed the runner will never see the whole pole fitting into the barn at one time.

———End Lecture 3.

### 1.2.5 Lorentz Transformations

So far, our conclusions about special relativity have been the result of cleverly designed thought experiments, which have been chosen to show off some of the important features of the theory—namely, time dilation and length contraction. But these are merely some components of the more complete theory, which has its own set of transformation rules akin to the Galilean coordinate and velocity transformations (1.1) and (1.2). Let us finally figure out the correct transformation law between coordinates in special relativity: the *Lorentz transformation*. Lorentz transformations are the relation between the position and time coordinates of the same events as seen in different reference frames, according to special relativity.

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[ The following content can be treated as supplementary material for those that wish to gain a deeper understanding of how these laws were actually derived; otherwise you can skip to the next horizontal line.]

To derive the Lorentz transformation, we label the coordinates as measured in the frame  $F$  by  $(t, x, y, z)$ , and the coordinates in the frame  $F'$  that moves to the right with velocity  $\vec{v} = v\hat{x}$  with respect to frame  $F$  as  $(t', x', y', z')$ . We begin with the following assumptions:

- Motion in the directions perpendicular to the direction of relative motion between the frames is unaffected. Therefore since the relative velocity between frames is in the  $\hat{x}$ -direction, we assume that the  $\hat{y}$  and  $\hat{z}$  directions are unaffected, so that

$$y' = y, \quad z' = z$$

On the other hand, we do expect that the coordinates  $x'$  and  $t'$  are some function of  $x$  and  $t$ , much as was the case for the Galilean coordinate transformation. The form of these functions can naively be anything, but in fact we will find that only one choice agrees with the postulates of special relativity, and reduces to Galilean relativity in the limit that the relative speed between frames is small compared to the speed of light.

- We next assume that the transformation of  $x$  and  $t$  is *linear* in their arguments  $t$  and  $x$ ,

$$t' = At + Bx + C, \quad x' = Dt + Ex + F,$$

where  $A, B, C, D, E, F$  are constants that are independent of  $x, y, z, t$ , but might depend on the constants  $v$  and  $c$ . The reason for this simplification (that, for instance, no  $t^2$  appears on the right-hand-side of either of these equations) is that we need to be consistent with the first postulate of relativity: that the laws of physics do not depend on the choice of inertial frame. If the transformations were not linear, then they would depend on the position/time that you started from. This would introduce a frame-dependence in the laws of physics, violating the first postulate.

- Next comes the familiar simplification to ask that the origins are synced—that  $x' = x = 0$  when  $t' = t = 0$ . This establishes a system for consistently comparing the two coordinate systems, and constrains the constants as,

$$\begin{aligned} t'(t = 0, x = 0) = 0 = C &\Rightarrow C = 0 \\ x'(t = 0, x = 0) = 0 = F &\Rightarrow F = 0 \end{aligned}$$

- We next need to ensure that frame  $F$  sees frame  $F'$  moving with velocity  $v$  to the right, while  $F'$  sees frame  $F$  moving with velocity  $-v$ , to the left. To do so, let us consider how  $F'$  measures velocity in that frame:

$$\frac{dx'}{dt'} = \frac{Ddt + Edx}{Adt + Bdx} = \frac{D + Edx/dt}{A + Bdx/dt} \quad (1.18)$$

The two frames should be moving with relative velocity  $v$ , so that  $F$  sees the origin  $x' = t' = 0$  of  $F'$  moving to the right with velocity  $dx/dt = v$ , while  $F'$  sees that point as stationary,  $dx'/dt' = 0$ , so that

$$0 = \frac{D + Ev}{A + Bv} \Rightarrow D = -Ev$$

The reverse condition is that  $F$  should see its own origin as stationary, while  $F'$  sees it moving to the left with velocity  $dx'/dt' = -v$ , so that substituting into (1.18) yields

$$-v = \frac{D + E(0)}{A + B(0)} = \frac{D}{A} = \frac{-Ev}{A}$$

so that together, we have obtained

$$A = E, \quad D = -Ev$$

To summarize, so far we have simplified the transformation laws to the following:

$$t' = Et + Bx, \quad x' = E(x - vt), \quad y' = y, \quad z' = z.$$

Two constants remain: the dimensionless constant  $E$ , and the dimensionful constant  $B$ , which has units of inverse velocity.

- Next we consider what each observer should see when we send a light pulse along the  $x$  direction. Both frames see the pulse as traveling with speed  $c$  (the second postulate!), so if the pulse originates at  $x = t = 0$  and  $x' = t' = 0$ , then both frames will agree that  $x = ct$  and  $x' = ct'$ . Therefore,

$$\begin{aligned} x' &= ct' \\ E(x - vt) &= c(Et + Bx) \\ E((ct) - vt) &= c(Et + B(ct)) \\ \Rightarrow B &= -\frac{Ev}{c^2} \end{aligned}$$

- How to determine the remaining constant  $E$ ? Since  $E$  is dimensionless, it is a function of  $v/c$ . In the limit that  $v \rightarrow 0$  we must reproduce  $x = x'$  and  $t = t'$ , so that

$$E \xrightarrow{v/c \rightarrow 0} 1.$$

To finally determine  $E$  as a function of  $v/c$ , we can consider one more thought experiment. Consider now sending a light pulse along the  $y$  direction in the frame  $F$ .  $F$  will track its position as  $x = 0$  and  $y = ct$ , but  $F'$  will track the beam moving in both the  $x'$  and  $y'$  directions, with  $y' = y$ . But the speed must be  $c$  in both frames, so the total distance the beam travels in frame  $F'$  must be equal to  $ct'$ :

$$\begin{aligned} ((x')^2 + (y')^2) &= (ct')^2 \\ E^2(0 - vt)^2 + y^2 &= (cE)^2(t - \frac{v(0)}{c^2})^2 \end{aligned}$$

Substituting for  $y = ct$ ,  $x = 0$ , and solving for  $E^2$ :

$$E^2(0 - vt)^2 + c^2t^2 = (cE)^2(t - 0)^2 \quad \Rightarrow \quad E = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} = \gamma$$

Indeed,  $E = \gamma \rightarrow 1$  when  $v/c \rightarrow 0$ . *[End supplemental derivation.]*

Let us summarize. By making the following assumptions:

- The first and second postulates: the laws of physics are not frame dependent, and the speed of light is  $c$  in every inertial frame.
- Motion in the directions perpendicular to the direction of relative motion is unaffected.
- The origins of frames are synced so that  $(t' = 0, x' = 0, y' = 0, z' = 0)$  when  $(t = 0, x = 0, y = 0, z = 0)$ ,

we obtain the *Lorentz transformation*,

$$\boxed{\begin{aligned} t' &= \gamma \left( t - \frac{v}{c^2} x \right) \\ x' &= \gamma(x - vt) \\ y' &= y, \quad z' = z \end{aligned}} \quad (1.19)$$

where again, we have defined  $\gamma = 1/\sqrt{1 - v^2/c^2}$  as the relativistic gamma-factor. These equations tell us how to transform between coordinates of events in a frame  $F$ , with those in a frame  $F'$  moving at speed  $v$  in the positive  $x$ -direction relative to  $F$ .

A few comments are in order:

- First, let us verify that we reproduce classical physics in the appropriate limit. In the limit that  $v \ll c$ , we can take ratios  $v/c \rightarrow 0$ . In this limit  $\gamma \rightarrow 1$ , and these equations reduce to<sup>6</sup>

$$\begin{aligned} \frac{v}{c} \rightarrow 0 : \quad t' &= t, & x' &= x - vt \\ y' &= y, & z' &= z \end{aligned}$$

which perfectly reproduce the Galilean coordinate transformation.

- A second comment is that we can invert these equations. The transformation (1.19) is useful when we know the coordinates of an event in the unprimed frame, and wish to determine the corresponding coordinates in the primed frame. If instead we know the coordinates in the primed frame and wish to determine the corresponding coordinates in the unprimed frame, we need the inverse equations. You *could* simply solve the system of equations for  $t, x, y, z$ , but this is a little cumbersome. The easier way to do it is to

<sup>6</sup>Note that we didn't take  $v \rightarrow 0$  in the second equation since it wasn't divided by  $c$ ; the correct version of the classical limit is that  $v$  is much smaller than  $c$ , not that  $v$  is necessarily 0! Galilean relativity works perfectly well in classical mechanics for nonzero speeds  $v$ , as long as  $v \ll c$ .

remember that according to an observer in frame  $F'$ , the frame  $F$  is moving at velocity  $-v\hat{x}'$ . Thus, the Lorentz transformation should be of precisely the same form, but with  $v \rightarrow -v$ . (Recall that  $\gamma$  depends on  $v^2$ , and so does not change under  $v \rightarrow -v$ , since  $v^2 = (-v)^2$ .) Either method gives the same result:

$$\boxed{\begin{aligned} t &= \gamma \left( t' + \frac{v}{c^2} x' \right) \\ x &= \gamma (x' + vt') \\ y &= y', \quad z = z' \end{aligned}} \quad (1.20)$$

Now that we know the Lorentz transformation, we can use it to derive our previous results of time dilation and length contraction as special cases of this more general framework. Let's first reconsider time dilation.

**Time dilation revisited:** Consider our light clock on a train from Section 1.2.2, at rest in frame  $F'$ . A pulse is emitted from the bottom mirror at time  $t'_1$ , and returns back to that mirror at time  $t'_2$ , so that  $\Delta t' = t'_2 - t'_1 \equiv \Delta\tau$  is the proper time between ticks of this clock. This clock appears to be moving to the right in frame  $F$ . What interval  $t_2 - t_1 = \Delta t$  does frame  $F$  measure between these events?

Let Event 1 correspond to the pulse being emitted, and Event 2 the pulse returning. In the  $F'$  frame these two events occur at the same point in space:

$$\text{Event 1 : } (t'_1, x'_1, y'_1, z'_1), \quad \text{Event 2 : } (t'_2, x'_2 = x'_1, y'_2 = y'_1, z'_2 = z'_1)$$

For the purpose of this exercise we'll let the spacetime location of Event 1 be some unspecified  $(t'_1, x'_1, y'_1, z'_1)$ , rather than setting it to the origin as we did in equation (1.6).

We can compute  $\Delta t = t_2 - t_1$  by substituting for the Lorentz transformation,

$$\begin{aligned} \Delta t = t_2 - t_1 &= \gamma(t'_2 + \frac{v}{c^2}x'_2) - \gamma(t'_1 + \frac{v}{c^2}x'_1) \\ &= \gamma(t'_2 + \frac{v}{c^2}x'_1) - \gamma(t'_1 + \frac{v}{c^2}x'_1) \\ &= \gamma(t'_2 - t'_1) = \gamma\Delta\tau \end{aligned}$$

and voila! We have re-derived the effect of time dilation:  $\Delta t = \gamma\Delta\tau$ .

**Length contraction revisited:** Next, let's reconsider length contraction. Consider an observer in frame  $F$  that wish to measure the length of a rod that lies on the  $x$ -axis and is moving to the right with speed  $v$  (at rest in the primed frame  $F'$ ). The measurement of the left and right ends of the rod will form the two events:

$$\begin{aligned} \text{Event 1} &= \text{measurement of left end of rod} \\ \text{Event 2} &= \text{measurement of right end of rod} \end{aligned}$$

In the rest frame of the rod, it is stationary, so  $\Delta x' = x'_2 - x'_1 \equiv L_0$  is the proper length.

In order to determine the length  $\Delta x = x_2 - x_1 \equiv L$  that an observer in  $F$  will measure, we need a simultaneous measurement of the ends of the ruler, at  $t_1 = t_2$ , so that

$$E_1 = (t_1, x_1, 0, 0), \quad E_2 = (t_2 = t_1, x_2, 0, 0)$$

(Again, the  $y$ - and  $z$ -directions play no role in this discussion.) So, we can calculate

$$\begin{aligned}\Delta x' &= x'_2 - x'_1 = \gamma(x_2 - vt_2) - \gamma(x_1 - vt_1) \\ &= \gamma(x_2 - x_1) - \gamma v(t_2 - t_1) = \gamma \Delta x \\ \Rightarrow L_0 &= \gamma L\end{aligned}$$

A word of caution, however: recall that events that are simultaneous in one frame are not simultaneous in another! Since we wanted to solve for the length of the rod in the frame  $F$  given its proper length  $L_0$  in the frame  $F'$ , we needed to impose that the measurements of the end of the rod are simultaneous in our unprimed frame. But these events will not be simultaneous in the primed frame; for example, if we use the Lorentz transformation on  $E_1$  and  $E_2$  to determine the time coordinates of those events in the primed frame, we would compute

$$\begin{aligned}t'_1 &= \gamma \left( t_1 - \frac{v}{c^2} x_1 \right), \quad t'_2 = \gamma \left( t_2 - \frac{v}{c^2} x_2 \right) \\ \Rightarrow t'_2 - t'_1 &= \gamma \cdot \frac{v}{c^2} (-x_2 + x_1) \\ &= -\frac{v}{c^2} L_0 \neq 0.\end{aligned}$$

where we used  $t_1 = t_2$ , and  $x_2 - x_1 = L = L_0/\gamma$ . Evidently,  $t'_2$  is *not* equal to  $t'_1$ . This is perfectly ok—since the rod is not moving in its rest frame (the primed frame), the measurement of the left end of the rod does not have to take place at the same time as the measurement of the right end of the rod; the rod is stationary, and so we can still conclude that  $\Delta x'$  for these non-simultaneous events in this frame indeed computes the proper length of the rod,  $L_0$ . The tricky part is that if we want to use the Lorentz transformation to say something about the length of an object *in a frame in which the object appears to be moving*, we must make sure that we take the measurements at the same instant in time.

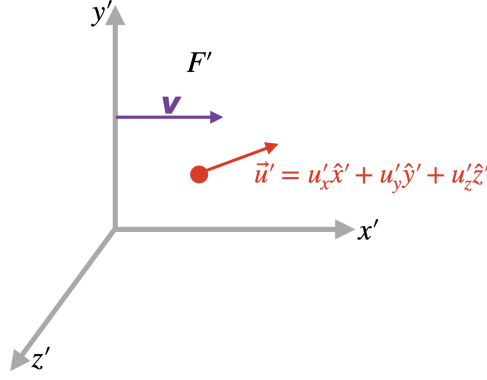
*Suggested exercise to test your understanding:* Reconsider the Pole Vault Paradox from Box (3).

- (a) Using the Lorentz transformation (1.19), re-derive the coordinates (1.17) of Events 1,2,3 in the primed frame, given the coordinates (1.16) in the unprimed frame.
- (b) Using the inverse Lorentz transformation (1.20), re-derive the coordinates (1.16) of Events 1,2,3 in the unprimed frame, given the coordinates (1.17) in the primed frame.

**Lorentz velocity addition** Next, let us consider the Special Relativity generalization of the velocity addition formulas (1.2). Recall that to derive the Galilean velocity transformation, we differentiated the Galilean coordinate with respect to time. We can do the analogous thing to derive the Special Relativistic version of these equations starting from the Lorentz transformation—the primary difference will be that since  $t$  also transforms between frames,  $dt \neq dt'$ , and we will instead need to use the form of the Lorentz transformation to relate the two.

For example, consider how the primed frame measures the velocity of an object in the





$x$ -direction, as  $u'_x = dx'/dt'$ . Substituting for the Lorentz transformation,

$$\begin{aligned} u'_x &= \frac{dx'}{dt'} = \frac{d(\gamma(x - vt))}{d(\gamma(t - \frac{v}{c^2}x))} \\ &= \frac{dx - vdt}{dt - \frac{v}{c^2}dx} \\ &= \frac{\frac{dx}{dt} - v}{1 - \frac{v}{c^2} \frac{dx}{dt}} = \frac{u_x - v}{1 - \frac{v}{c^2} u_x} \end{aligned}$$

In going from the first to the second line we used the fact that  $\gamma$  is a constant since it only depends on the constant  $v/c$ , so that  $d\gamma = 0$ , so that the factors of  $\gamma$  in both the numerator and denominator cancel. In going from the second to the third line we divided both the numerator and denominator by  $dt$ , and then identified  $dx/dt = u_x$ .

Performing the same exercise for  $u_y = dy/dt$  and  $u_z = dz/dt$  yields the following Lorentz velocity transformation laws for an object moving more generally in the  $\hat{x}'$ ,  $\hat{y}'$ , and  $\hat{z}'$  directions,

$$\begin{aligned} u'_x &= \frac{u_x - v}{1 - \frac{vu_x}{c^2}} \\ u'_y &= \frac{u_y}{\gamma \left(1 - \frac{vu_x}{c^2}\right)} \\ u'_z &= \frac{u_z}{\gamma \left(1 - \frac{vu_x}{c^2}\right)} \end{aligned} \tag{1.21}$$

Inverting these equations to express  $u_x, u_y, u_z$  in terms of  $u'_x, u'_y, u'_z$  yields,

$$\begin{aligned} u_x &= \frac{u'_x + v}{1 + \frac{vu'_x}{c^2}} \\ u_y &= \frac{u'_y}{\gamma \left(1 + \frac{vu'_x}{c^2}\right)} \\ u_z &= \frac{u'_z}{\gamma \left(1 + \frac{vu'_x}{c^2}\right)} \end{aligned} \tag{1.22}$$

These inverted equations can be derived by simply taking  $v \rightarrow -v$  in the previous formulae, since the primed frame sees the unprimed frame as moving with velocity  $v$  in the  $-\hat{x}'$  direction.

A first comment on these relations is that **the velocities perpendicular to the direction of relative motion also transform!** While the Lorentz coordinate transform leaves directions

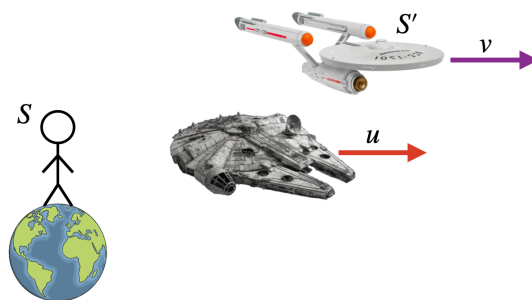
perpendicular to the relative motion between the frames unchanged, components of velocities in these directions *do* transform between frames. The reason is that the different frames see time itself pass differently, and velocity measures how the location of an object changes with time; even though  $dy' = dy, dz' = dz$ , since  $dt' \neq dt$  there will be a nontrivial transformation for these components.

The next comment is that in the classical limit  $v \ll c$ , these transformation laws reduce exactly to the Galilean velocity transformation laws. In that limit we take ratios  $v/c \rightarrow 0$ , so that  $\gamma \rightarrow 1$ , and we are left with

$$\begin{aligned} u'_x &= \frac{u_x - v}{1 - \frac{vu_x}{c^2}} \xrightarrow{v/c \rightarrow 0} u_x - v \\ u'_y &= \frac{u_y}{\gamma \left(1 - \frac{vu_x}{c^2}\right)} \xrightarrow{v/c \rightarrow 0} u_y \\ u'_z &= \frac{u_z}{\gamma \left(1 - \frac{vu_x}{c^2}\right)} \xrightarrow{v/c \rightarrow 0} u_z \end{aligned}$$

This is, as usual, an important consistency check on these laws.

### Clicker Question: Lorentz velocity addition



An observer  $S'$  traveling along the  $+\hat{x}$  direction with velocity  $v$  overtakes a slower spaceship traveling in the same direction. Observer  $S$  tells observer  $S'$  that the spaceship is traveling with velocity  $u$ . Observer  $S'$ , forgetting relativity, mistakenly calculates her velocity relative to the other spaceship as  $u - v$ .

Her *actual* velocity relative to the spaceship is:

- (a) greater than his mistaken calculation.
- (b) less than his mistaken calculation.

The mistaken observer  $S'$  would calculate the velocity of the slower ship as  $u' = u - v$ , but, but according to the Lorentz velocity addition, the correct answer is

$$u' = \frac{u - v}{1 - \frac{uv}{c^2}} > u - v.$$

Here  $u' > u - v$  since the denominator  $1 - uv/c^2$  is always less than 1, since both  $u$  and  $v$  are always less than  $c$ . The correct answer is (a).

### Example Problem: Competing spaceships

Two spaceships  $A$  and  $B$  leave Earth traveling in opposite directions with velocities  $v_A = -(3/4)c$  and  $v_B = +(4/5)c$  respectively. How fast does each spaceship see the other move?

There are three frames of reference: the rest frame of Earth, which sees the ships moving at speeds  $v_A$  and  $v_B$ ; the rest frame of spaceship  $A$  (call it frame  $F'_A$ ), and the rest frame of spaceship  $B$  (call it frame  $F'_B$ ).

First consider frame  $F'_A$ , in which ship  $A$  is at rest. Since we are given the velocity of  $B$  in the rest frame of Earth, and the Earth moves with speed  $v_E = +(3/4)c$  relative to this frame, the velocity of  $B$  as measured in this frame is

$$u'_B = \frac{v_B + v_E}{1 + \frac{v_B v_E}{c^2}} = \frac{(4/5)c + (3/4)c}{1 + \frac{(4/5)(3/4)c^2}{c^2}} = \frac{\frac{31}{20}c}{1 + \frac{12}{20}} = \frac{31}{32}c$$

So, spaceship  $A$  sees spaceship  $B$  traveling faster than the observer on Earth sees spaceship  $B$  traveling ( $v_B$ ), which makes sense since spaceship  $A$  is moving in the opposite direction.

Next consider frame  $F'_B$ . In this frame the Earth moves with speed  $v_E = -(4/5)c$ , and we are given the velocity of  $A$  as  $v_A = -(3/4)c$  in the Earth frame. So  $B$  will compute  $A$ 's speed as,

$$u'_A = \frac{v_A + v_E}{1 + \frac{v_A v_E}{c^2}} = \frac{-(3/4)c - (4/5)c}{1 + \frac{(-3/4)(-4/5)c^2}{c^2}} = \frac{-\frac{31}{20}c}{1 + \frac{12}{20}} = -\frac{31}{32}c$$

Spaceship  $B$  sees spaceship  $A$  traveling with the opposite speed that spaceship  $A$  sees spaceship  $B$  traveling—good! And, the relativistic velocity addition formulas ensured that neither sees the other as traveling *faster* than the speed of light.

———End Lecture 4.

### 1.2.6 The Relativistic Doppler Shift

On a daily basis, we experience the Doppler effect in sound. The frequency of a sound increases if the emitter moves towards the observer. This is why, for example, when an ambulance moves towards us we hear it as sounding higher pitched, and when it moves away, we hear it as sounding lower pitched. The speed of sound  $v$  is related to its frequency  $f$  and wavelength  $\lambda$  by  $v = f\lambda$ , so this means that while the frequency increases, the wavelength decreases if the emitter moves towards the observer.

Now we consider the same effect on electromagnetic waves in relativity, known as the relativistic Doppler effect. We can use the Lorentz transformation (again!) to derive this effect.

**Derivation** Consider the following setup: a very fast car is driving away from me at speed  $v$  in my  $\hat{x}$ -direction, sending pulses back towards me at frequency  $f'$  in the car's rest frame (the primed frame,  $F'$ ). Call my rest frame the unprimed frame,  $F$ . We'll derive the frequency of light  $f$  that I observe when the light reaches me. Our strategy is to examine how long it takes me to see two successive wavefronts emitted by the source. Recall that light travels with velocity  $c$ , related to its wavelength and frequency as  $c = \lambda f$ .

Let event  $E_1$  correspond to the spacetime location of one node of the emitted light wave being sent out of the car right as it passes me at  $x = x' = 0$ , and let event  $E_2$  refer to the spacetime location of the subsequent node of the wave being sent out of the car. Let the first event  $E_1$  take place at  $t' = 0$  and  $x' = 0$  in the car's rest frame  $F'$ .

For a wave with frequency  $f'$  in the frame  $F'$ , the period of the wave is  $T' = \frac{1}{f'}$ . (The speed is still  $c$ , satisfying  $c = \lambda' f'$ .) Then if Event 1 is at  $E'_1 = (0, 0)$ , Event 2 occurs a time of  $T'$  later but at the same place (since the car remains at the origin in its own frame), so

$$\begin{aligned} E'_1 &= (t'_1, x'_1) = (0, 0), \\ E'_2 &= (t'_2, x'_2) = (T', 0). \end{aligned}$$

We have neglected the  $y', z'$  coordinates as they will play no role in this derivation. The Lorentz transformation that relates these coordinates in the primed frame to my coordinates in the unprimed frame is,

$$\begin{aligned} t &= \gamma\left(\frac{v}{c^2}x' + t'\right) \\ x &= \gamma(x' + vt') \end{aligned}$$

Plugging in for  $t' = x' = 0$  tells us that in the unprimed frame, Event 1 occurs at  $E_1 = (t_1, x_1) = (0, 0)$ , i.e. the origins of the two coordinate systems coincide (by construction), while Event 2 occurs at

$$\begin{aligned} t &= \gamma(0 + T'), \quad x = \gamma(0 + vT') \\ \Rightarrow E_2 &= (t_2, x_2) = (\gamma T', \gamma v T'). \end{aligned}$$

The light from Event 2 takes additional time to reach me since the car is traveling away from me; it needs to travel the distance of  $x_2 - x_1$  at speed  $c$ . This additional time is then,

$$\Delta t = \Delta x / c = (x_2 - x_1) / c = \gamma v T' / c$$

Thus, even though Event 2 occurs at our time  $t_2 = \gamma T'$ , we don't actually see it until a time  $\Delta t_{\text{tot}}$  of

$$\Delta t_{\text{tot}} = \gamma T' + \gamma v T' / c = \gamma T' \left(1 + \frac{v}{c}\right).$$

$\Delta t_{\text{tot}}$  is precisely the period  $T$  of the wave as observed in my unprimed frame, since I saw the first node at  $t_1 = 0$ , and the second node reached me a time  $\Delta t_{\text{tot}}$  later.

Thus, the period of the wave as observed in my frame is,

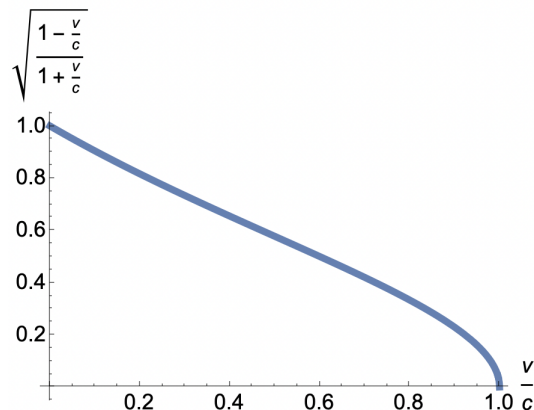
$$\begin{aligned} T &= \frac{1}{f} = \gamma T' \left(1 + \frac{v}{c}\right) = \frac{\gamma}{f'} \left(1 + \frac{v}{c}\right) \\ \Rightarrow f &= f' \frac{\sqrt{1 - \left(\frac{v}{c}\right)^2}}{1 + \frac{v}{c}} = f' \sqrt{\frac{1 - \frac{v}{c}}{1 + \frac{v}{c}}}. \end{aligned}$$

This is the relativistic doppler shift formula, written in the conventions that the source of the light is traveling *away* from me (in my  $+\hat{x}$  direction) with speed  $v$ . To summarize, the frequency of light observed by a stationary observer when the light is emitted by a source that is traveling with speed  $v$  away from the observer is,

$$\boxed{f_{\text{obs}} = \sqrt{\frac{1 - \frac{v}{c}}{1 + \frac{v}{c}}} f_{\text{source}}} \quad (1.23)$$

with the convention that  $+v$  is a source moving away from the observer. If the source is moving towards the observer, we need to take  $v \rightarrow -v$  in the above formula.

To understand the result of this effect on the frequency, we can plot the proportionality factor in (1.23). As we can see in the plot, this factor is always less than or equal to 1; it is equal to 1 in the limit that  $v \rightarrow 0$ , and approaches 0 as  $v$  approaches  $c$ . Therefore, the observed frequency of the wave is *smaller* for a wave whose source is moving away from the observer.



### Example Problem: Problem

How fast must you be moving away from a blue light ( $\lambda = 460 \text{ nm}$ ) for it to appear red ( $\lambda = 650 \text{ nm}$ )?

Since the problem asks about a source and observer moving away from each other, we can use the Doppler shift formula as written, substituting for  $c = f\lambda$ :

$$f_{\text{obs}} = \sqrt{\frac{1 - \frac{v}{c}}{1 + \frac{v}{c}}} f_{\text{source}} \quad \Rightarrow \quad \frac{c}{\lambda_{\text{obs}}} = \sqrt{\frac{1 - \frac{v}{c}}{1 + \frac{v}{c}}} \frac{c}{\lambda_{\text{source}}}$$

Solving for  $v$ , we obtain

$$\begin{aligned} \frac{\lambda_{\text{source}}}{\lambda_{\text{obs}}} &= \sqrt{\frac{1 - \frac{v}{c}}{1 + \frac{v}{c}}} \\ \lambda_{\text{source}}^2 \left(1 + \frac{v}{c}\right) &= \lambda_{\text{obs}}^2 \left(1 - \frac{v}{c}\right) \\ \Rightarrow v &= \frac{c(\lambda_{\text{obs}}^2 - \lambda_{\text{source}}^2)}{(\lambda_{\text{obs}}^2 + \lambda_{\text{source}}^2)} \end{aligned}$$

Substituting for  $\lambda_{\text{obs}} = 650 \text{ nm}$ , and  $\lambda_{\text{source}} = 460 \text{ nm}$ , we obtain

$$v = 0.33c = 9.98 \times 10^7 \text{ m/s}.$$

**Comments** We derived that the frequency of the wave is observed as *smaller* when the source is moving away from us, corresponding to the wavelength observed as being *larger*, so a shift towards the red end of the spectrum. On the other hand, when the source is moving towards us (take  $v \rightarrow -v$ ), we observe the frequency as higher, corresponding to observing smaller wavelengths, corresponding to a blue shift in the spectrum.

This effect is important in making astronomical observations. Astronomers can study a galaxy through the light it emits. An astronomer will often spread the light received by a galaxy into its constituent wavelengths, which will be seen as different colors for visible light. The resulting plot of the brightness against the wavelength is called a *spectrum*. These plots of spectra can tell us about what kind of stars make up the galaxy.

When we view the spectral lines from galaxies in the universe, they appear shifted towards the red end of the spectrum if the galaxy is moving away from us, and towards the blue end of the spectrum if the galaxy is moving towards us. From these observations, scientists have concluded that stars and galaxies are moving *away* from us, since they appear red-shifted. In fact, we now understand that this is because the universe is expanding! Galaxies are moving away from each other, like dots on a balloon that's being blown up. The rate of expansion is characterized by the Hubble parameter  $H$ , which is related to the measured recessional velocity of galaxies. By extrapolating backwards, scientists believe that the universe is about 10 billion years old.

### 1.2.7 Four-vectors and Spacetime

Lorentz transformations offer a powerful tool for handling scenarios in special relativity. They also carry a geometric interpretation: they are the transformations that leave invariant “distances” in spacetime. In this section we'll explore this point, and understand how drawing spacetime diagrams are a convenient tool for visualizing these scenarios.

In 3d space, positions are specified by coordinates  $(x, y, z)$ , with the distance  $d$  between points computed by

$$d^2 = (\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2$$

where  $\Delta x = x_2 - x_1$ , *etc.* However, we have emphasized that in special relativity the time coordinate  $t$  also has important significance; specifying the coordinates of an event in spacetime requires specifying the time coordinate as well as the spatial coordinates, and we have learned that  $t$  itself transforms between frames of reference with the Lorentz transformation. Thus in relativity, it is useful to think of time together with the three spatial coordinates as a 4-component vector, or *4-vector*, in spacetime. In order that each of the components of this 4-vector has the same dimensions, it is useful to label the time component of this 4-vector by  $ct$  rather than  $t$ , which then has units of distance matching the units of  $(x, y, z)$ . We therefore label coordinates in spacetime by,

$$(ct, x, y, z)$$

The distance  $d$  between points in space is invariant under (1) changes of basis of my coordinate system (for example, changing Cartesian to radial coordinates), and (2) Galilean coordinate transformations—you will check this explicitly in your homework. This makes sense: in classical physics, the spatial distance between two events should be the same regardless of which coordinate system I choose to use, and which inertial frame of reference I am in—lengths are invariant in Newtonian mechanics!

However,  $d$  is *not* invariant under Lorentz transformations. This makes sense—in special relativity, lengths contract between different frames, so measuring the spatial distance between points cannot possibly be an invariant of observers moving with different relative velocities. What *is* the invariant notion of distance in special relativity?

The answer is the *spacetime interval*  $\Delta s$ , defined between two events separated by  $(c\Delta t, \Delta x, \Delta y, \Delta z)$  as,

$$\Delta s^2 = -(c\Delta t)^2 + (\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2$$

(Note the funny minus sign in front of  $(c\Delta t)^2$ !) If two events occur simultaneously at the same value of  $t$  so that  $\Delta t = 0$ , then  $\Delta s$  is simply the distance  $d$  that we would normally measure between the two points in space. But more generally,  $\Delta s$  should be thought of as the distance in *spacetime* which is invariant under Lorentz transformations. If we consider two different events, all inertial frames of reference would agree on the value of  $\Delta s$  regardless of which frame it is computed in.

Let's get a feel for what different values of  $\Delta s$  mean. Suppose I consider the path of a light beam in just 1 spatial dimension, so we will only track the  $ct$  and  $x$  coordinates (and drop the  $y, z$  coordinates for now). Say the beam travels at the speed of light in the  $x$  direction between points  $(ct_1, x_1)$  and say  $(ct_2, x_2)$ . Then between the two set of coordinates, it travels a spatial distance of

$$\text{distance light traveled} = x_2 - x_1 = c(t_2 - t_1)$$

Thus, the spacetime interval  $\Delta s$  between these coordinates computes to,

$$(\Delta s)^2 = -c^2(t_2 - t_1)^2 + (x_2 - x_1)^2 = -c^2(t_2 - t_1)^2 + c^2(t_2 - t_1)^2 = 0$$

**The spacetime interval  $\Delta s$  is zero for anything traveling the speed of light.**

The importance of  $\Delta s$  can be illustrated with the help of spacetime diagrams. A spacetime diagram is a plot of  $ct$  against the spatial coordinates  $x, y, z$ , although since it is difficult to draw a 4-dimensional plot, we will focus on spacetime diagrams of just  $ct$  plotted against  $x$ , with  $y$  and  $z$  set to constant values and not depicted. In our example of the light beam, if we put  $ct$  on the vertical axis and  $x$  on the horizontal axis, then the path of the light beam moving to the right with speed  $c$  is a straight line at a  $45^\circ$  angle, since it satisfies  $c\Delta t = \Delta x$  and therefore corresponds to a line with slope 1. This path of the light beam through spacetime is called the *worldline* of the beam. Similarly, if the light beam were moving to the left with speed  $c$ , we would have that its path satisfies  $\Delta x = -c\Delta t$ , so that its worldline corresponds to a line with slope  $-1$  at  $45^\circ$  angle to the negative  $x$ -axis.

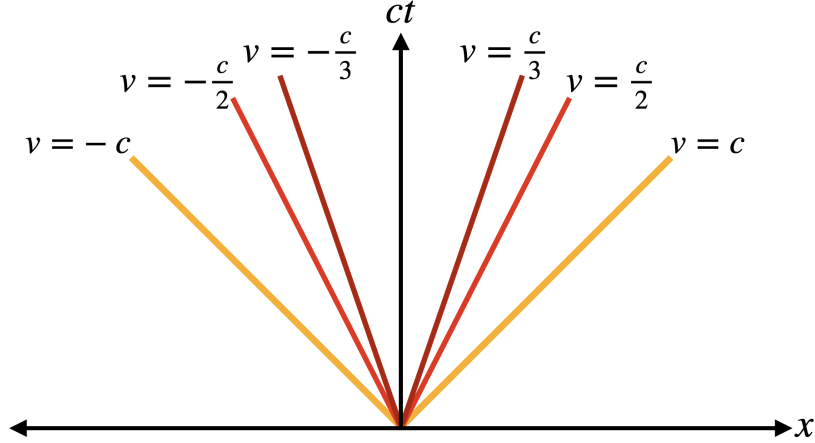
What about a particle moving at constant speed  $v$ ? Since the spatial distance traveled of the object in an interval  $\Delta x$  is equal to  $v\Delta t$ ,  $(\Delta s)^2$  for the path of this object is equal to

$$(\Delta s)^2 = -c^2(\Delta t)^2 + (\Delta x)^2 = -c^2(\Delta t)^2 + v^2(\Delta t)^2 = c^2(\Delta t)^2\left(\frac{v^2}{c^2} - 1\right)$$

Since  $v^2$  is always smaller than  $c^2$ , the factor  $(\frac{v^2}{c^2} - 1)$  is always smaller than 0, so for a particle moving with speed  $v < c$  we have that  $(\Delta s)^2 < 0$ .  **$(\Delta s)^2$  for a particle moving with speed  $v < c$  is always negative.** Plotting the worldline of such a particle on the spacetime diagram means plotting the path

$$\Delta x = v\Delta t \quad \Rightarrow \quad c\Delta t = \frac{c}{v}\Delta x$$

This corresponds to a straight line with slope  $c/v > 1$  in the spacetime diagram. Some examples of worldlines of particles moving with different constant velocities are plotted in the figure.

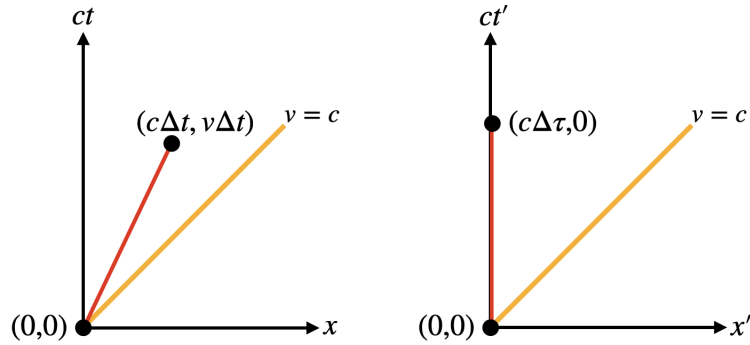


The “cone” of space bounded by the two  $45^\circ$  degree lines that describe the worldlines of light traveling at speed  $c$  is known as the *light cone*. Any worldline of anything moving with speeds less than  $c$  lies within the light cone.

### Example Problem: Lifespan of a particle

A subatomic particle has a lifetime of  $\tau$ .

- (1) On a spacetime diagram, draw the worldline of the particle in its rest frame.
- (2) On a separate diagram, draw the worldline of the particle in a frame in which the particle appears to be moving to the right with speed  $v$ .
- (3) Compute  $(\Delta s)^2$  between the birth and death of the particle in each of the frames of reference. What can you conclude?



In the rest frame of the particle (which we'll call the primed frame  $F'$ ), we compute

$$(\Delta s)^2 = -c^2(\Delta\tau)^2$$

whereas in frame  $F$ ,

$$(\Delta s)^2 = -c^2(\Delta t)^2 + (\Delta x)^2 = -c^2(\Delta t)^2 + v^2(\Delta t)^2 = -c^2(\Delta t)^2 \left(1 - \frac{v^2}{c^2}\right) = -\frac{c^2}{\gamma^2}(\Delta t)^2$$



Equating  $(\Delta s)^2$  in both frames, we find

$$-c^2(\Delta\tau)^2 = -\frac{c^2}{\gamma^2}(\Delta t)^2 \Rightarrow \Delta t = \gamma\Delta\tau$$

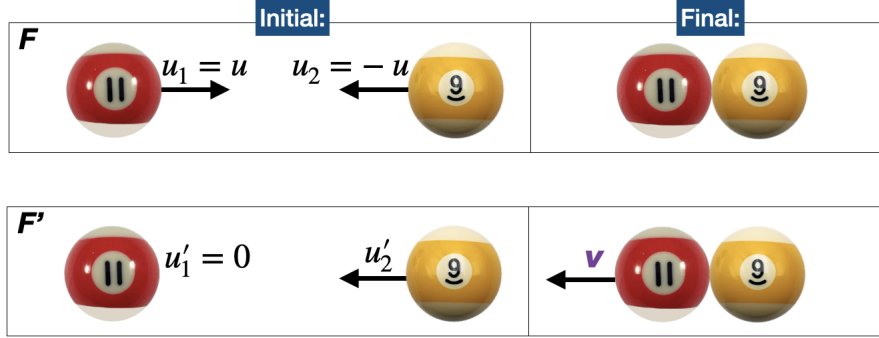
This rederives time dilation between the two frames.

———End Lecture 5.

## 1.3 Energy and Momentum in Special Relativity

### 1.3.1 Relativistic Momentum

We will now examine how the laws of Newtonian mechanics must be generalized to be compatible with the Lorentz transformation and theory of special relativity. In particular, we will see that enforcing that momentum is conserved in every inertial frame will require a reformulating of how momentum is defined.



To motivate this redefinition, let us begin by considering the following inelastic collision between two putty balls: In one frame  $F$ , two putty balls of mass  $m$  come towards each other from opposite directions with the same speed  $u_1 = u_2 \equiv u$ , and stick together to form a stationary mass of putty. In this frame, classical momentum conservation says  $p_i = p_f$ . Indeed,

$$p_i = mu + (-mu) = 0, \quad p_f = 2m(0) = 0 \Rightarrow p_i = p_f.$$

Now, consider the situation in a frame  $F'$  in which the first putty ball is stationary,  $u'_1 = 0$ , and the second is moving towards it with speed  $u'_2$ . According to the Lorentz velocity addition formulae, this frame is related to frame  $F$  by a relative speed  $v$ , where the velocities satisfy

$$u'_1 = \frac{u_1 - v}{1 - \frac{u_1 v}{c^2}} = \frac{u - v}{1 - \frac{uv}{c^2}} = 0, \quad u'_2 = \frac{u_2 - v}{1 - \frac{u_2 v}{c^2}} = \frac{-u - v}{1 - \frac{(-u)v}{c^2}}$$

The first equation says that  $u - v = 0$ , or  $v = u$ . Thus, the frame  $F'$  is related to the frame  $F$  by a boost by velocity  $u$ ; according to frame  $F$ , frame  $F'$  moves to the right with speed  $u$ . Since initially the final mass of putty was stationary, the final mass of putty is now moving with speed  $v = u$  to the left, in this frame.

Then, the second equation says that

$$u'_2 = \frac{-2u}{1 + \frac{u^2}{c^2}}.$$

Thus, in this frame,

$$p_i = mu'_1 + mu'_2 = \frac{-2mu}{1 + \frac{u^2}{c^2}}, \quad p_f = -2mu$$

$$\Rightarrow p_i \neq p_f!$$

*Momentum is not conserved in the frame  $F'$ !*

We require a definition of momentum that is conserved in both frames simultaneously. We will state the result without proof: the required definition of *relativistic momentum* of an object of rest mass  $m$  and velocity  $\vec{u}$  that is conserved in all inertial frames is as follows:

Relativistic momentum: $\vec{p} = \gamma_u m \vec{u}, \quad \gamma_u = \frac{1}{\sqrt{1 - \frac{u^2}{c^2}}}$	(1.24)
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Relativistic momentum defined this way holds in all inertial frames, whenever the net external force on a system is zero, just as in the case for classical momentum. Take care that  $u$  is the speed of the object, not a relative speed between reference frame, and we've put a subscript  $u$  on  $\gamma_u$  to remind ourselves that this gamma-factor is a function of this speed  $u$ .

This definition of momentum requires a new concept: the concept of rest mass. In relativity, mass itself is a relativistic quantity! By rest mass, we mean the mass of an object in the frame in which it's at rest. Mass is not a conserved quantity in special relativity, which we'll see in more detail later.

Some comments on this definition of relativistic momentum:

- Relativistic momentum has the same units as Newtonian momentum (as it had to!), since  $\gamma$  is dimensionless.
- As usual, let us consider the classical limit. When  $u \ll c$  so that the object is moving slow compared to the speed of light,  $\gamma \rightarrow 1$ , and we reproduce  $\vec{p} = m\vec{u}$ . We are thus consistent with classical physics at small velocities compared to the speed of light.
- Next consider the ultrarelativistic limit, when  $u \sim c$  so that  $\gamma \rightarrow \infty$ . For a massive object moving at ultrarelativistic speeds, the momentum goes to infinity! This is another indication that anything with mass cannot go the speed of light—such an object would have to have infinite momentum!
- *Aside:* Where does this definition come from? It's the formula for the classical momentum, but computed in the rest frame of the object, so with  $\vec{u} = d\vec{x}/d\tau$  computed in increments of proper time, and with  $m$  the proper mass in the rest frame. You can verify (as your book does) that  $\frac{dx}{d\tau} = \frac{dx}{dt} \frac{dt}{d\tau} = \gamma \frac{dx}{dt}$ .

**Newton's second law made relativistic** As a quick aside, let us note that Newton's second law takes a new form in special relativity. We define force the same way in special relativity as in Newtonian mechanics,

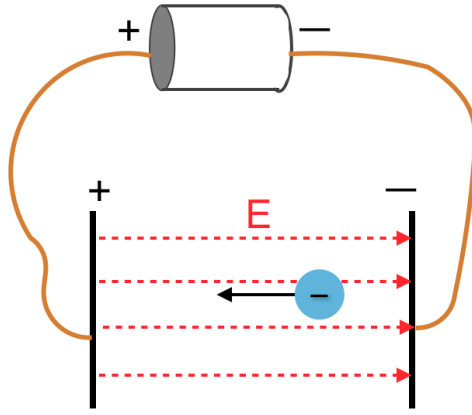
$$\vec{F} = \frac{d\vec{p}}{dt},$$

except that now, we apply the new definition of relativistic momentum,  $\vec{p} = \gamma m \vec{u}$ . Taking the derivative,

$$\begin{aligned}\vec{F} &= \frac{d\vec{p}}{dt} = \frac{d}{dt} \left( \frac{m\vec{u}}{\sqrt{1 - \frac{u^2}{c^2}}} \right) = \frac{d\vec{u}}{dt} \cdot \frac{d}{du} \left( \frac{mu}{\sqrt{1 - \frac{u^2}{c^2}}} \right) = m \frac{d\vec{u}}{dt} \left( \frac{1}{\sqrt{1 - \frac{u^2}{c^2}}} - \frac{1}{2} \frac{(-2u)}{c^2} \frac{1}{\left(1 - \frac{u^2}{c^2}\right)^{\frac{3}{2}}} \right) \\ \Rightarrow \quad \vec{F} &= \left(1 - \frac{u^2}{c^2}\right)^{-\frac{3}{2}} m \frac{d\vec{u}}{dt} = \gamma^3 m \frac{d\vec{u}}{dt}\end{aligned}\tag{1.25}$$

where we can define the acceleration as the rate of change of velocity,  $\vec{a} = \frac{d\vec{u}}{dt}$ . We see that Newton's second law adjusts; forces in different frames need to be scaled by a factor of  $\gamma^3$ .

—————End Lecture 6.



This relativistic version of Newton's second law is crucial to how linear particle accelerators work. Consider the following experiment: A particle of charge  $e$  and mass  $m$  moves in a straight line with speed  $u$  in a uniform electric field  $\vec{E}$  in between parallel plates that are separated by a distance  $d$ . It accelerates under the force due to the electric field,  $\vec{F} = e\vec{E}$ . The field between the plates is related to the potential difference  $V$  between the plates,

$$\vec{F} = e\vec{E}, \quad E = \frac{V}{d}.$$

Using  $F = \gamma_u^3 ma$ , the magnitude of the acceleration of the particle is then

$$a = \frac{du}{dt} = \left| \frac{\vec{F}}{m} \right| \left(1 - \frac{u^2}{c^2}\right)^{\frac{3}{2}} = \frac{qE}{m} \left(1 - \frac{u^2}{c^2}\right)^{\frac{3}{2}} = \frac{eV}{dm} \left(1 - \frac{u^2}{c^2}\right)^{\frac{3}{2}}.$$

The larger the potential difference  $V$  across the plates, the larger the force on the particle, and the larger the resulting acceleration of the particle. Linear accelerators operating on this principle are used to accelerate particle to high speeds and collide them with other particles, resulting in high energy collisions that can be used to probe the structure of matter!

**A note on units:** remember that  $e$  (sometimes called  $q$ ) is the elementary charge, which is the electric charge carried by a single proton, or equivalently  $-e$  is the charge carried by a single electron. In SI units,

$$e = 1.602 \times 10^{-19} \text{ C}.$$

Often in particle physics, the combination  $e$  times a potential difference comes up, as it did in this last problem. This combination has units of energy. Define an *electron-volt*, or 1 eV, as the work done on an electron in accelerating it through a potential difference of one volt. In SI units, this is

$$1 \text{ eV} = 1 \cdot (1.602 \times 10^{-19} \text{ C}) \cdot \frac{(kg \cdot m^2 \cdot s^{-2})}{C} = 1.602 \times 10^{-19} \text{ kg} \cdot m^2/s^2 = 1.602 \times 10^{-19} \text{ J}.$$

Then, an MeV is a mega-electron-volt ( $10^6$  eV), a giga-electron-volt is  $10^9$  eV, and so on. Typical particle physics processes occur at energies of around 1 MeV= $10^6$  eV or 1 keV= $10^3$  eV.

Momentum has units of [Energy]/ $c$ , and mass has units of [Energy]/ $c^2$ , thus it is usual to measure momentum in units of eV/ $c$ , and mass in units of eV/ $c^2$ .

### 1.3.2 Total Energy and Rest Mass in Special Relativity

In much the same way that we had to redefine momentum to find a version which is conserved in the relativistic setting, we must do the same for energy. The result is as follows: the total relativistic energy of a particle with mass  $m$  and speed  $u$  is

Total relativistic energy:  $E = \gamma_u m c^2, \quad \gamma_u = \frac{1}{\sqrt{1 - \frac{u^2}{c^2}}}$

(1.26)

The subscript on  $\gamma_u$  is meant to indicate that the velocity in its argument is the velocity of the particle,  $u$ . The *rest energy* is the part of the total energy with  $u = 0$  (the energy of the particle when it is at rest), given by

Rest energy:  $E_0 = m c^2$ .

(1.27)

$m$  is the *rest mass*, a “fingerprint” of a particle. This is Einstein’s famous formula! It implies that even stationary mass has energy associated to it. Unlike in Newtonian mechanics, in relativistic physics mass and energy are two sides of the same coin. Mass can convert to energy, and vice versa, with conversion factor  $c$ . Think of  $c$  like the exchange rate of mass to energy conversion.

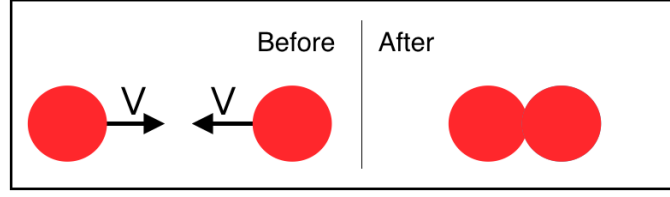
We’ve just learned that energy is conserved, but mass is not! As a result, in an interaction between particles mass does not need to be conserved. Let’s see this effect at play in the following example:

#### Clicker Question: An inelastic collision

*Concepts: conservation of relativistic energy, mass in relativity*

Return to the example with which we started this section. Consider two particles of mass  $m$  coming towards each other from opposite directions, each with speed  $u$ . The particles collide and stick together, so that afterwards there is just one stationary mass.

Use relativistic energy conservation to determine: Is the mass  $M$  of the final state object bigger than, equal to, or smaller than  $2m$ ?



By relativistic energy conservation, the sum of the relativistic energy of a system of particles before interaction must equal the sum after the interaction. Initially, the energy of each particle is  $\gamma_u mc^2$ , while the energy of the stationary final state (which is at rest) is  $Mc^2$ . Solving for  $M$ ,

$$\begin{aligned} \frac{mc^2}{\sqrt{1 - \frac{u^2}{c^2}}} + \frac{mc^2}{\sqrt{1 - \frac{u^2}{c^2}}} &= Mc^2 \\ \Rightarrow M &= \frac{2m}{\sqrt{1 - \frac{u^2}{c^2}}} > 2m. \end{aligned}$$

Thus, the total mass of the final state is *bigger* than the sum of the masses of the initial two particles! As we see here, mass is not an invariant quantity—mass is not conserved, but rather the total relativistic energy is conserved.

### 1.3.3 Relativistic Kinetic Energy

We've discussed that the total energy of a particle is given by  $E = \gamma_u mc^2$ , and the rest energy is given by  $E_0 = mc^2$ . If we just subtract off the rest energy to find the kinetic portion of the energy, we obtain,

Relativistic kinetic energy:  $K_{\text{rel}} = E - E_0 = (\gamma_u - 1)mc^2$

(1.28)

In our example of an inelastic collision, we can ask: Where did the increase in mass come from? It came from the kinetic energy of the initial particles. Each initial particle has kinetic energy

$$K_{\text{rel}} = (\gamma_u - 1)mc^2,$$

and the increase in mass between the initial and final states is precisely equal to,

$$\Delta M = M - 2m = 2(\gamma - 1)m = \frac{2K_{\text{rel}}}{c^2}.$$

We can conclude that the kinetic energy of the initial particles is not lost, but is transformed into more mass in the final state.

Some comments are in order:

- At first glance, this expression looks nothing like the classical version,  $K = \frac{1}{2}mu^2$ . So far when we've been taking the classical limit  $v/c \rightarrow 0$ , we've taken  $\gamma \rightarrow 1$ , so that the relativistic kinetic energy (1.28) goes to zero in this limit. Is this a violation of the correspondence principle, that our special relativistic formulas should reduce to classical physics in the right limit?

The answer is no—we simply need to keep higher order terms in  $\gamma_u$ . From the definition of the relativistic gamma factor, we can rewrite it as,

$$\gamma_u = \frac{1}{\sqrt{1 - \frac{u^2}{c^2}}} = \left(1 - \frac{u^2}{c^2}\right)^{-\frac{1}{2}}$$

We are interested in the classical limit that all speeds are small compared to the speed of light,  $u/c \ll 1$ . Perhaps you remember the binomial theorem, which states that for a small number  $\epsilon \ll 1$ ,

$$(1 + \epsilon)^a = 1 + a\epsilon + \text{even smaller terms}, \quad \epsilon \ll 1$$

In our definition of  $\gamma_u$  we can identify that  $\epsilon = -u^2/c^2$  as our small number, so that indeed  $\gamma_u$  takes the form  $\gamma_u = (1 + \epsilon)^a$  with exponent  $a = -1/2$ . Then,

$$\gamma_u = \left(1 - \frac{u^2}{c^2}\right)^{-\frac{1}{2}} \approx 1 + \left(-\frac{1}{2}\right)\left(-\frac{u^2}{c^2}\right) = 1 + \frac{1}{2} \frac{u^2}{c^2}, \quad \frac{u}{c} \ll 1.$$

Substituting into our formula for the kinetic energy, we obtain,

$$K_{\text{rel}} = (\gamma_u - 1)mc^2 \approx \left(1 + \frac{1}{2} \frac{u^2}{c^2} - 1\right) mc^2 = \frac{1}{2} mu^2$$

in the limit that  $u \ll c$ . At leading order in this expansion in  $\epsilon$  the relativistic kinetic energy vanishes, but by keeping the subleading order term we obtain something nonvanishing. Thus, we in fact do reproduce the classical formula, we just needed to keep track of one higher order term in our approximation for  $\gamma_u$  in this limit! At small velocities compared to the speed of light, our relativistic formula for the kinetic energy reproduces that of the kinetic energy of a particle of mass  $m$  moving at speed  $u$ .

- What about the ultra relativistic limit? The classical expression for the kinetic energy goes to infinity as  $u \rightarrow \infty$ , but this is not physical since we've learned that  $c$  is a fundamental speed limit in nature. The relativistic expression fixes this non-relativistic expression, so that the  $K_{\text{rel}} \rightarrow \infty$  when  $u \rightarrow c$ . One way to read this is that no matter how energetic the particle is (even if it has infinite kinetic energy!) it will never go faster than the speed of light.

A further comment is in order. Combining our definitions of  $E$  and  $p$ , we find a very useful expression:

$$\begin{aligned} E^2 - p^2 c^2 &= (\gamma m c^2)^2 - (\gamma m v)^2 c^2 = \gamma^2 m^2 c^4 \left(1 - \frac{v^2}{c^2}\right) = m^2 c^4 \\ &\Rightarrow \boxed{E^2 = p^2 c^2 + m^2 c^4}. \end{aligned} \tag{1.29}$$

This is a formula that relates the total relativistic energy of a particle of mass  $m$  with its momentum  $p$ , and is independent of the particle's speed!

What about particles with no mass? According to this formula, the total energy of a particle with zero rest mass is

$$\boxed{\text{Energy of massless particle : } E = pc}, \tag{1.30}$$

or put another way, the momentum of a massless particle is

$$p = \frac{E}{c}.$$

Photons are examples of particles with no mass. This equation then means that light itself has momentum, even though it doesn't have any mass!

### 1.3.4 Examples

We've introduced several new definitions: relativistic momentum, rest energy, total energy, and kinetic energy. We'll now do a few examples to further explore these concepts.

#### Example Problem: Sunshine won't be forever!

*Concepts: rest energy*

Solar energy reaches the Earth at a rate of  $1.4 \text{ kW}$  per square meter of surface perpendicular to the direction of the sun. By how much does the mass of the sun decrease per second owing to energy loss? The mean radius of the Earth's orbit is  $1.5 \times 10^{11} \text{ m}$ .

First we need to find the total power lost by the sun,  $P_{\text{lost}}^{\text{sun}}$ , when we are given the power per square meter received by Earth,  $P_{\text{incident}}^{\text{Earth}}/m^2$ . The surface area of a sphere of radius  $r$  is  $A = 4\pi r^2$ . The total power radiated by the sun out to a distance of radius  $r$  is equal to the power received by a sphere whose radius is equal to Earth's orbit radius. However, only  $P_{\text{incident}}^{\text{Earth}} = 1.4 \text{ kW}$  of power is incident on Earth per square meter. So, the total power lost is,

$$P_{\text{lost}}^{\text{sun}} = \frac{P_{\text{incident}}^{\text{Earth}}}{m^2} (4\pi r^2) = (1.4 \times 10^3 \text{ W/m}^2) \cdot 4\pi (1.5 \times 10^{11} \text{ m})^2 = 4.0 \times 10^{26} \text{ W}.$$

Power (given in Watts) is equal to energy (in joules) per second. Therefore, the sun loses  $E_0 = 4.0 \times 10^{26} \text{ J}$  of energy per second. This is rest energy, since we can approximate the sun as at rest relative to the Earth. Converting this rest energy to a mass, the sun is losing

$$m = \frac{E_0}{c^2} = \frac{4.0 \times 10^{26} \text{ J}}{(3 \times 10^8 \text{ m/s})^2} = 4.4 \times 10^9 \text{ kg/s}.$$

The sun will eventually lose all of its mass: given that the mass of the sun is approximately  $2.0 \times 10^{30} \text{ kg}$ , this will happen in about

$$t = \frac{2.0 \times 10^{30} \text{ kg}}{4.4 \times 10^9 \text{ kg/s}} = 4.5 \times 10^{20} \text{ s} \approx 14 \text{ billion years}.$$

One day the sun will be gone, and the solar system will not be a hospitable place for life.

#### Clicker Question: Fast proton

*Concepts: total relativistic energy and momentum*

A proton of mass  $m_p$  has a kinetic energy that is 3 times larger than its rest energy.

- (a) Find the total energy.
- (b) Find the speed and momentum of the particle.

We are told the  $K_{\text{rel}} = 3E_0$ , so the total energy is given by,

$$E = K_{\text{rel}} + E_0 = 3E_0 + E_0 = 4E_0$$

The rest energy is  $E_0 = m_p c^2$ , therefore

$$E = 4m_p c^2.$$

Given the total energy, we can find the momentum from,

$$\begin{aligned} E^2 &= p^2 c^2 + m_p^2 c^4 \\ \Rightarrow p &= \sqrt{E^2/c^2 - m_p^2 c^2} = \sqrt{(4m_p c^2)^2/c^2 - m_p^2 c^2} = \sqrt{15} m_p c \end{aligned}$$

Having solved for the momentum, we can solve for the speed using the relation,

$$p = \gamma_u m_p u = \frac{m_p u}{\sqrt{1 - \frac{u^2}{c^2}}}$$

Isolating the speed  $u$  results in,

$$p^2 \left(1 - \frac{u^2}{c^2}\right) = m_p^2 u^2 \quad \Rightarrow \quad u^2 = \frac{p^2}{(m_p^2 + p^2/c^2)} = \frac{15m_p^2 c^2}{m_p^2 + 15m_p^2} = \frac{15}{16} c^2$$

Or in other words,  $u = \sqrt{\frac{15}{16}} c$ . Now that's a fast proton!

### Clicker Question: Relativistic kinetic energy

*Concepts: total relativistic energy and momentum*

A particle has a relativistic momentum of  $6 \text{ MeV}/c$  and a mass of  $8 \text{ MeV}/c^2$ . Its kinetic energy is:

- (a) 2 MeV
- (b) 10 MeV
- (c) 14 MeV
- (d) 6 MeV

We've learned that the kinetic energy is

$$K_{\text{rel}} = E - mc^2,$$

and the total energy is

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

Using  $pc = 6 \text{ MeV}$ , and  $mc^2 = 8 \text{ MeV}$ , we obtain,

$$K_{\text{rel}} = \sqrt{p^2 c^2 + m^2 c^4} - mc^2 = \sqrt{36 \text{ MeV}^2 + 64 \text{ MeV}^2} - 8 \text{ MeV} = 2 \text{ MeV}.$$

Correct answer is (a).

—————End Lecture 7.



The following two problems we will not cover in class, but if you want some extra practice I encourage you to work on them at home.

### Example Problem: Accelerating electrons

*Concepts: total relativistic energy, practice with units*

Setup: an electron is accelerated from rest through a potential difference of  $10^6$  volts (1 Megavolt) from a metal cathode to a metal anode. Find its speed at the anode, expressed as a fraction of  $c$ . (Note that the mass of an electron in units of electron-volts per  $c^2$  is  $0.511 \text{ MeV}/c^2$ .)

It takes one electron-volt (eV) to accelerate an electron from rest through a potential difference of 1 volt. If the electron is accelerated through a potential difference of  $V = 10^6$  volts, then the kinetic energy of the electron after the acceleration will be 1 MeV. The rest energy of the electron is  $E_0 = m_e c^2 = 0.511 \text{ MeV}$ . Thus, the total energy of the electron at the anode is

$$E = K_{\text{rel}} + E_0 = 1 \text{ MeV} + 0.511 \text{ MeV} = 1.511 \text{ MeV}.$$

The total energy is  $E = \gamma_u m_e c^2$ , so we can use this to solve for  $u$ :

$$\begin{aligned} E = \gamma_u m_e c^2 &= \frac{m_e c^2}{\sqrt{1 - \frac{u^2}{c^2}}} \Rightarrow 1 - \frac{u^2}{c^2} = \left( \frac{m_e c^2}{E} \right)^2 \\ \frac{u}{c} &= \sqrt{1 - \left( \frac{m_e c^2}{E} \right)^2} = \sqrt{1 - \left( \frac{0.511}{1.511} \right)^2} = \sqrt{1 - 0.11} = 0.94 \\ &\Rightarrow u = 0.94c. \end{aligned}$$

### Clicker Question: Accelerating electrons

*Concepts: relativistic momentum, practice with units*

In the previous example, obtain the electron's momentum when it reaches the anode, in units of  $\text{MeV}/c$ .

- (a)  $0.16 \text{ MeV}/c$
- (b)  $1.96 \text{ MeV}/c$
- (c)  $1.41 \text{ MeV}/c$
- (d)  $0.48 \text{ MeV}/c$

We can either use  $p = \gamma m_e u$ , or  $p^2 c^2 = E^2 - m_e^2 c^4$ . Using the former, the relevant quantities from the previous example are  $m_e c^2 = 0.511 \text{ MeV}$ , and  $u = 0.94c$ .

$$p = \gamma_u m_e u = \frac{m_e u}{\sqrt{1 - \frac{u^2}{c^2}}} = \frac{0.511 \text{ MeV}/c^2 \cdot 0.94c}{\sqrt{1 - (0.94)^2}} = 1.41 \text{ MeV}/c.$$

The correct answer is (c).

### 1.3.5 Beyond Special Relativity (not tested)

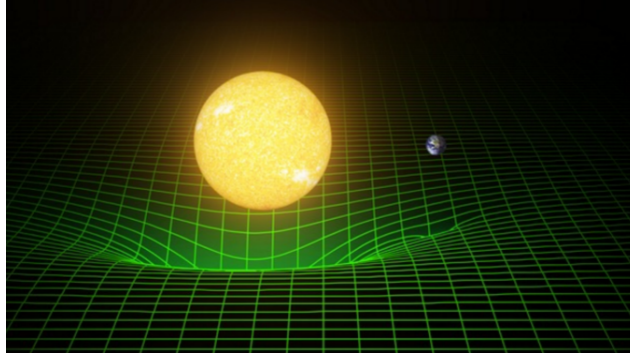


Figure 2: Curvature bends in the vicinity of massive objects. Credit: T. Pyle/Caltech/MIT/LIGO lab.

The consistency of special relativity relied on the existence of inertial frames of reference: frames in which a particle at rest in it stays at rest if no force acts on it. In Newtonian mechanics, gravity is regarded as a force.

However, it turns out that gravity is distinguished from all the other forces in a very important way: *all* particles, regardless of their internal composition, follow exactly the same trajectory in a gravitational field. What this means for us as experimentalists on Earth is that we can't experimentally find the trajectory of a particle that's unaffected by gravity, and so can't define an inertial frame at rest on Earth.

Consider the following example: imagine yourself on a uniformly accelerating rocket ship in empty space, where there is no gravity. From your point of view inside the rocket, there is a gravitational field inside the rocket: if I drop a ball, it accelerates downwards, much like dropping a ball on Earth. Just standing stationary in the ship, I have a weight equal to the force required to keep myself accelerating along with the ship that's proportional to my mass—just as I do on Earth.

In fact, any experiment I could do in such a uniformly accelerating reference frame of acceleration  $a$  is completely indistinguishable from the same experiments performed in a non-accelerating reference frame situated in a uniform gravitational field in which the acceleration due to gravity is  $g = -a$ . This is the (*weak*) *principle of equivalence* between gravity and acceleration. Another way to put this is that an object's *inertial mass*—the mass that measures resistance to being accelerated by a force,  $m_i = F/a$ —and *gravitational mass*—the degree to which it's affected by a gravitational field,  $m_g = F_g/g$ —are the same.

This observation, made by Einstein in 1915, is the starting point for the theory of **general relativity**. General relativity reduces to special relativity in the limit that gravitational effects become less important.

Einstein developed an ingenious way to deal with these accelerating frames: by replacing the concept of gravitational force with curvature of spacetime. The presence of a mass causes a curvature of spacetime in the vicinity of the mass, and this curvature dictates the path in spacetime that all objects must follow. As summarized by American theoretical physicist John Wheeler, “Space tells matter how to move and matter tells space how to curve.”

**One consequence of general relativity: Gravitational waves** You might have heard in the news a couple of years ago that gravitational waves were directly detected experimentally for the first time. Gravitational waves can be thought of as ripples in the fabric of spacetime caused by massive accelerating objects. These wavelike solutions are a lot like electromagnetic waves, and travel at the speed of light.

In 2016, the Laser Interferometer Gravitational-Wave Observatory (LIGO) announced that they'd detected gravitational waves from a merger of 2 black holes. LIGO uses laser interferometry (like what you learned in studying the Michelson-Morley interferometry experiment) to search for signals of gravitational waves from astrophysical events.

The signal came from an event in which two black holes which were each about 30 times the mass of the sun spiraled in towards each other, collided, and merged 1.3 billion years ago. The 2017 Nobel Prize in Physics was awarded for this work on the detection of gravitational waves!

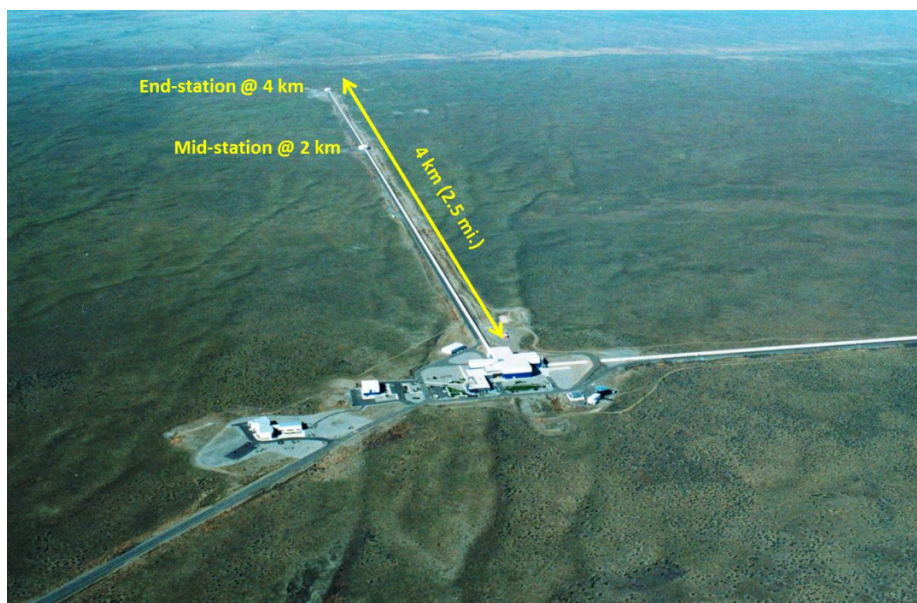


Figure 3: One of twin LIGO observatories, this one in Washington state. Credit: Caltech/MIT/LIGO Lab.

## 2 Part II: Wave-Particle Duality and Motivations for Quantum Physics

### 2.1 The Quantum Theory of Light

In the late 19th century, classical physics assumed the following:

- That Newton's laws apply universally.
- Light is an electromagnetic wave, described by Maxwell's equations.
- Atoms are the basic constituents of matter.

However, there were several experiments that could not be explained by classical physics. Sorting out these inconsistencies led to a revolution in scientific thought at the turn of the 20th century, which led to the birth of quantum theory and a radical change in how we think about nature. The resolutions to these inconsistencies will imply that Newton's laws do not apply to the microscopic world of the electron; that light also has a particle-like nature; and that atoms are not the most microscopic objects. The new theory of quantum mechanics will be needed to describe the world of the subatomic particles, and this theory is probabilistic by nature, as compared to the deterministic nature of classical physics.

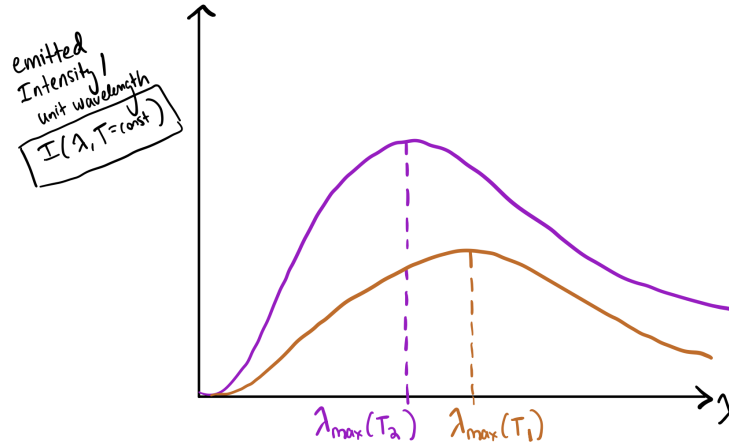
In this section, we will explore a series of classical puzzles and their resolutions (blackbody radiation, the photoelectric effect, the Compton effect) that led to a quantum theory of light. We will go on a journey of discovery through trial and error, making classical assumptions and seeing where they go wrong, and seeing what new assumptions are needed to fix them up. In this sense, our discussion Part II of this course will be somewhat less clean than our presentation of special relativity. Later when we get to quantum mechanics, we will understand a top-down theory starting from the postulates of quantum mechanics that can satisfactorily explain these results.

#### 2.1.1 Blackbody Radiation

When heated, all objects emit light. An object at any temperature will emit electromagnetic radiation of a variety of wavelengths, some wavelengths with more intensity than others. Objects around room temperature radiate mainly in the infrared part of the spectrum. If we heat up an object to about  $1500^\circ$  it will glow red. The sun, whose surface temperature is around 5000-6000 Kelvin, radiates most strongly in a range of wavelengths around 560 nm, corresponding to the yellow part of the electromagnetic spectrum.

We can plot  $I(\lambda, T)$  the intensity per unit wavelength that the object emits at a given temperature as a function of  $\lambda$ , and the result will look something like the the figure above.

Radiation that is incident on an object will be partially absorbed, and partially reflected. A *blackbody* refers to a system which is a perfect absorber: it absorbs all electromagnetic radiation incident upon it, and re-radiates out energy which is characteristic of the blackbody and *not* the type of light incident upon it. In order to stay in thermal equilibrium, it must emit radiation at the same rate that it absorbs it, and so thus it is also a perfect emitter. So in other words, a blackbody is a system in perfect thermal equilibrium at a particular temperature, that is opaque and non-reflecting.



There are two important experimental facts related to the graph of blackbody radiation intensity:

- There will typically be some wavelength where this plot peaks, so that light of those wavelengths is most strongly radiated by the object at the given temperature. The larger the temperature and so the hotter the body, the shorter the wavelength corresponding to this peak in the radiation curve. This is encapsulated by the Wien displacement law:

$$\boxed{\text{Wien displacement law: } \lambda_{\max} T = 2.898 \times 10^{-3} \text{ m} \cdot \text{K}} \quad (2.1)$$

- The total intensity of the light integrated over all wavelengths is equal to the area under the curve. Experimentally the data follows Stefan's law, that the total intensity is proportional to  $T^4$  as,

$$\begin{aligned} \text{total intensity (integrated over all wavelengths)} &= \text{area under curve of } I(\lambda, T) \\ &= \frac{\text{Power}}{\text{Area}} = \sigma T^4 \end{aligned}$$

In other words,

$$\boxed{\text{Stefan's law: } P(T) = \sigma A T^4} \quad (2.2)$$

where  $A$  is the surface area of the blackbody, and  $\sigma$  is the Stefan-Boltzman constant,  $\sigma = 5.670 \times 10^{-8} \text{ W}/(\text{m}^2 \cdot \text{K}^4)$ . So if we know the size of the object at a given temperature that is emitting blackbody radiation, we can compute its total power emitted (i.e. energy per unit time).

*Aside:* The universe is filled with radiation! If you look at the energy spectrum, it matches the spectrum of a perfect blackbody very well, whose temperature is 2.7 Kelvin. This is known as cosmic microwave background (CMB) radiation, which you can think of as the “fossil” radiation that was released soon after the big bang, and so is the furthest any telescope can see. It's the thermal relic of a hot, dense era of the universe. The CMB provides arguably the best evidence for the big bang.

### Example Problem: The power of the early universe

The CMB radiation very well approximates a blackbody with temperature 2.7 K. What is the average power per unit area?

*Solution:* Using Stefan's law, the power per unit area is,

$$\frac{P}{A} = \sigma T^4 = (5.670 \times 10^{-8} \text{ W/(m}^2 \text{K}^4)) (2.7 \text{ K})^4 = 3 \times 10^{-6} \text{ W/m}^2$$

**The ultraviolet catastrophe of classical physics** Rayleigh and Jeans calculated the emission spectrum of a blackbody as follows. A good example of a blackbody is a cubic cavity with a small hole, so that any light incident upon the hole goes into the cavity and is essentially trapped. Rayleigh and Jeans treated the radiation as waves trapped inside the cavity, and then calculated the energy density of the radiation inside the cavity. Since the cavity is a perfect emitter, this also gives the emission spectrum, i.e. the energy density emitted from the blackbody. We'll use the variable  $u(\lambda, T)$  for this energy density per unit wavelength, which is related to the emitted intensity per unit wavelength by an annoying factor of  $4/c$  (which has to do with the fact some smaller fraction of the radiation bouncing around the 3d cavity actually leaves through the small hole),

$$u(\lambda, T) = \text{energy} / \text{unit volume} / \text{unit wavelength} = \frac{4}{c} I(\lambda, T)$$

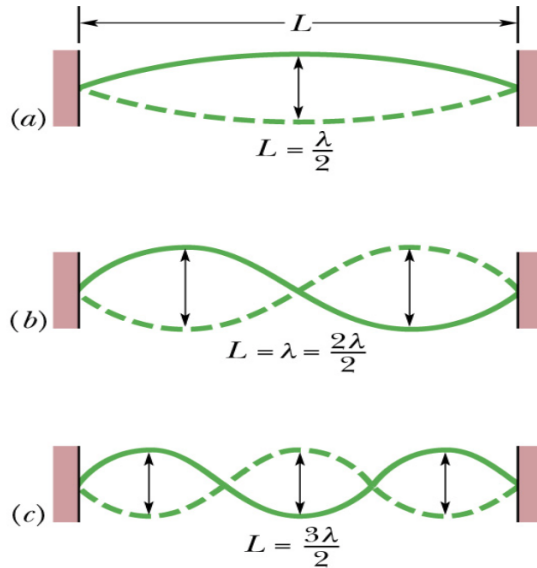


Figure 4: Standing waves on a string of length  $L$ .

It is instructive to review their classical calculation. Consider a cubic cavity with sides of lengths  $L$  filled with electromagnetic radiation. Radiation is reflected back and forth between the walls, and is in thermal equilibrium with the walls of the box. As the system comes to thermal equilibrium, only the standing waves with nodes at the walls will persist.

The strategy of the calculation is to solve for the energy density of the radiation is as follows.

**Step 1:** We first ask, how many standing waves of wavelength  $\lambda$  can fit inside the box? Standing waves are labeled by integers called *modes*. Since the radiation in a given range of

wavelengths should be proportional to the number of standing waves in that range, we need to find the number of modes  $n(\lambda)$  per unit wavelength per unit volume that can fit inside the cavity:

$$n(\lambda) d\lambda = \# \text{ of modes per unit volume with wavelengths between } \lambda \text{ and } \lambda + d\lambda$$

Below we will review this step in some detail, since it will not change between the classical and quantum pictures.

**Step 2:** The electromagnetic energy per unit volume at temperature  $T$  in a range of wavelengths between  $\lambda$  and  $\lambda + d\lambda$ , which we call  $u(\lambda, T)$ , is therefore, given by the *average* energy per mode of wavelength  $\lambda$ ,  $E_{\text{avg}}(\lambda)$ , times the number of modes per unit volume in the range  $(\lambda, \lambda + d\lambda)$ :

$$u(\lambda, T) d\lambda = E_{\text{avg}}(\lambda) n(\lambda) d\lambda$$

Thus, the second step is to determine this average energy per mode.

To accomplish the first step and solve for  $n(\lambda)$ , let us first recall some basics about standing waves. A standing wave (also called a stationary wave) is a wave that oscillates in time, but appears to just vibrate in place. A standing wave in one dimension of length  $L$  occurs when a half-integer number of wavelengths fits in the length  $L$ , such that the amplitude of the wave is zero (a node) at the walls.

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

The integer  $n$  labels the *mode* of the standing wave.

An electromagnetic standing wave in a 3d cavity at equilibrium is a solution to Maxwell's equations inside the cavity, which imply that the  $\vec{E}$  and  $\vec{B}$  fields satisfy the 3d wave equation,

$$\frac{\partial^2 \vec{E}}{\partial x^2} + \frac{\partial^2 \vec{E}}{\partial y^2} + \frac{\partial^2 \vec{E}}{\partial z^2} = \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2}. \quad (2.3)$$

The boundary conditions are that the electric field at the metal walls are zero, so a mode for an electromagnetic wave in a cavity must satisfy the condition of zero electric field at the wall. Let the walls be at  $x = L, y = L, z = L$ . Solutions to this equation with these boundary conditions are of the form

$$\vec{E} = \vec{E}_0 \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) \sin\left(\frac{n_z \pi}{L} z\right) \sin\left(\frac{2\pi c}{\lambda} t\right), \quad n_i \in \mathbb{Z}, > 0 \quad (2.4)$$

labeled by the positive integers  $n_x, n_y, n_z$  that are constrained to satisfy

$$n_x^2 + n_y^2 + n_z^2 = \frac{4L^2}{\lambda^2} \quad (2.5)$$

These integers label the possible solutions to the allowed standing modes inside the box.

*Suggested Exercise:* check by substituting (2.4) into the wave equation (2.3) that this is indeed a solution to the wave equation, if the integers  $n_x, n_y, n_z$  satisfy (2.5). Furthermore, check that substituting  $x = 0, L$  and/or  $y = 0, L$  and/or  $z = 0, L$  yields  $\vec{E} = 0$ , so that this solution satisfies the necessary boundary conditions.

So, how many modes labeled by  $n_x, n_y, n_z$  are in the cavity; i.e., how many modes meet the constraint for a given  $\lambda$ ? This requires that we count all the possible combinations of the



integer values  $n_x, n_y, n_z$ . This counting problem is a little tricky, and so I've relegated it to a supplemental reading (the blue text below), and we will just quote the result:

$$n(\lambda) d\lambda = \frac{8\pi}{\lambda^4} d\lambda$$

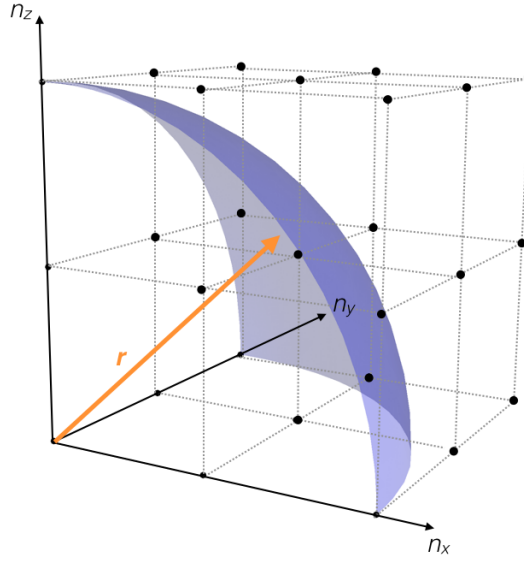
This completes step 1 of the calculation.

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Treat  $n_x, n_y, n_z$  as components of a vector  $\vec{n}$  in a 3-dimensional “ $n$ -space”,

$$\vec{n} = n_x \hat{x} + n_y \hat{y} + n_z \hat{z}.$$

Then, our condition  $n_x^2 + n_y^2 + n_z^2 = \frac{4L^2}{\lambda^2}$  says that the allowed points are within a sphere of



radius  $r$  given by

$$r^2 = \vec{n} \cdot \vec{n} = n_x^2 + n_y^2 + n_z^2 = \left( \frac{2L}{\lambda} \right)^2$$

The total number of combinations allowed is the volume of the 3d grid of values of  $n$  within this radius, i.e. the volume of the sphere,

$$\text{“volume” of } n's = \frac{4\pi r^3}{3} = \frac{4\pi}{3} (n_x^2 + n_y^2 + n_z^2)^{\frac{3}{2}}.$$

This is an approximation that is valid for  $L \gg \lambda$ , which is a good approximation for electromagnetic waves in a finite cavity. But we still have some corrections to make. In using a sphere (rather than the cube we care about!) we allowed both positive and negative values of  $n$ , while our wave equation solutions should only have positive or zero values; thus, we actually only need 1/8th of the volume computed here. Another point is that light can be polarized in two perpendicular directions, so we have to multiply by a factor of 2 to account for both polarizations. With these corrections, this volume is a good approximation for the total number of modes  $N$ , given by

$$N = \frac{\pi}{3} (n_x^2 + n_y^2 + n_z^2)^{\frac{3}{2}} = \frac{8\pi L^3}{3\lambda^3}.$$



From here, we can compute the number of modes per unit wavelength,

$$\frac{dN}{d\lambda} = \frac{d}{d\lambda} \frac{8\pi L^3}{3\lambda^3} = -\frac{8\pi L^3}{\lambda^4}.$$

The minus sign means that the number of modes *decreases* as wavelength increases. Then, the number of modes per unit volume in the cavity of volume  $L^3$ , with wavelengths between  $\lambda$  and  $\lambda + d\lambda$ ,  $n(\lambda)$ , is

$$n(\lambda)d\lambda = \frac{1}{L^3} \left| \frac{dN}{d\lambda} \right| d\lambda = \frac{8\pi}{\lambda^4} d\lambda \quad (2.6)$$

*End supplemental material.*

### Clicker Question: Changing variables

If the number of waves which exist in a cavity with wavelengths between  $\lambda$  and  $\lambda + d\lambda$  is  $n(\lambda) d\lambda = \frac{8\pi}{\lambda^4} d\lambda$ , then what is the number of waves with frequencies between  $f$  and  $f + df$ ?

- (a)  $\frac{8\pi}{f^4} df$
- (b)  $\frac{8\pi f^2}{c^3} df$
- (c)  $\frac{8\pi f^4}{c^3} df$

We need to substitute for  $\lambda$  both in the denominator and in the differential, the latter of which requires the chain rule:

$$\lambda = \frac{c}{f}, \quad d\lambda = d\left(\frac{c}{f}\right) = c \frac{d}{df} \left(\frac{1}{f}\right) df = -\frac{c}{f^2} df$$

Then, we can compute

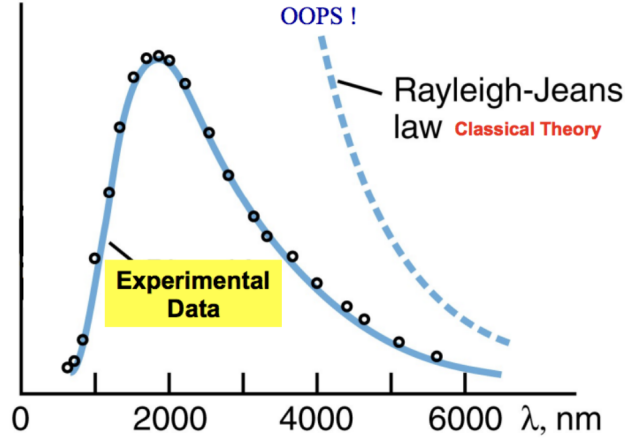
$$\begin{aligned} n(\lambda)d\lambda &= \frac{8\pi}{\lambda^4} d\lambda = \frac{8\pi}{(c/f)^4} \left(-\frac{c}{f^2}\right) df \\ &= -\frac{8\pi f^2}{c^3} df \end{aligned}$$

The relative minus sign just indicates that the number of modes  $n(f)$  increases as the frequency increases, which is the opposite of  $n(\lambda)$ , since the number of modes decreases as the wavelength increases. The answer is (b).

**Step 2** of the Rayleigh-Jeans computation follows from a theorem of statistical mechanics, the *equipartition theorem*. This theorem states that the average value of the kinetic energy for each independent direction of motion for a system at temperature  $T$  is  $k_B T/2$ . In our model of blackbody radiation, we treat each mode as a harmonic oscillator, which has both kinetic and potential energy and so gets an extra factor of 2, so that each mode has an average energy of  $E_{\text{avg}} = k_B T$ . It is this step that will need to change to account for the experimental results!

We have thus derived the Rayleigh-Jeans law,

$$u(\lambda, T)d\lambda = E_{\text{avg}} n(\lambda)d\lambda = \frac{8\pi k_B T}{\lambda^4} d\lambda.$$



Now, this law has several serious problem. Clearly, this function looks nothing like the function we were expecting based on experimental data, especially at smaller wavelengths. At small wavelengths ( $\lambda \rightarrow 0$ ), according to this law the intensity per unit wavelength diverges,  $u(\lambda, T) \rightarrow \infty$ , so that the total intensity of light (and total radiation emitted) goes to infinity. This is called the ultraviolet catastrophe, and was the beginning of the end for classical physics

**Resolution of the UV catastrophe: quantization of electromagnetic energy** So, how do we fix it? In 1900 Max Planck proposed a revolutionary idea: that electromagnetic energy is quantized. Planck proposed that we should model the cavity radiation as the exchange of energy between electromagnetic radiation and “atomic” oscillators present in the walls of the cavity. (Back in Planck’s time, he didn’t yet know about electrons, the nucleus, or anything else about atomic structure—hence the charged oscillators idea.) The oscillators can have any frequency  $f = c/\lambda$ , but the energy exchange between the radiation and the oscillators is *not* continuous and arbitrary, but instead is discrete, always exchanged in packets of the same amount:

$$E = nhf = nhc/\lambda, \quad n = 1, 2, 3, \dots, \infty$$

so that the energy exchange is always a multiple of

$$\boxed{\text{Energy quantum of radiation: } \Delta E = hf = \frac{hc}{\lambda}} \quad (2.7)$$

$h$  is called Planck’s constant, a very very small number:

$$\boxed{\text{Planck’s constant : } h = 6.626 \times 10^{-34} \text{ J} \cdot \text{s}} \quad (2.8)$$

So now we need to count how many standing waves fit inside the cavity, except we assume the radiation energy in the cavity is quantized. This is a hybrid approach to quantizing the radiation that uses both its wave-like and particle-like nature: we are modeling the radiation inside the cavity as waves, but assuming that it can be absorbed in only quantized amounts. (Later we’ll understand in much more detail what the how to get a consistent overall picture in the framework of quantum mechanics!) This changes the average energy of a mode of wavelength  $\lambda$ , which can be found to be (we’ll skip the details, since it relies on statistical mechanics..)

$$E_{\text{avg}}(\lambda) = \frac{hc/\lambda}{e^{hc/(\lambda k_B T)} - 1}$$

so that

$$u(\lambda, T) d\lambda = E_{\text{avg}}(\lambda) n(\lambda) d\lambda \quad \Rightarrow \quad \boxed{u(\lambda, T) d\lambda = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{hc/(\lambda k_B T)} - 1} d\lambda}$$

You can verify that this expression for the integrand  $u(\lambda, T)$  indeed has units of Energy / Volume / Wavelength, *i.e.* Energy /  $m^4$ .

Some comments:

- Fitting this new formula to the experimental data allows the constant  $h$  to be determined, yielding the number quoted in (2.8).
- Again, we point out that this expression differs from the expression of  $I(\lambda, T)$  in your book by a factor of  $c/4$ ; either expression contains the same physics.
- Using the result from the clicker question to replace  $n(\lambda)d\lambda$  with  $n(f)df$ , and substituting variables  $\lambda = c/f$ , we can equivalently rewrite this in terms of the frequency  $f$  as,

$$\boxed{u(f, T) df = \frac{8\pi h}{c^3} \frac{f^3}{e^{hf/(k_B T)} - 1} df}$$

- In your homework (Pset problem 2), you will explore how Planck's formula reduces in the low and high frequency limits, and see how Planck's formula makes contact with both the classical Rayleigh-Jeans law, and Stefan's law.
- How would you then derive Wien's displacement law for  $\lambda_{\text{max}}$ ? You would differentiate with respect to  $\lambda$  at constant  $T$  to find the peak,

$$\left. \frac{du(\lambda, T)}{d\lambda} \right|_{\lambda=\lambda_{\text{max}}} = 0$$

You can numerically check by doing this that you reproduce the earlier formula we gave for  $\lambda_{\text{max}}$ . *Supplemental: check out [this link](#) for more details!*

### Example Problem: The size of quantum effects for a classical oscillator

*Supplementary problem, not covered in lecture:*

Let's run with Planck's idea of energy quantization. Suppose a mass  $m$  oscillates at the end of a spring with spring constant  $k$ , and the amplitude of these oscillations is  $\Delta x$ . If this oscillator's energies were quantized *a la* Planck, how does the discrete energy spacing compare to the energy of the oscillations?

*Solution:* For a spring of spring constant  $k$  and mass  $m$ , the frequency of oscillations is

$$f = \frac{1}{2\pi} \sqrt{\frac{k}{m}},$$

which would correspond to an energy quantum of,

$$\Delta E = hf = \frac{h}{2\pi} \sqrt{\frac{k}{m}}$$

For vibrations with an amplitude of  $\Delta x$ , the energy of the oscillations is,

$$E = \frac{1}{2} k (\Delta x)^2$$

so we can compare,

$$\frac{\Delta E}{E} = \frac{h}{\pi(\Delta x)^2 \sqrt{km}}$$

How large or small this ratio is will depend on the size of the parameters involved, and in particular how small  $h$  is compared to  $\pi(\Delta x)^2 \sqrt{km}$ . Suppose for a typical oscillator that  $m = 1 \text{ kg}$ ,  $k = 10^3 \text{ N/m}$ , and  $\Delta x = 0.1 \text{ m}$ . Then this number evaluates to

$$\frac{\Delta E}{E} = \frac{6.626 \times 10^{-34} \text{ J} \cdot \text{s}}{\pi(0.1 \text{ m})^2 \sqrt{(10^3 \text{ N/m})(1 \text{ kg})}} = 6.7 \times 10^{-34}$$

This is an extremely small number, due to the fact that  $h$  is so tiny! If the oscillator's energy levels were quantized, you would never notice because the spacing would be so close together that they would appear to be continuous.

—————End Lecture 8.

### 2.1.2 The Photoelectric Effect

Classical disaster number (2) which we'll discuss is known as the photoelectric effect. The photoelectric effect describes what happens when light is incident on a metal. The basic idea is that light above a certain frequency shining on a metal will eject electrons. In this scenario we shine light on a metal, and we can tune the intensity  $I$ , as well as the wavelength  $\lambda$  or frequency  $f$  of the light, satisfying  $c = \lambda f$ . The metal absorbs energy from the light, and emits electrons, which are called *photoelectrons*.

We can measure the kinetic energy of the photoelectrons by stopping them with an electric field—practically speaking, we see how much voltage is needed to stop them. The voltage needed to stop *all* the electrons (including the most energetic ones) is called the stopping voltage  $V_s$ ; it tells us the maximum kinetic energy of the emitted electrons,  $K_{\max}$ ,

$$K_{\max} = eV_s,$$

where recall that  $1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$ . Applying the stopping voltage  $V_s$  completely stops the flow of current.

The basic characteristics of this experiment are as follows:

- The intensity of the light controls how many electrons come off the metal, but does not affect their speed—in particular, the maximum kinetic energy  $K_{\max}$  does not depend on the intensity of the incident light.

This contradicts the classical picture of light as an electromagnetic field, according to which the energy in a light wave is spread out uniformly and continuously over the wavefront, so the amount of energy an electron in the surface of the metal absorbs would be proportional to the intensity  $I$  of that wave.

- If the wavelength is too high (frequency too low), then no electrons come off of the metal, regardless of how high you crank up the intensity of the light. *There is a minimum frequency* for the effect to exist.

Again this contradicts the classical picture, since classically the intensity of a light wave is proportional to the amplitude squared of the electric field associated to the wave,  $I \sim |E|^2$ , which does not depend at all on the frequency of the light.

- There is no time lag between the time the light is incident on the metal and the time a photoelectron is ejected.

Yet again, this is puzzling from the classical point of view; if we model the light with a spherical wavefront over which energy is uniformly distributed, we would expect it to take time for the electrons in the metal to absorb enough energy from the light to overcome the attractive Coulomb force that binds it to the atom in order to be emitted. We call this energy the *binding energy*, or the *work function*. How could there be no time lag?

**Einstein's explanation** These results were explained by Einstein in 1905 (for which he got the 1922 Nobel prize).<sup>7</sup> Einstein took Planck's proposal that electromagnetic energy is quantized all the way to its logical conclusion that light itself is quantized, and modeled the light as a stream of photons with discrete energies

$$\boxed{\text{photon energy/momentum: } E = hf = pc} \quad (2.9)$$

According to this theory, energy is *not* uniformly distributed over a wave-front, but rather in packets of "stuff", the photons. Each photon delivers exactly energy  $hf$  to each electron. It transfers all of its energy to an electron, which gets absorbed by the metal to release the electron, and give the electron a boost of kinetic energy. By conservation of energy, this effect is summed up with the following formula:

Energy of incident photon = Energy required to release  $e^-$  + Kinetic energy of ejected  $e^-$

$$\Rightarrow hf = \phi + K_{\max}$$

where  $\phi$  is the work function of the metal, meaning the energy required for the metal to release an electron. Therefore, the stopping voltage is related to the maximum kinetic energy as

$$\boxed{eV_s = K_{\max} = hf - \phi}$$

Some comments on this result:

- This result is completely independent of the intensity of the light; even if you decrease the intensity to one photon per second shining on the metal, you will get the same results. Larger intensity means more photons, but does *not* change how much energy per photon can be transferred to an electron.
- There is a threshold frequency for electrons to be emitted, when  $K_{\max} = 0$ . The incident light needs to have *at least* this threshold frequency  $f_*$  in order for the photons to carry enough energy to overcome the work function of the metal and free an electron,

$$hf_* = \frac{hc}{\lambda_*} = \phi$$

Any leftover energy goes into the kinetic energy of the electron.

### Clicker Question: Photoelectric effect 1

In a photoelectric experiment, suppose the metal is illuminated by light which is held constant in intensity while its frequency is increased. The resulting photo-current will:

- (a) increase

<sup>7</sup>Einstein wrote 4 revolutionary papers in 1905: two on relativity, one on Brownian motion, and the other on the photoelectric effect.

- (b) decrease
- (c) stay the same

*Solution:* (c)! Increasing the frequency increases the maximum kinetic energy of the emitted electrons, but this doesn't change the current (the rate of flow of electric charge).

### Example Problem: Photoelectric effect 2

What is the threshold frequency for electron emission from aluminum, with work function 4.28 eV? (Note that  $h = 4.136 \times 10^{-15} \text{ eV} \cdot \text{s}$ .)

*Solution:* The threshold frequency is given by setting

$$\phi = hf_* \Rightarrow f_* = \frac{\phi}{h} = \frac{4.28 \text{ eV}}{4.136 \times 10^{-15} \text{ eV} \cdot \text{s}} = 1.03 \times 10^{15} \text{ Hz}$$

This is just past the UV end of the visible spectrum.

### Clicker Question: Photoelectric effect 3

The photoelectric work function of potassium is 2.3 eV. If light having a wavelength of 250 nm falls on potassium, find:

- (a) The kinetic energy in eV of the most energetic electrons ejected. (Note that  $h = 4.136 \times 10^{-15} \text{ eV} \cdot \text{s}$ .)
- (b) The speed of these electrons. (Note that  $m_e = 0.511 \text{ MeV}/c^2$ .)

*Solution:* Use

$$\begin{aligned} K_{\max} &= hf - \phi = (4.136 \times 10^{-15} \text{ eV} \cdot \text{s}) \frac{3 \times 10^8 \text{ m/s}}{250 \times 10^{-9} \text{ m}} - 2.3 \text{ eV} \\ &= 2.66 \text{ eV} \end{aligned}$$

For part (b), we can solve for the speed using

$$\begin{aligned} K_{\max} &= (\gamma - 1)mc^2 = \left( \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} - 1 \right) mc^2 \\ \Rightarrow \frac{K_{\max}}{mc^2} + 1 &= \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \\ \Rightarrow \frac{1}{\left( \frac{K_{\max}}{mc^2} + 1 \right)^2} &= 1 - \frac{v^2}{c^2} \\ \Rightarrow \frac{v}{c} &= \sqrt{1 - \frac{1}{\left( \frac{K_{\max}}{mc^2} + 1 \right)^2}} = 3.2 \times 10^{-3} \end{aligned}$$

Or in other words,

$$v = (3.2 \times 10^{-3})c = 9.6 \times 10^5 \text{ m/s}$$

At this point, you may be wondering: is light a wave, or a particle? The answer is, really, both. The photons associated with electromagnetic waves are massless particles that travel with speed  $c$ . Relativity says that  $E^2 = (pc)^2 + (mc^2)^2$ , so these photons have energy  $E = pc$ . But Planck and Einstein tell us that this energy is quantized, as  $E = hf$ . Putting these two ideas together,

$$E = hf = \frac{hc}{\lambda} = pc \quad \Rightarrow \quad \boxed{p = \frac{h}{\lambda}} \quad (2.10)$$

Photons have momentum that is inversely proportional to the wavelength of the associated EM wave. What's going on is that we need a new language with which to talk about subatomic particles, which is the theory of quantum mechanics. This is where we're headed.

### 2.1.3 Compton Scattering

Classical disaster (3) is known as Compton scattering. Compton Scattering refers to the scattering of light (a photon) from a target electron at rest. It is named after Arthur H. Compton, who observed the scattering of X-rays from electrons in a carbon target.

X-rays are electromagnetic waves with high frequency (low wavelengths on the order of  $\lambda \sim 10^{-10} \text{ m}$ ) that allow us to probe subatomic structures. In general, to probe into a structure you need a light source with a wavelength much smaller than the features of the object being probed.

The classical theory of light would describe X-rays as waves with frequency  $f_0$ . When the X-rays hit the electron, the electron oscillates, and re-radiates waves at frequency  $f'$ , where  $f'$  depends on the intensity of the incident radiation. Since the electron would need some time to soak up enough energy to radiate, we would expect a time delay.

Experimentally, Compton found that  $f'$  is actually independent of the incident intensity, and in fact only depends on the scattering angle: the angle that the scattered X-ray makes with the collision axis. The explanation of this observation comes from describing light as made up of photons. Compton was awarded the Nobel prize in 1927 for this discovery, since it gave clear evidence of the particle-like behavior of light.

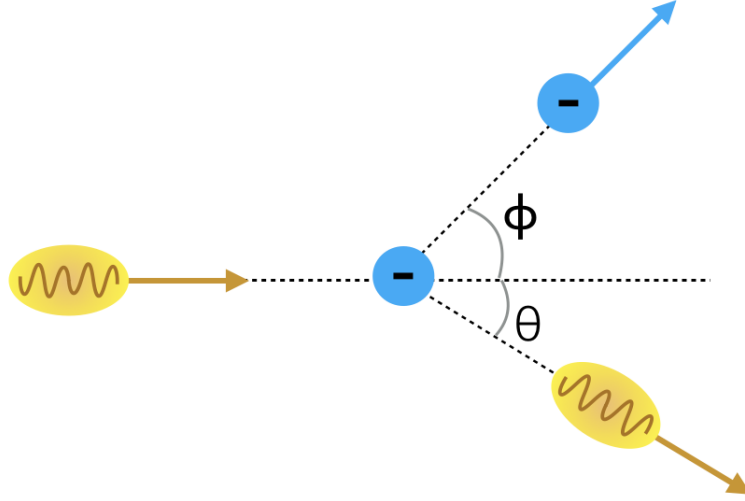
To derive this result, consider an X-ray (a photon) with frequency  $f_0$  incident on a stationary electron. Recall that for a massless particle, its energy is related to its frequency, wavelength, and momentum as

$$E = hf = \frac{hc}{\lambda} = pc \quad (\text{massless particle}),$$

while for a massive particle,

$$E = \gamma mc^2 = \sqrt{p^2 c^2 + m^2 c^4}, \quad (\text{massive particle}),$$

where  $\vec{p}$  for the massive particle is the relativistic momentum,  $\vec{p} = \gamma m \vec{v}$ . Call the energy and momentum of the incident photon  $E_0, p_0$ ; of the target electron  $E_e^i, p_e^i$ ; of the scattered electron



$E_e^f, p_e^f$ , and of the scattered photon  $E', p'$ . We will use

$$\text{Conservation of energy: } E_0 + E_e^i = E' + E_e^f$$

$$\text{Conservation of momentum: } \vec{p}_0 + \vec{p}_e^i = \vec{p}' + \vec{p}_e^f.$$

Assume that the frequency  $f_0$  of the initial radiation is known, and that we've measured the angle  $\theta$  at which the light scattered from the horizontal axis. Then, this is 3 equations for 3 unknowns: (1) the frequency  $f'$  of the scattered photon, (2) the velocity  $v$  of the scattered electron, and (3) the angle  $\phi$  that the scattered electron makes with the horizontal axis.

The energy of the incident photon is  $E_0 = hf_0$ , and its wavelength is related to its frequency as

$$\lambda_0 f_0 = c,$$

while the energy of the target electron is

$$E_e^i = \gamma m_e c^2 = m_e c^2.$$

We used that  $\gamma$  for the target electron is 1, since it's velocity is zero. The energy of the scattered electron is  $E_e^f$ , and the energy of the scattered photon is  $E' = hf'$ . Then, conservation of energy lets us solve for the energy of the scattered electron:

$$hf_0 + m_e c^2 = hf' + E_e^f \quad \Rightarrow \quad E_e^f = h(f_0 - f') + m_e c^2.$$

Next, conservation of the  $x$ -component of momentum (see the figure for the definition of the angles) is

$$p_0 = p_e^f \cos \phi + p' \cos \theta \quad \Rightarrow \quad p_e^f \cos \phi = p_0 - p' \cos \theta$$

where we used that  $p_e^i = 0$  since the electron is initially at rest. Initially neither particle has a component of momentum in the  $y$ -direction, so conservation of the  $y$ -component of momentum is

$$0 = p_e^f \sin \phi - p' \sin \theta \quad \Rightarrow \quad p_e^f \sin \phi = p' \sin \theta. \quad (2.11)$$

We want to solve for  $f'$ , the frequency of the scattered photon. To do this, we can eliminate  $\phi$  from the conservation of momentum equations by squaring them and adding them:

$$\begin{aligned} (p_e^f)^2 \cos^2 \phi &= (p_0 - p' \cos \theta)^2 \\ (p_e^f)^2 \sin^2 \phi &= (p')^2 \sin^2 \theta \\ (p_e^f)^2 \cos^2 \phi + (p_e^f)^2 \sin^2 \phi &= (p_e^f)^2 = (p_0 - p' \cos \theta)^2 + (p')^2 \sin^2 \theta. \end{aligned}$$



Simplifying, we can express the momentum of the scattered electron as

$$(p_e^f)^2 = (p_0 - p' \cos \theta)^2 + (p')^2 \sin^2 \theta = p_0^2 + (p')^2 - 2p_0 p' \cos \theta.$$

Express the momenta of the photons in terms of their frequency,  $p' = hf'/c$ ,  $p_0 = hf_0/c$ , and then

$$(p_e^f)^2 = \frac{h^2}{c^2} (f_0^2 + (f')^2 - 2f_0 f' \cos \theta).$$

Finally, use

$$(E_e^f)^2 = (p_e^f)^2 c^2 + m_e^2 c^4$$

$$(h(f_0 - f') + m_e c^2)^2 = h^2 (f_0^2 + (f')^2 - 2f_0 f' \cos \theta) + m_e^2 c^4$$

Simplifying, we can solve for  $f'$  as a function of  $f_0$ ,  $m_e$ ,  $h$ ,  $c$ ,  $\theta$  (I suggest you work out the final bit of algebra as an exercise!). We'll express our final answer in terms of the wavelength  $\lambda'$  (using  $f' = c/\lambda'$ ):

Compton scattering: $\lambda' - \lambda_0 = \frac{h}{m_e c} (1 - \cos \theta)$	(2.12)
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———End Lecture 9.

This result says that the wavelength of the scattered photon depends *only* on the wavelength of the incident photon, and the scattering angle. Further, since  $-1 \leq \cos \theta \leq 1$ ,  $0 \leq 1 - \cos \theta \leq 2$ , so the scattered wavelength is *larger* than the wavelength of the incident photon (and therefore the scattered photon has smaller energy than the incident one).

### Clicker Question: Compton scattering

Assume that a photon of energy 100 keV is about to Compton scatter off of a stationary electron. What is the minimum possible energy of the scattered photon?

*Solution:* If the initial photon has energy 100 keV, its wavelength is

$$E = \frac{hc}{\lambda} \Rightarrow \lambda = \frac{hc}{E} = \frac{(4.136 \times 10^{-15} \text{ eV} \cdot \text{s})(3 \times 10^8 \text{ m/s})}{100 \times 10^3 \text{ eV}} = 1.2 \times 10^{-11} \text{ m}$$

This is  $\lambda_0$  in the Compton scattering formula. The scattered photon has an energy of

$$E' = \frac{hc}{\lambda'}$$

where  $\lambda'$  satisfies

$$\lambda' = \frac{h}{m_e c} (1 - \cos \theta) + \lambda_0$$

$\lambda'$  is its largest value, so that  $E'$  is its minimum value, when  $\cos \theta = -1$  (or  $\theta = \pi$ ), so that the photon scatters backwards off of the electron. Then, we can solve for

$$(\lambda')_{\max} = \frac{(4.136 \times 10^{-15} \text{ eV} \cdot \text{s})}{(0.511 \times 10^6 \text{ eV}/c^2)c} (2) + (1.2 \times 10^{-11} \text{ m})$$

$$= 1.7 \times 10^{-11} \text{ m}$$

This allows us to solve for the minimum possible energy of the scattered photon as,

$$E' = \frac{hc}{(\lambda')_{\min}} = \frac{(4.136 \times 10^{-15} \text{ eV} \cdot \text{s})(3 \times 10^8 \text{ m/s})}{1.7 \times 10^{-11} \text{ m}} = 7.2 \times 10^4 \text{ eV}$$

or in other words,

$$E' = 72 \text{ keV}$$

This is *smaller* than the energy of the initial photon, as it should be.

Note that if the problem had instead asked for the maximum energy, it would be when  $\theta = 0$  so that  $\cos \theta = 1$ , and  $\lambda' = \lambda_0$  and the whole energy of the initial photon goes into the final state photon without scattering the electron at all.

## 2.2 The Particle Nature of Matter

*“If, in some cataclysm, all scientific knowledge were to be destroyed, and only one sentence passed on to the next generation of creatures, what statement would contain the most information in the fewest words? I believe it is the atomic hypothesis (or atomic fact, or whatever you wish to call it) that all things are made of atoms - little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another. In that one sentence you will see an enormous amount of information about the world, if just a little imagination and thinking are applied.” ~Richard Feynman*

In the first section of these notes we focused on light, where we came to the conclusion that light behaves both as a wave and as a particle. For this next section we will focus on matter (stuff with mass), and eventually come to the same conclusion. First, we will focus on the particle nature of matter, and discuss the evolution of scientist’s understanding of what makes up the atom. In the subsequent section we will focus on the wave nature of matter, seeing that some properties of matter can be best explained by thinking of matter as coming in wavelike packets, just like with photons.

### 2.2.1 Rutherford Scattering

We begin with some historical aspects of the discovery of the structure of the atom.

Before 1897, many people thought that atoms were the smallest indivisible units of matter. By experimenting with cathode rays, J.J. Thomson was the first to discover a subatomic particle, the electron. He proposed the “plum pudding” model of the atom in order to explain the fact that atoms have electric charges (electrons) on their interior. In this model, the electric charges in the atom are uniformly distributed like raisins in a plum pudding, with positive charge homogeneously distributed over the whole atom, such that the positive charges cancel the negative charges and the atom is net neutral.

In order to probe the charge and mass distribution inside the atom, Ernest Rutherford and his Ph.D. students Ernest Marsden and Hans Geiger conducted a series of experiments involving shooting  $\alpha$  particles at thin gold foils and observing their scattering. The  $\alpha$  particles are ionized Helium atoms, which act as charged bullets being shot at the foil. They have charge  $2e$ , and nonrelativistic velocity  $v_\alpha \approx 0.1c$ . The hypothesis based on the plum-pudding model of the atom was that the  $\alpha$  rays would hardly scatter, because:

- With the assumption that positive charge is distributed over the whole size of the atom,  $\sim 10^{-10}m$ , the  $\alpha$  particles would probably not be scattered at too large angles.
- The mass of the  $\alpha$  particles  $m_\alpha$  satisfies  $m_\alpha \gg m_e$ , so hitting the electrons would be like a moving truck hitting a bicycle.

Thus, the prediction was that  $\alpha$ -rays would pass through an array of atoms with little scatter.

The experiment was set up with a radioactive substance that emits  $\alpha$  particles, that are then narrowed into a collimated beam and shot at a piece of thin metallic foil. A viewing screen is set up around the foil, so that the angles of the scattered  $\alpha$  particles could be measured.

What was observed was surprising. Most of the  $\alpha$  particles passed straight through the foil with no deflection whatsoever, but some ( $\sim 10^{-4}$ ) were scattered at large angles, and even fewer scattered almost backwards. The plum pudding model of the atom could not account for the large angle scattering.

What could explain these results is a model in which all of the positive charge in the atom is concentrated at a single central point, the nucleus. Then, the electric repulsion experienced by an incident  $\alpha$  particle in a head on collision would be much greater. Most of the particles would go right through, but some would be deflected at large angles, and even almost backwards, by the nucleus. Rutherford was awarded the Nobel prize in chemistry for this work in 1908.

**Explanation** Assume that there is a heavy nucleus of positive charge at the center of an atom. We can compute the resulting force on an  $\alpha$ -particle, and predict where we should find the scattered particles in the detector. Suppose the  $\alpha$  particle comes in at velocity  $v_\alpha$  (which is  $\ll c$ , so we don't need relativistic mechanics) towards a nucleus of an atom in the gold foil. The particle is scattered by the repulsive Coulomb force from the positively charged nucleus,

$$\vec{F} = \frac{kq_\alpha Q}{r^2} \hat{r}, \quad q_\alpha = 2e, \quad Q = Ze$$

where  $Z$  is the atomic number of the gold atoms. Assume that the nucleus is so heavy that it doesn't move after the collision. Then, the trajectory of the  $\alpha$  particle will be hyperbolic, and the final angle at which the particle moves away after colliding with the nucleus is the scattering angle  $\theta$ .

One can work out this scattering problem, but it is a bit complicated. The result is that the number of scattered  $\alpha$  particles entering the detector per unit time at an angle  $\theta$ ,  $\Delta n$ , turns out to be proportional to  $1/\sin^4(\theta/2)$ :

Rutherford scattering: $\Delta n \propto \frac{1}{\sin^4 \frac{\theta}{2}}$
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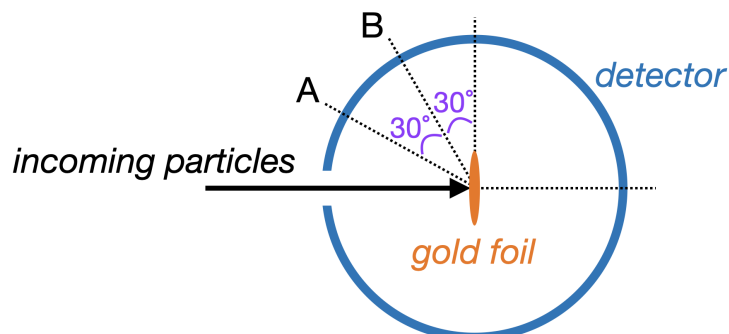
(2.13)

This implies that the number of scattered  $\alpha$  particles detected goes *down* with an increase in the scattering angle—most are scattered at small angles, but some will be scattered at large angles.

Rutherford realized that this scattering setup can also be used to probe the size of the nucleus. The scattering assumes a constant, static gold nucleus. This is ok as long as the  $\alpha$  particles don't have enough energy to penetrate into the nucleus...there is a certain kinetic energy of  $\alpha$  particles where the theory starts to disagree with experiment. Using this critical value of the kinetic energy, we can deduce the size of the nucleus, with result that it is on the order of  $10^{-15}m$ .

### Clicker Question: Rutherford scattering

In one hour, the detector measures 1000 alpha particles at location A. How many alpha particles would be measured at location B in this same hour?



*Solution:* We are told in Rutherford's formula that  $\Delta n = \frac{\text{constant}}{\sin^4 \frac{\theta}{2}}$  where  $\theta$  is the angle between the incident direction of the  $\alpha$  particles, and the direction from the target to the detector. In this problem,  $\theta_A = 90^\circ + 2(30^\circ) = 150^\circ$ , and  $\theta_B = 90^\circ + 30^\circ = 120^\circ$ . Therefore,

$$\Delta n_A \sin^4(\theta_A/2) = \text{constant} = \Delta n_B \sin^4(\theta_B/2)$$

$$\Delta n_B = \Delta n_A \frac{\sin^4(\theta_A/2)}{\sin^4(\theta_B/2)} = (1000 \text{ particles/hour}) \frac{\sin^4(75^\circ)}{\sin^4(60^\circ)} = 1550 \text{ particles/hour}.$$

At this point, Rutherford and his students had shown that the mass and the positive charge of the atom were concentrated in a tiny nucleus with radius  $\sim 10^{-15}$ . But how are electrons located inside an atom, and how are they held in orbits in a stable fashion? To answer this question, we need new experiments and observations to point the way.

### 2.2.2 Observations of Atomic Spectra

Throughout the 1800s, scientists were able to measure emission / absorption lines of various materials, identifying elements of different types based on their spectroscopic signatures. As we learned when we studied blackbodies, a blackbody radiates a continuous spectrum of wavelengths. Heated solids and liquids, and high density gases, in general emit a continuous spectrum of wavelengths.

However, some materials absorb and emit only certain wavelengths of light. For example, a low pressure, low density, hot gas radiates only at a few specific wavelengths. The emission lines correspond to photons of discrete energies that are emitted when excited atomic states in the gas transition to lower-lying energy levels, and are characteristic of the elements that comprise the gas. Similarly, when light passes through a cool, dilute gas, atoms in the gas absorb light at certain discrete frequencies, resulting in an absorption spectrum that is characteristic of the elemental composition of the gas.

The spectrum of atomic hydrogen is of particular interest for astronomical observation, since it's such an abundant element in the universe. An empirical model to describe the emission of atomic hydrogen was made by Johan Balmer, and is known as the Balmer formula. The series of emission lines for hydrogen described by the Balmer formula is called the Balmer series, and

are given by taking  $n_f = 2$  and  $n_i = 2, 3, 4, \dots$ , in the following formula,

An empirical model to describe the emission of atomic hydrogen was proposed by Johannes Rydberg,

$$\frac{1}{\lambda} = R_H \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right), \quad n_i > n_f, \quad n_f = 1, 2, \dots$$

In this formula, the Balmer series (proposed by Johan Balmer) corresponds to  $n_f = 2$  and  $n_i$  an integer greater than 2; the Lyman series corresponds to  $n_f = 1$ , the Paschen series to  $n_f = 3$ , and so on. Fitting to the spectral line series data yields  $R_H = 1.09737 \times 10^7 \text{m}^{-1}$ , called the Rydberg constant.

This model fit remarkably well with the discrete emission spectrum data, but was perplexing from the perspective of the Rutherford model.

### 2.2.3 The Bohr Model of the Atom

**Postulates of the Bohr model** Neil Bohr gave the first successful theory of atomic line spectra, taking a key step in the development of quantum mechanics. He applied Planck's ideas to orbiting atomic electrons, to propose the following semi-classical model:

- Electrons are confined to circular orbits around the nucleus, with velocity  $v$ . (so far, nothing new!)
- Only stable, non radiating stationary orbits of certain frequencies are allowed. The electron does not radiate when in these stationary orbits.

Why is this point important? The Rutherford model of electrons rotating around a nucleus, bound by the Coulomb force, is unstable. Because rotating objects accelerate, and according to the laws of classical electromagnetism charges release electromagnetic radiation when accelerating, this means that in this model the electrons release radiation when orbiting the nucleus. This causes the electron to lose energy, and spiral to an orbit of smaller radius, where it radiates more, and spirals to lower radius, and so on, until it spirals towards the nucleus and the atom collapses. Bohr corrects for this by positing that electrons only orbit in so-called *stationary*, non-radiating orbits.

- These stationary state orbits have quantized angular momentum,

$$L_n = m_e v_n r_n = \frac{n\hbar}{2\pi} \equiv n\hbar, \quad n = 1, 2, 3, \dots \quad (2.14)$$

This is a quantum condition imposed on the electron's orbital angular momentum!

Note that in this equation a factor of  $h/(2\pi)$  appears. This combination will appear over and over again, so we define a *reduced Planck's constant* as,

$$\hbar = \frac{h}{2\pi} = 1.05 \times 10^{-34} \text{J} \cdot \text{s} = 6.58 \times 10^{-16} \text{eV} \cdot \text{s} \quad (2.15)$$

- Electrons can gain or lose energy by jumping between the allowed orbits. Radiation is emitted when an electron "jumps" from a stable orbit of higher energy to a stable orbit of lower energy. This energy change is quantized,

$$|E_f - E_i| = hf = \frac{hc}{\lambda},$$

where  $f$  is the frequency of the radiation.

An atomic transition occurs when the electron jumps from a more energetic initial stationary state to a less energetic final stationary state, emitting a photon of frequency  $f$ —this fact will explain the observed absorption / emission spectra.

———*End Lecture 10.*

**Deriving the allowed energy levels and radii of orbit** With these assumptions, we can ask: What are the allowed energy levels? Consider this question for hydrogen, where one electron orbits one proton. The key concepts we will use are:

- Coulomb's law provides a centripetal force acting on the electron.
- Angular momentum is quantized (one of Bohr's postulates).
- The electron is in an orbit with constant energy (one of Bohr's postulates).

The Hydrogen atom is an example of motion in a central force, the Coulomb force. This is a two body system, with two bodies of different masses (a proton and an electron), each with the same but opposite charge, under a central force. Both the proton and electron revolve around their common center of mass. Such a system is equivalent to a single particle of reduced mass  $\mu$  that revolves around the center of mass. Thus, we can model the Hydrogen atom as a particle of reduced mass

$$\mu = \frac{m_e m_p}{m_e + m_p}.$$

orbiting around the center of mass, at

$$r = r_e - r_p = \text{distance between proton and electron}$$

Since  $m_p \gg m_e$ , ( $m_e/m_p \approx \frac{1}{1836} \approx 0.0005$ )

$$\mu = \frac{m_e m_p}{m_e + m_p} = \frac{m_e}{1 + \frac{m_e}{m_p}} \approx m_e.$$

(We *cannot* do this when calculating *equal* mass charges rotating around each other—this approximation only works because the mass of the electron is so small compared to that of the proton!) Thus, a Hydrogen atom is approximately equivalent to a particle of reduced mass  $m_e$  in a Coulomb potential.

The potential and kinetic energies of an electron in orbit around the proton are

$$U(r) = \frac{kq_e q_p}{r} = -\frac{ke^2}{r}, \quad K = \frac{1}{2}m_e v^2.$$

For the purposes of this problem, it will be sufficient to assume the electron moves at a nonrelativistic speed. The total energy is

$$E = K + U = \frac{1}{2}m_e v^2 - \frac{ke^2}{r}.$$

For a stable orbit, we need the force from Coulomb attraction between the electron and proton to equal the central potential force; applying Newton's second law,

$$F = m_e a$$

$$\frac{ke^2}{r^2} = m_e a = \frac{m_e v^2}{r} \quad \Rightarrow \quad K = \frac{m_e v^2}{2} = \frac{ke^2}{2r}.$$

Thus, the total energy of the system is

$$E = K + U = \frac{ke^2}{2r} - \frac{ke^2}{r} \quad \Rightarrow \quad \boxed{E = -\frac{ke^2}{2r}}. \quad (2.16)$$

The energy is negative, meaning that it's a bound system—the electron and proton are bound together. This says that an energy of  $ke^2/(2r)$  must be added to the system to break up the bound atom.

Now, to calculate the radius of the electron's orbit, we start with the assumption that angular momentum is quantized,

$$m_e v r = n \hbar \quad \Rightarrow \quad v_n = \frac{n \hbar}{m_e r}.$$

Substitute this into the kinetic energy,

$$K = \frac{1}{2} m_e v^2 = \frac{ke^2}{2r}$$

$$\Rightarrow \boxed{r_n = \frac{n^2 \hbar^2}{m_e k e^2}, \quad n = 1, 2, \dots, \infty} \quad (2.17)$$

(The  $n$  subscripts are just to emphasize that these quantities are quantized.) We see that this model of the hydrogen atom along with the assumption of angular momentum quantization leads to the conclusion that **the electron can only be found at certain radii**, labeled by the integer  $n$ ! The radius of the first stationary orbit,  $n = 1$ , is called the Bohr radius,

$$\boxed{a_0 = \frac{\hbar^2}{m_e k e^2} = 0.0529 \text{ nm} \quad \Rightarrow \quad r_n = a_0 n^2} \quad (2.18)$$

Quantization of the orbital radii immediately leads to energy quantization! Substitute  $r = n^2 a_0$  into the energy of the atom, and the allowed energy levels have energies

$$\boxed{E_n = -\frac{ke^2}{2a_0} \left( \frac{1}{n^2} \right)}. \quad (2.19)$$

The ground state of Hydrogen corresponds to the lowest energy level,

$$E_1 = -\frac{ke^2}{2a_0} = -13.6 \text{ eV}.$$

So it is useful to express the energies as

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

### Clicker Question: Quantization of electron speed

Given the quantization of the orbital radius of an electron in orbit around a proton in the Hydrogen atom,

$$r_n = a_0 n^2, \quad n = 1, 2, 3, \dots$$

what are the possible speeds that the electron could have?

*Solution:* Using angular momentum quantization,

$$m_e r_n v_n = n \hbar$$

and substituting for  $r_n = a_0 n^2$ , we obtain,

$$m_e a_0 n^2 v_n = n \hbar \quad \Rightarrow \quad v_n = \frac{\hbar}{m_e a_0 n} = \frac{2.19 \times 10^6}{n} \text{ m/s}$$

Note that larger  $n$  corresponds to orbits at larger radii, which then have smaller velocities and smaller energies.

An atomic transition occurs when the electron jumps from a more energetic initial stationary state to a less energetic final stationary state, emitting a photon of frequency  $f$ . This atomic transition has an energy

$$\begin{aligned} E_i - E_f &= hf = \frac{hc}{\lambda} = -\frac{ke^2}{2a_0} \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \\ \Rightarrow \frac{1}{\lambda} &= \frac{ke^2}{2a_0 hc} \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right). \end{aligned}$$

Defining  $ke^2/(2a_0 hc)$  as a constant  $R$ ,

$$\boxed{\frac{1}{\lambda} = R_H \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right), \quad R_H = \frac{ke^2}{2a_0 hc}.} \quad (2.20)$$

This  $R$  turns out to be the same as the experimentally determined Rydberg constant,  $R = 1.0973732 \times 10^7 \text{ m}^{-1}$ ! This agreement was recognized as the crowning achievement of the quantum theory of hydrogen.

These results explain the spectral series for Hydrogen. When an electron in a hydrogen atom makes a transition from an  $n > 1$  state to a lower state, it releases a photon of frequency  $f$  that is given by the formulae we've derived, resulting in an emission line. Similarly, an absorption line results when an electron in a given energy state absorbs a photon of the exact frequency required to produce a "jump" to a higher energy state. Since ordinarily hydrogen atoms are in the ground state, usually only the Lyman series corresponding to transitions from the ground state to higher energy states are seen. This is why typically not every line present in an emission spectrum is present in the element's absorption spectrum.

However, the Bohr model could not explain the intensities of the lines in atomic spectra, and the degeneracies of the energy levels, and also did not provide a first-principles motivation of the quantization of angular momentum in stationary orbits. The theory of quantum mechanics would solve all these problems.



### Clicker Question: A transition in Hydrogen

The electron in an at-rest hydrogen atom makes a transition from the  $n = 3$  energy state to the  $n = 1$  ground state. What is the frequency of the emitted photon?

- (a)  $2.9 \times 10^{15} \text{ Hz}$
- (b)  $2.2 \times 10^{15} \text{ Hz}$
- (c)  $1.0 \times 10^{-7} \text{ Hz}$

*Solution:* The wavelength of the photon is given by

$$\frac{1}{\lambda} = R_H \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

For the case of  $n_f = 1$ , and  $n_i = 3$ ,

$$\frac{1}{\lambda} = R_H \left( \frac{1}{1} - \frac{1}{9} \right) = (1.097 \times 10^7 \text{ m}^{-1}) \frac{8}{9}.$$

Solving for  $f = c/\lambda$ ,

$$f = \frac{c}{\lambda} = (3 \times 10^8 \text{ m/s})(1.097 \times 10^7 \text{ m}^{-1}) \frac{8}{9} = 2.9 \times 10^{15} \text{ Hz}.$$

The answer is (a).

### Example Problem: The Bohr model of Hydrogen

*Question:* An electron in a Bohr orbit of hydrogen has momentum  $p = 745.9 \text{ eV}/c$ . What is the radius of its orbit?

*Solution:* Using angular momentum quantization,

$$\begin{aligned} L = mvr = pr = n\hbar, \quad r = a_0 n^2 \\ \Rightarrow pa_0 n^2 = n\hbar \quad \Rightarrow n = \frac{\hbar}{a_0 p}. \end{aligned}$$

Plugging in, we can solve for  $n$ :

$$n = \frac{\hbar}{a_0 p} = \frac{6.58 \times 10^{-16} \text{ eV} \cdot \text{s}}{(5.29 \times 10^{-11} \text{ m})(745.9 \text{ eV}/(3 \times 10^8 \text{ m/s}))} = 5.$$

With  $n = 5$ , we can solve for

$$r = a_0 n^2 = 25a_0.$$

A comment:

- Note that Bohr's method can be applied in general to all Hydrogen-like atoms: meaning, all systems of an electron, with charge  $-e$ , orbiting a nucleus with atomic number  $Z$  and

charge  $e$ . For a single electron orbiting a fixed nucleus of charge  $+Ze$ , these formulae are modified to

$$r_n = n^2 \frac{a_0}{Z}, \quad E_n = -\frac{ke^2}{2a_0} \left( \frac{Z^2}{n^2} \right).$$

You will explore this idea in Homework 6.

### Example Problem: Emission and absorption spectra

*Question:* Photons with wavelengths in the range  $24 \text{ nm} \leq \lambda \leq 25 \text{ nm}$  are incident on a gas of  $\text{He}^+$  ions ( $Z = 2$ ), whose electrons are all initially in the ground state. Photons are absorbed, and subsequently emitted.

Considering only photons emitted during the first transition after absorption, what are the possible wavelengths of the emitted photons?

*Solution:* For  $Z = 1$ , we've learned that

$$\frac{1}{\lambda} = R_H \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right),$$

where  $R$  is a constant,

$$R_H = \frac{ke^2}{2\hbar a_0 c} = -\frac{E_1}{\hbar c} = 1.097 \times 10^7 \text{ m}^{-1}$$

for  $E_1$  the energy of the ground state of the hydrogen atom,  $-13.6 \text{ eV}$ . We've learned that for more general  $Z$ ,  $E_1 \rightarrow Z^2 E_1^{\text{hydrogen}}$ , so the formula for the wavelength gets modified to

$$\frac{1}{\lambda} = Z^2 R_H \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right).$$

We can rewrite the factor  $Z^2 R_H$  as follows:

$$\frac{1}{R_H} = \frac{1}{1.097 \times 10^7 \text{ m}^{-1}} = 91.1 \text{ nm} \quad \Rightarrow \quad \frac{1}{Z^2 R_H} = \frac{91.1 \text{ nm}}{4} = 22.8 \text{ nm}.$$

Thus, we'll solve for  $\lambda$ ,

$$\lambda = \frac{1}{Z^2 R_H} \left( \frac{1}{\frac{1}{n_f^2} - \frac{1}{n_i^2}} \right) = (22.8 \text{ nm}) \left( \frac{1}{\frac{1}{n_f^2} - \frac{1}{n_i^2}} \right)$$

To start with, all the electrons are in the ground state, so  $n_f = 1$ . Plugging in for  $n_i = 2, 3, \dots$ , we'll see which possible wavelengths can correspond to an absorption that

fall in the range  $24 \text{ nm} < \lambda < 25 \text{ nm}$ :

$$\begin{aligned} n_i = 2, \quad \lambda &= \frac{(22.8 \text{ nm})}{1 - \frac{1}{2^2}} = 30.4 \text{ nm} \\ n_i = 3, \quad \lambda &= \frac{(22.8 \text{ nm})}{1 - \frac{1}{3^2}} = 26.7 \text{ nm} \\ n_i = 4, \quad \lambda &= \frac{(22.8 \text{ nm})}{1 - \frac{1}{4^2}} = 24.3 \text{ nm} \\ n_i = 5, \quad \lambda &= \frac{(22.8 \text{ nm})}{1 - \frac{1}{5^2}} = 23.8 \text{ nm}. \end{aligned}$$

Thus, we see that if we only have photons of wavelengths  $24 \text{ nm} < \lambda < 25 \text{ nm}$ , the only possibility of absorption occurs for  $n_i = 4$ , so so the electrons can be excited to the  $n_i = 4$  energy level.

Then, photons can be emitted in the transition from  $n_i = 4$ , down to  $n_f = 3, 2, 1$ . Plugging in the numbers, this corresponds to emission of photons of wavelengths

$$\begin{aligned} n_f = 3, \quad \lambda &= \frac{(22.8 \text{ nm})}{\frac{1}{3^2} - \frac{1}{4^2}} = 469 \text{ nm} \\ n_f = 2, \quad \lambda &= \frac{(22.8 \text{ nm})}{\frac{1}{2^2} - \frac{1}{4^2}} = 121.6 \text{ nm} \\ n_f = 1, \quad \lambda &= \frac{(22.8 \text{ nm})}{\frac{1}{1^2} - \frac{1}{4^2}} = 24.3 \text{ nm}. \end{aligned}$$

These are the possible wavelengths of emitted photons.

**Bohr's correspondence principle** If quantum theory is truly describing nature, then it should recover classical physics in the right limit, when quantum effects become unimportant. What is the classical limit for a quantum system? The classical limit is defined as the regime where the quantized variables become much larger than their minimum quantum size. In Bohr's theory of hydrogen, this is the limit that the quantum number  $n \rightarrow \infty$ , so that the angular momentum  $L$  is much larger than  $\hbar$ . Since the energies of the orbits go as  $1/n^2$ , for  $n$  large, these energies become very close together—so close, that for all intents and purposes, they become indistinguishable from one another, so that we would see a “classical” continuum of allowed energies.

—————*End Lecture 11.*

## 2.3 The Wave Nature of Matter

### 2.3.1 de Broglie Matter Waves

The Bohr model was successful at explaining the emission and absorption spectra of Hydrogen, but failed to predict the intensity of spectral lines, and to make more complicated predictions for multi-electron atoms (like, Helium). The “hodge-podge” nature of the model, with the semi-classical description of electrons orbiting an atom, but semi-quantum notions of quantized angular momentum, left many unconvinced. This model could not explain the wave nature of light—a fact that comes from the model's overemphasis on the particle nature of matter.

Further, it can't predict the time evolution of a system from some initial state, or apply more generally to non-periodic motion in atomic systems.

So, without fundamental insight, why was Bohr successful? The key to the Bohr model of the atom was angular momentum conservation. It was Prince Louis de Broglie who was able to give a *reason* for this quantization, with the following conjecture (which he made in his Ph.D. thesis!): since photons have both wave-like and particle-like properties, it's only logical that other particles should have wave-like properties as well. de Broglie conjectured that—much like photons have accompanying electromagnetic waves—electrons have accompanying “pilot waves”, or “matter waves”, which guide through spacetime. Then, the formulas we've learned apply to photons should *also apply to particles like electrons*:

$$\lambda = \frac{h}{p}, \quad f = \frac{E}{h} \quad (\text{Matter waves}) \quad (2.21)$$

Electrons (and other particles with mass) also have accompanying waves, with frequency and wavelength related to their momentum.

Note that the relations (2.21) always work, no matter if relativity is needed to describe the particle (i.e. the speed of the particle is close to the speed of light) or not. The relations between energy, momentum, and velocity should be chosen appropriately based on the situation (classical or relativistic), but the relations between momentum and wavelength, as well as energy and frequency, are always the same!

As a warning, note that for a matter wave,  $\lambda f$  does *not* equal the speed of the particle!

$$\lambda f = \frac{E}{p} \neq u.$$

For a massless particle like a photon,  $E/p = c$  is the particles speed, but for a particle with mass this is not true—for example we can use  $E = \gamma mc^2$  and  $p = \gamma mu$  to find that  $\lambda f = \frac{c^2}{u} > c$ ! Later we will return to the interpretation of “what is waving?” in a matter wave, and understand how to interpret this velocity.

### Clicker Question: de Broglie wavelength of a baseball

Say we have a baseball with mass  $m = 140 \text{ g}$ , that a pitcher throws with speed  $v = 27 \text{ m/s}$ . What is the de Broglie wavelength of the ball? Does it make sense why we don't normally encounter wavelike properties of particles in everyday life?

*Solution:* The associated de Broglie wavelength for the baseball is

$$\lambda_b = \frac{h}{p} = \frac{6.63 \times 10^{-34} \text{ J} \cdot \text{s}}{0.14 \text{ kg} \cdot 27 \text{ m/s}} = 1.75 \times 10^{-34} \text{ m}.$$

This wavelength is much, much smaller than the size of the nucleus ( $10^{-15} \text{ m}$ ), which means it will be impossible to detect with even the finest instruments—let alone, the naked eye. This is why we would never notice interference effects from the baseball's associated wavelength, and why the baseball “looks” like a particle.

What about an electron? Say we have a non-relativistic electron with kinetic energy  $K = 120 \text{ eV}$ . The electron's momentum would be

$$K = \frac{p^2}{2m_e} \Rightarrow p = \sqrt{2m_e K} = \sqrt{2(0.511 \times 10^6 \text{ eV}/c^2)(120 \text{ eV})} = 1.11 \times 10^4 \text{ eV}/c$$

Then, the de Broglie wavelength of the electron is

$$\lambda_e = \frac{h}{p} = \frac{4.136 \times 10^{-15} \text{ eV} \cdot \text{s}}{1.11 \times 10^4 \text{ eV} / (3 \times 10^8 \text{ m/s})} = 1.12 \times 10^{-10} \text{ m}.$$

This is about the size of an atom! Then, when studying the behavior of an electron in an atom, we absolutely need to take into account the wave-like nature of the electron.

*Aside:* Why is this a non-relativistic kinetic energy? Relativistically, the momentum can be expressed in terms of the kinetic energy as

$$K_{\text{rel}} = E - mc^2 = \sqrt{p^2 c^2 + m^2 c^4} - mc^2 \Rightarrow p = \frac{K}{c} \sqrt{1 + \frac{2mc^2}{K}}$$

whereas nonrelativistically,

$$K_{\text{non-rel}} = \frac{1}{2}mv^2 = \frac{p^2}{2m} \Rightarrow p = \sqrt{2mK}$$

The relativistic expression reduces to the non-relativistic one when  $K \ll 2mc^2$ : in this limit, we can drop the +1 under the square root, so that

$$p = \frac{K}{c} \sqrt{1 + \frac{2mc^2}{K}} \approx \sqrt{2mK}$$

The kinetic energy is non-relativistic if  $K \ll 2mc^2$ , so that the relativistic and non-relativistic expressions agree. In the example we just did, the electron's kinetic energy was given as 120 eV, leading to

$$\frac{K}{2mc^2} = \frac{120 \text{ eV}}{2(0.511 \times 10^6 \text{ eV}/c^2)c^2} \approx 10^{-4} \ll 1$$

which justifies our use of the non-relativistic expressions for the electron's kinetic energy.

### Example Problem: de Broglie wavelength

*We didn't cover this question in class, so it's a good practice problem to try on your own.*

Suppose an electron accelerated through 1 Volt has an associated wavelength  $\lambda$ . If the electron were accelerated through 4 V, it would have a wavelength of: (you may use non-relativistic expressions)

- (a)  $4\lambda$
- (b)  $\lambda/4$
- (c)  $\lambda/2$
- (d)  $2\lambda$

It takes 1 eV to accelerate an electron through a potential difference of 1 Volt, so the electron after 1 Volt has kinetic energy 1 eV. Using the non-relativistic expression for the kinetic energy in terms of the momentum,

$$K = \frac{p^2}{2m} \Rightarrow p = \sqrt{2mK}$$

Substituting into the formula for the de Broglie wavelength, we find

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m(1\text{ eV})}}$$

If the electron were instead accelerated through a potential difference of 4 volts, we would find a wavelength of

$$\lambda' = \frac{h}{\sqrt{2m(4\text{ eV})}} = \frac{\lambda}{2}$$

The answer is (c).

Notice that we can justify the use of the non-relativistic expression since

$$\frac{K}{2mc^2} = \frac{(1 - 4)\text{ eV}}{2(0.511 \times 10^6 \text{ eV}/c^2)c^2} \approx 10^{-6} \ll 1.$$

This is an incredible conjecture, with widespread implications. In particular, if matter has wave-like properties, then matter should show interference effects. This is precisely what C.J. Davisson and L. H. Germer tested in 1927, by shining an electron beam onto a layer of nickel atoms, which act as a diffraction grating. If you shine light on the layer, then you can calculate the pattern of light you will see scattered off the grating based on when you will get constructive versus destructive interference, and therefore predict the resulting interference pattern. The experimental results showed a diffraction pattern for the electrons, demonstrating that electrons diffract in crystals just as light does, with the experimentally verified wavelength of the electrons related to their momentum a la de Broglie. (See your book for more reading on the Davisson Germer experiment!)

A practical application of this fact is the electron microscope. Because the associated wavelengths of electrons can be so small, they can be used to resolve very fine distances.

**Explanations for the Bohr orbits** The wave-like nature of light explained the quantized Bohr orbits. The quantization of orbits of electrons around a nucleus correspond in a wave-like language to “standing waves of electrons.” An electron is in a stable orbit when an integral number of the electron’s corresponding wavelength fits into the circumference of the orbit. The possible standing waves correspond to stable “modes of vibration” of the electron in orbit. Meanwhile, non-standing wave solutions do not persist, since a fractional number of waves in the orbit loop will die from destructive interference.

Requiring constructive interference of the electron’s matter wave in a circular orbit around an atom, i.e. requiring the electron be in a standing wave configuration, follows directly from angular momentum quantization! Constructive interference along a circle of radius  $r$  exists when

$$n\lambda = 2\pi r, \quad n = 1, 2, \dots$$

Using  $\lambda = h/p$ , we have,<sup>8</sup>

$$\begin{aligned}\lambda = \frac{h}{p} = \frac{h}{mv} &\Rightarrow n\lambda = n\frac{h}{mv} = 2\pi r \\ &\Rightarrow n\hbar = mvr \quad \left(\hbar \equiv \frac{h}{2\pi}\right)\end{aligned}$$

The stationary states with quantized angular momentum are *precisely* the states that correspond to standing waves where an integral number of the electron's de Broglie wavelengths fit into the orbit.

———End Lecture 12.

### 2.3.2 What Waves in a Matter Wave?

So, just what is it that's waving in matter waves? For light, it's the electric and magnetic fields that wave. For matter, it's *the probability of finding the particle at some location* that waves. This is radically different from what you're used to in classical physics, and an example of the fact that things on a small scale behave nothing like anything we have any direct experience about.

Let's be a bit more specific. (We'll wait until Part III to develop the general, consistent theory of what these waves are and how they should behave—consider this section an introduction.) Recall that the intensity of a wave is proportional to its amplitude squared. For instance, let's say my wave is described by a function  $\Psi(x, t)$ ; then, the intensity of the wave is proportional to  $|\psi(x, t)|^2$ . If my wave describes a particle, then the claim is that the intensity of the matter wave is equal to the probability of the particle being found in some location,

$$\text{Probability of being at } x \text{ and } t \equiv P(x, t) = |\psi(x, t)|^2.$$

This probabilistic nature of reality is at the heart of quantum mechanics.

So, what kinds of waves can describe particles? The matter wave representing a particle should incorporate the fact that a particle is *localized*, *i.e.* has a large probability of being found in a small region of space at a specific time. We will now take a math break to learn how to describe waveforms that are localized in space. These ideas are covered in more detail in the supplementary notes posted to the class website, so I recommend taking a look through those if this material is unfamiliar to you.

**Math Break! Building a wave packet** We need to learn how to describe waveforms that are localized in space. This can be achieved by adding sinusoidal waves with different wavelengths.

Let's start with our good old 1-dimensional plane wave, which we can write as

$$\psi(x, t) = A \cos(kx - \omega t) \tag{2.22}$$

<sup>8</sup>If we use the relativistic formula for the electron's momentum, we would just find that  $n\hbar = \gamma mvr$ , which says that the relativistic momentum of the electron is quantized.

where  $k$  is the wavenumber and  $\omega$  is the angular frequency, related to the wavelength  $\lambda$  and frequency  $f$  as,

$$k = \frac{2\pi}{\lambda}, \quad \omega = 2\pi f.$$

These are in turn related to the speed of the wave as,

$$\lambda f = \frac{\omega}{k} = v_p$$

where we put a subscript  $p$  on the speed because this is more specifically the *phase speed* of the wave. In particular,  $v_p$  is the speed that a point of constant phase (*e.g.* the crest) travels.

Our claim is that the intensity of the wave describes the probability of finding the particle at some location and some time. For the plane wave (2.22), we can compute

$$P(x, t) = |\psi(x, t)|^2 = |A|^2 \cos^2(kx - \omega t)$$

which is periodic both in time and space. Clearly such a probability density cannot well describe a particle—we're after something localized in space.

Instead, we can consider adding up two such plane waves with different  $k$  and  $\omega$  (and the same amplitude). Then, the total wave group takes the form

$$\begin{aligned} \psi(x, t) &= \psi_1(x, t) + \psi_2(x, t) \\ &= A (\cos(k_1 x - \omega_1 t) + \cos(k_2 x - \omega_2 t)) \\ &= 2A \cos\left(\frac{1}{2}((k_2 - k_1)x - (\omega_2 - \omega_1)t)\right) \cos\left(\frac{1}{2}((k_2 + k_1)x - (\omega_2 + \omega_1)t)\right) \end{aligned} \tag{2.23}$$

where in the second line we used trigonometric formulas to add the cosines. If  $k_1 \approx k_2$  and  $\omega_1 \approx \omega_2$ , then  $k_1 - k_2$  and  $\omega_1 - \omega_2$  are very small, while  $k_1 + k_2 \approx 2k_1$  and  $\omega_1 + \omega_2 \approx 2\omega_1$  is relatively large. This total waveform describes *beats*: there is a broad sinusoidal envelope described by the cosine with large wavelength  $\lambda = 4\pi/(k_1 - k_2)$  and small frequency  $(\omega_1 - \omega_2)/2$ , which modulates a wave with small wavelength  $\lambda = 4\pi/(k_1 + k_2)$  and high frequency  $(\omega_1 + \omega_2)/2$ .

The high frequency waves moves at the phase velocity,

$$v_p = \frac{(\omega_1 + \omega_2)/2}{(k_1 + k_2)/2} \approx \frac{\omega_1}{k_1}$$

while the low frequency envelope moves at what's known as the *group velocity*,

$$v_g = \frac{(\omega_1 - \omega_2)/2}{(k_1 - k_2)/2}$$

This sum of two plane waves still isn't a great description for a matter wave describing a particle, since it's still periodic (even if we have achieved localized beats). What we're really after is a wave group that doesn't repeat. We can accomplish this with a wave group formed from adding up an infinite number of plane waves, whose amplitudes vary as a function of the wavelength and frequency of the individual waves. (This leads us to the subject of *Fourier analysis*, the study of the way a general function can be represented by summing up simpler trigonometric functions with definite frequencies. We won't need to cover the full machinery of Fourier analysis in this course, we are just going to review the points we need for our analysis of quantum mechanics!)



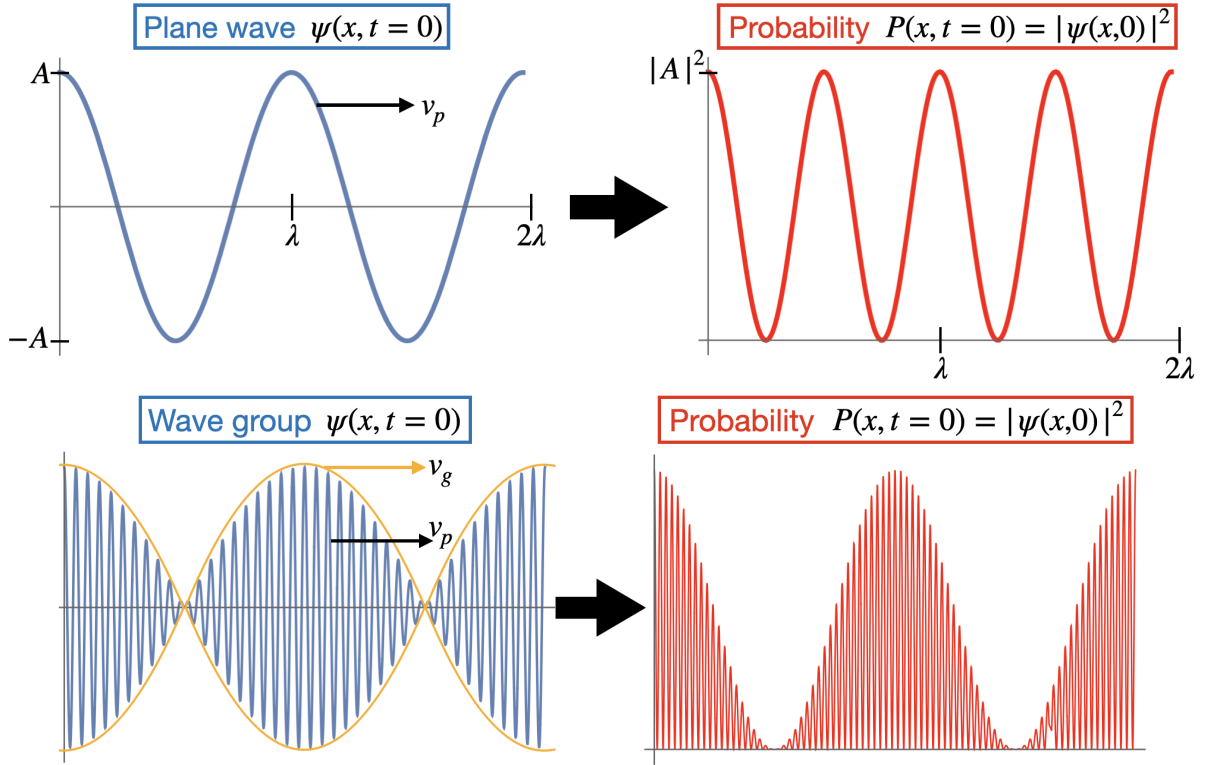


Figure 5: The plane wave (2.22) and its associated probability density (top), and the wave group (2.23) and its associated probability density (bottom).

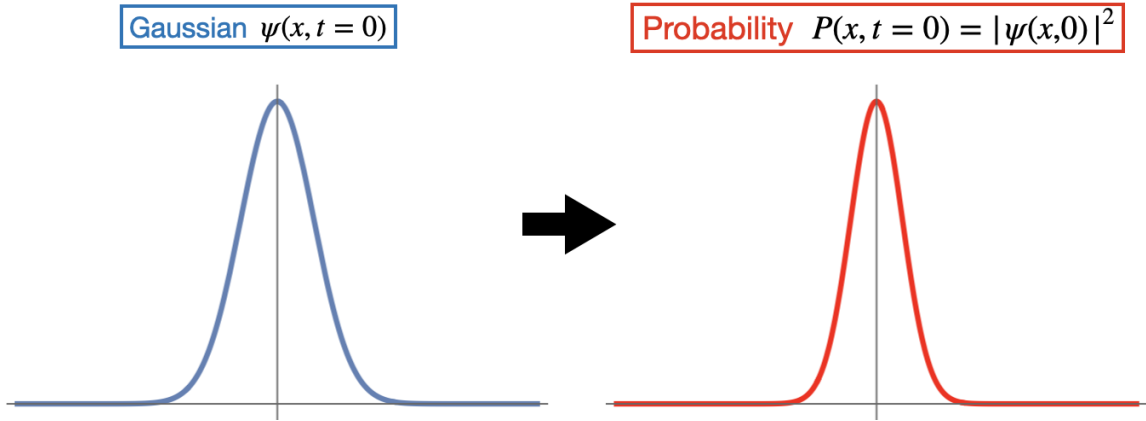


Figure 6: A Gaussian wavepacket, plotted at constant  $t = 0$ .

The classic example of a localized wave packet is the Gaussian wavepacket. The idea is to add up an infinity of plane waves whose amplitudes take a very particular form,

$$\psi_k(x, t = 0) = A(k)e^{ikx}, \quad A(k) = e^{-k^2}$$

where we'll focus on the wave at just  $t = 0$ . Since  $e^{ikx} = \cos(kx) + i\sin(kx)$ , the real part of  $\psi_k(x)$  is precisely the plane wave we wrote in (2.22), except we've chosen it to have the special  $k$ -dependent amplitude  $A(k)$ . Summing up an infinity of these plane waves with  $k$  ranging from  $-\infty$  to  $\infty$  means doing the following integral,

$$\Psi(x) = \int_{-\infty}^{\infty} \psi_k(x) dk = \int_{-\infty}^{\infty} e^{ikx - k^2} dk = \sqrt{\pi} e^{-\frac{x^2}{4}} \quad (2.24)$$

(This is a famous integral called a Gaussian integral—if you ever need to do it in class you’ll be given the formula to do so.) The function (2.24) is called a Gaussian; it is a packet of an infinite number of waves with different wavenumbers/frequencies clustered around a value of  $x$ .

### Example Problem: Practice with waves

*These are some practice problems to make sure you are comfortable working with plane waves. I highly recommend doing these on your own to make sure you are prepared for the next part of the course.*

1. Write the complex form of a plane wave with wavelength  $\lambda = 2m$  and frequency  $f = 1/4s^{-1}$ , and amplitude 1.
2. Write the real part of this wave.
3. Consider the wave  $\psi_1(x, t) = \sin(k(x - 3t))$ . What is the angular frequency of this wave?
4. Consider the wave  $\psi_2(x) = Ae^{ikx} + Be^{-ikx}$ . Using  $e^{i\theta} = \cos \theta + i \sin \theta$ , rewrite this wave in the form

$$\psi_2(x) = A' \cos(kx) + B' \sin(kx).$$

What are the coefficients  $A'$  and  $B'$  in terms of  $A$  and  $B$ ?

5. Impose the boundary condition that  $\psi_2(x = 0) = 0$ . What does this tell you about the coefficients  $A', B'$ ?
6. Suppose that  $\psi_2(x)$  satisfying the boundary condition from part (5) describes a matter wave. For which values of  $x$  is the probability of finding the particle at that location equal to 0?

*Answers:*

- 1.

$$\psi(x, t) = e^{i(\frac{2\pi}{2m}x - 2\pi(1/4s^{-1})t)} = e^{\pi i(x - \frac{1}{2}t)}$$

where  $x$  is measured in meters and  $t$  in seconds.

2. Since  $e^{i\theta} = \cos \theta + i \sin \theta$ , the real part of the complex exponential is cosine of its exponent. We have that:

$$\text{Re}(\psi) = \cos\left(\pi\left(x - \frac{1}{2}t\right)\right)$$

3. The angular frequency is what is in front of the  $t$ , so  $\omega = 3k$ . (It doesn’t matter that this is sine versus cosine, since we can just rewrite

$$\sin(k(x - 3t)) = \cos\left(k(x - 3t) - \frac{\pi}{2}\right)$$

which differs from the cosine by an  $x$  and  $t$  independent phase.

4. We can use

$$\begin{aligned}
\psi_2(x) &= Ae^{ikx} + Be^{-ikx} \\
&= A(\cos(kx) + i\sin(kx)) + B(\cos(-kx) + i\sin(-kx)) \\
&= A(\cos(kx) + i\sin(kx)) + B(\cos(kx) - i\sin(kx)) \\
&= \cos(kx)(A + B) + \sin(kx)(iA - iB) \\
\Rightarrow A' &= A + B, \quad B' = i(A - B)
\end{aligned}$$

where we used that  $\cos(-\theta) = \cos(\theta)$  and  $\sin(-\theta) = -\sin(\theta)$  since cosine is a symmetric function and sine an antisymmetric one.

5. Imposing  $\psi_2(0) = 0$  leads to  $0 = A'\cos(0) + B'\sin(0) = A'$ , since  $\cos(0) = 1$  and  $\sin(0) = 0$ . Therefore, we have learned that  $A' = 0$  in order to satisfy the boundary condition.
6. If we suppose that  $\psi_2(x) = B'\sin(kx)$  describes a matter wave, then the probability of finding the particle as position  $x$  is proportional to

$$P(x) \propto \psi_2(x)^*\psi_2(x) = (B')^*B'\sin^2(kx) = |B'|^2\sin^2(kx)$$

(I say “proportional to” because there is an overall constant normalization that we haven’t determined here.) Assuming  $B'$  isn’t 0 so that this isn’t just trivially 0, the probability of finding the particle at position  $x$  is only 0 when  $\sin^2(kx) = 0$ . Since  $\sin$  is a periodic function which is zero when its argument is equal to an integer multiple of  $\pi$ , this is true when

$$P(x) = 0 \quad \Leftrightarrow \quad x = \frac{n\pi}{k}, \quad n = 0, 1, 2, 3, \dots$$

*End math break.*

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So, the types of waves that will describe particles localized in space are wave packets consisting of sinusoids whose amplitudes depend on  $k$  (the most idealized version being the Gaussian wave packet). As we saw, a wave packet has two different kinds of velocity: phase velocity and group velocity. These are defined as

$$\boxed{v_p = \frac{\omega}{k}, \quad v_g = \frac{d\omega}{dk}} \quad (2.25)$$

The phase velocity describes how quickly the wiggles inside the envelope are moving, and is in general *NOT* the actual velocity of the particle. In fact,  $v_p$  can be larger than the speed of light! On the other hand, the group velocity describes how quickly the envelope is moving, and *does* correspond to the actual velocity of the particle.

These relations become somewhat more familiar once we apply the de Broglie relations. If my electron has relativistic momentum  $p$  and relativistic energy  $E$ , then according to de Broglie its associated matter wave has wavelength and frequency

$$\lambda = \frac{h}{p} \quad \Rightarrow \quad \boxed{p = \hbar k}, \quad f = \frac{E}{h} \quad \Rightarrow \quad \boxed{E = \hbar\omega} \quad (2.26)$$

where we used  $\omega = 2\pi f$  and  $k = 2\pi/\lambda$ . We see then that we can rewrite the expression for the

phase and group velocity in terms of the particle's energy and momentum as

$$\boxed{v_p = \frac{E}{p}, \quad v_g = \frac{dE}{dp} = u \text{ (the particle's speed)}} \quad (2.27)$$

The energy  $E$  of the particle in general depends on  $p$ —relativistically  $E = \sqrt{p^2 c^2 + m^2 c^4}$ , and non-relativistically  $E = p^2/(2m)$ , which implies that the angular frequency  $\omega$  depends on  $k$ . (In general, we call the function  $E(p)$  or equivalently  $\omega(k)$  a *dispersion relation*.)

On your Homework, you will show that  $v_g$  defined in this way indeed reproduces the particle's speed, which is always less than or equal to the speed of light. While the velocity of individual waves making up the wave packet ( $v_p$ ) can be bigger than  $c$ , these don't represent the speed of any physical object—the physical speed always satisfies the laws of relativity.

### 2.3.3 The Uncertainty Principle & The Meaning of Observation

We've seen that in order to localize a wave in space, we need to add together sine waves of different wavelengths. In general, the more we want to localize a wave (the smaller we want its spatial spread  $\Delta x$  to be), the larger the range of wavelengths we need to include in the superposition (the larger  $\Delta k$  needs to be) in order to form the pulse. Mathematically, we can state this as the fact that these two quantities are inversely proportional,

$$\Delta x \Delta k \approx 1.$$

Similarly, the smaller we want the time duration of the pulse to be ( $\Delta t$ ), the larger the spread of frequencies  $\Delta \omega$  we will need to add up to form the wave group,

$$\Delta t \Delta \omega \approx 1.$$

These reciprocity relations hold for pulses of any kind—water waves, sound waves, electromagnetic waves, and matter waves. The content of these statements is that as the spatial spread (temporal spread) of my waveform decreases, the spread in the number of wavelengths (frequencies) I need to make that waveform must increase, and vice versa—both  $\Delta x$  and  $\Delta k$  cannot become arbitrarily small, since as one goes to zero the other goes to infinity.

Applying this fact about general wave groups to matter waves is the essence of the uncertainty principle. Since  $k$  is related to the particle's momentum as  $k = p/\hbar$ , and  $\omega$  to its energy as  $\omega = E/\hbar$ , we can rewrite the above equations in terms of momentum and energy. This leads us to the uncertainty principle,

$$\boxed{\text{Uncertainty principle: } \Delta x \Delta p \geq \frac{\hbar}{2}, \quad \Delta E \Delta t \geq \frac{\hbar}{2}} \quad (2.28)$$

These principles are statements about the simultaneous measurement of position and momentum of a particle, or of the energy and time taken to measure that energy. With regards to the position-momentum uncertainty relation, It is impossible to simultaneously measure both the position and momentum of a particle with unlimited precision.<sup>9</sup> This statement does *not* arise from any sort of imperfection in a measuring device, but rather arises from the inherent uncertainty relation governing any type of wave pulse that is formed by the superposition of waves of different wavelengths/frequencies, with  $\Delta x$  and  $\Delta k$  (and similarly  $\Delta E$  and  $\Delta t$ ) equal

<sup>9</sup>The meaning of the energy-time uncertainty relation is somewhat less clear—what do we mean by uncertainty in time? If we have an unstable particle, then  $\Delta t$  means its lifetime, so that its energy is not exact.

to the standard deviations of the waveforms constructed in this manner. This is a fundamental constraint, which shakes the foundations of classical physics which we have relied on for so long. (All of classical mechanics is built around position and momentum—if we cannot measure them at the same time, then none of our classical ideas have any use!)

### Example Problem: Uncertainty principle for an electron in a box

For example, let's say that at some moment in time I've trapped an electron in a box of length  $L$ . What is the minimum uncertainty in the electron's momentum?

Since the electron is confined in a box of length  $L$ , this means that the uncertainty in the position of the electron is  $\Delta x = L$ . So, according to the uncertainty principle, the minimum uncertainty in my knowledge of the momentum of the electron at this moment is

$$\Delta x \Delta p \geq \frac{\hbar}{2} \Rightarrow \Delta p_{\min} = \frac{\hbar}{2\Delta x} = \frac{\hbar}{2L}.$$

What this result says is that the smaller the box in which I know I've trapped my electron, the less I can pinpoint its momentum.

One can prove that the wave form that saturates the lower bound is the Gaussian waveform,

$$\Delta x \Delta p = \frac{\hbar}{2} \quad \text{for a Gaussian wave packet.}$$

Put another way, the Gaussian wave packet represents the perfect balance of how precisely we can know both the position and momentum of a particle simultaneously as allowed by the laws of nature. I can tell its position and momentum reasonably well, but not exactly. What about plane waves?

### Clicker Question: Uncertainty principle for a plane wave

I have a particle whose corresponding matter wave is a plane wave,  $\psi(x, t) = A \cos(kx - \omega t)$ . What is  $\Delta p$  for this particle?

- (a) 0
- (b)  $h/(4\pi)$
- (c) Infinity
- (d) None of the above

A plane wave has definite value  $k = \frac{2\pi}{\lambda}$ , meaning the associated particle's momentum  $p = \hbar k$  is also definite. Since the plane wave has a definite momentum, so  $\Delta p = 0$ , and the answer is (a).

The plane wave is on the opposite end of the spectrum as the Gaussian, since a plane wave is infinitely spread out in space (so that the uncertainty in our knowledge of  $x$ ,  $\Delta x$ ,  $= \infty$ ), but has a precise value of  $k$  (so that the uncertainty in our knowledge of  $k$ ,  $\Delta k$ ,  $= 0$ ).

Note that [this link](#) has a nice discussion of the uncertainty principle and wave groups.

—————End Lecture 13.

### Example Problem: A world in a grain of sand

Suppose we measure the position of a grain of sand of mass 1mg to the nearest atom—an uncertainty of 0.1nm. What does the uncertainty principle imply about the uncertainty in the speed of the grain?

*Answer:* Using  $p = mv$  for  $v$  the speed of the grain and  $m$  its mass,  $\Delta p = m\Delta v$ , and

$$\Delta v \geq \frac{\hbar}{2m\Delta x} = \frac{1.0546 \times 10^{-34} J}{2(1 \times 10^{-6} kg)(0.1 \times 10^{-9} m)} = 5.3 \times 10^{-19} m/s$$

This is a *tiny* number. It would take *6 years* to see the grain of sand move a distance of just 0.1nm—the precision to which we could measure its position in the first place. This is why the uncertainty principle is not evident in our everyday experience;  $\hbar$  is such a small number that you have to be measuring either very tiny distances or speeds to see the effect.

**A physical motivation for the uncertainty principle** As we’ve stated it, the uncertainty principle arises from the fact that particles have associated waves. We can also, however, give a more physical motivation for the impossibility of measuring the position and momentum of a particle with infinite precision at the same time on the basis of classical optics. In reality, all measurements have limited precision, no matter what measurement instrument is used. Since measurement is an experimental procedure, measurement errors are unavoidable.

Consider that when I look at something I am observing the light scattering off of it, which necessarily disturbs (to at least some small degree) whatever it is I’m looking at. You learned in our discussion of Compton scattering (for instance) that when I scatter a photon off of an electron, the electron will move off with some change in its momentum, and the photon goes off with some change in its frequency—the act of observation disturbs the electron.

Consider the following thought experiment for observing an electron (known as “Heisenberg’s microscope”, since this was first considered by Heisenberg). I have a very powerful microscope that works by scattering a single photon from an electron initially at rest, and viewing the scattered photon through the lens of the microscope. The scattered photon passes through the lens and lands somewhere on the viewing screen. I will only make an observation when the photon is scattered within the range of the lens, so when the scattering angle  $\theta$  of the photon is not larger than  $1/2$  the angle subtended by the lens.

As we learned in Compton scattering, when the photon scatters off the electron the electron gains some momentum,  $\Delta p$ . Let  $p_x$  denote the component of momentum in the  $x$ -direction of Figure 7, which satisfies

$$p_x = \frac{hf'}{c} \sin \theta$$

(This result follows from conservation of momentum in the  $x$ -direction of the figure, equation (2.11) from our previous discussion of the Compton effect, where we have switched the  $x$ - and  $y$ - axes between the two setups.) The magnitude of this momentum can range from  $\frac{hf'}{c} \sin \theta$  to  $-\frac{hf'}{c} \sin \theta$  depending on whether  $\theta$  is positive or negative, so the total possible range of the

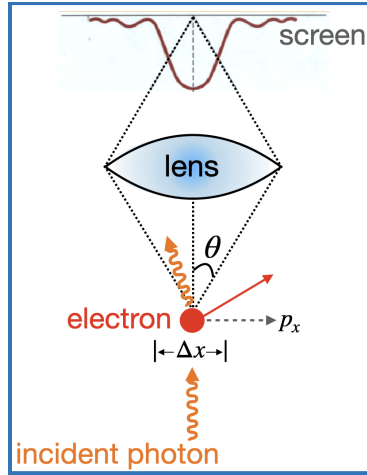


Figure 7: Setup for Heisenberg's microscope.

electron's momentum is

$$\Delta p_x = \frac{2hf'}{c} \sin \theta$$

This says that the amount of recoil of the electron is only determined up within this range, since we can only know the path of the scattered photon within the range angle  $2\theta$  subtended by the lens.

Meanwhile, it is a fact from optics that since light diffracts like a wave, instruments have limited resolution. The resolution of a microscope made with such a lens is

$$\Delta x = \frac{\lambda'}{2 \sin \theta} = \frac{c}{2 f' \sin \theta}$$

The microscope can then only resolve the position of the electron up to this accuracy. Together, we see that

$$\Delta x \Delta p_x = h$$

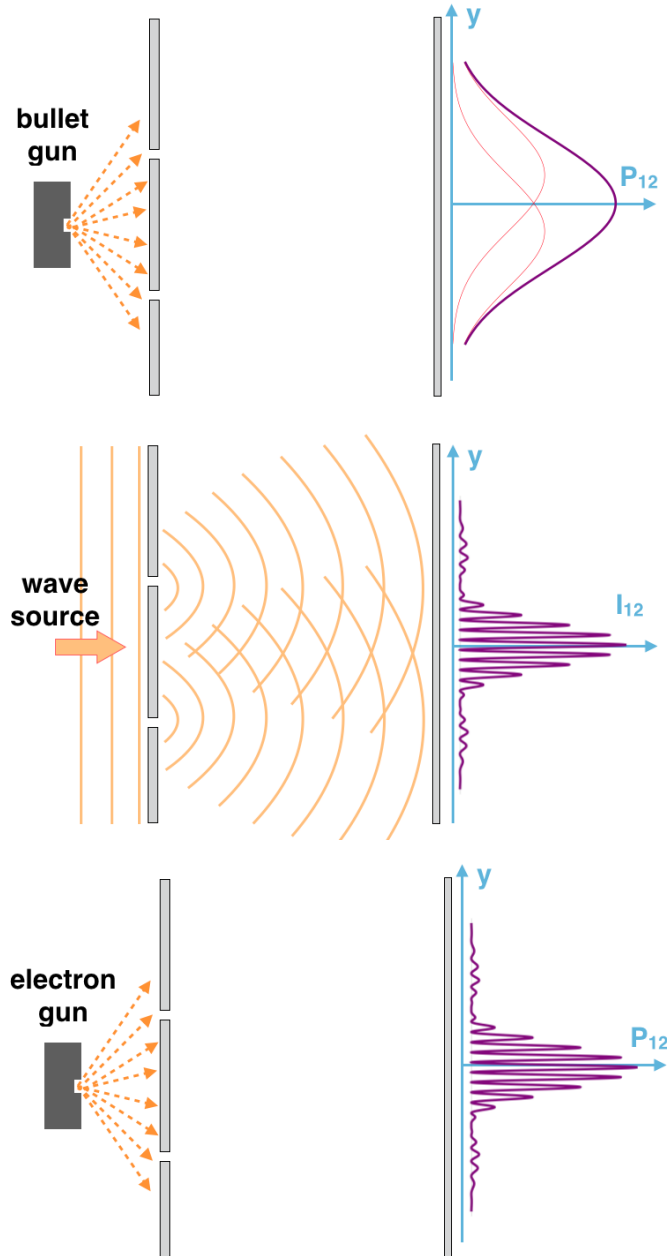
which approximates the uncertainty principle!

In sum, because light is made up of discrete packets of energy and therefore imparts some of that energy onto whatever particle it is scattering off of, and furthermore a physical microscope can only resolve the path of the scattered light within some accuracy, it is impossible to know both the precise position and momentum of the electron.

### 2.3.4 Matter Diffraction

To understand the quantum behavior of particles like electrons, we'll do an experiment. Set up an electron gun in front of a screen with two slits. A detection screen is set up a distance  $L$  from the screen with the slits, which records whenever an electron hits the screen. What do we see?<sup>10</sup>

<sup>10</sup>We closely follow the presentation of this material from Richard Feynman's lectures, which can be found online at [www.feynmanlectures.caltech.edu](http://www.feynmanlectures.caltech.edu).



**The indestructible bullets experiment** First, let's think about what would happen if I shot bullets at the screen. Imagine that the gun shoots a stream of indestructible bullets that sprays randomly over a large angular spread, and the screen with the slits is made of hard armor plate, with two slits just big enough to let a bullet through. Question: What is the probability that a bullet which passes through the holes in the wall will arrive at the detection screen a distance  $x$  from the center?

The bullets arrive in lumps on the observation screen. Of course, a bullet which reaches the detection screen either went through hole 1 or hole 2. When hole 1 is covered, bullets can only pass through hole 2, and we would get the probability curve  $P_2$ . When hole 2 is covered, bullets can only pass through hole 1, and we would get the probability curve  $P_1$ . With both holes open, the probabilities just add together:  $P_{12} = P_1 + P_2$ .



**Interference patterns of waves through slits** Next, let's recall what happens when we shine light at a double slit. We have a source of coherent light incident on the screen with the slits, and the waves diffract at each of the slits. According to the Huygens principle, the wave-front at each of the slits can be regarded as a source of spherical wavefronts. The light waves emanating from each slit are superimposed on the detection screen, which records the intensity of the incident light. Question: What is intensity of light recorded on the detection screen a distance  $x$  from the center?

The answer is that light undergoes interference (overlapping waves interfere) and diffraction (waves spread out beyond a narrow opening), leading to an intensity profile of light and dark spots on the screen. For example, let's consider the interference between two light waves. If we cover hole 1, we see an intensity pattern  $I_2$ , while when we cover hole 2, we see an intensity pattern  $I_1$ . The intensity observed when both holes are open is *not*, however, the sum of  $I_1$  and  $I_2$ , due to interference of the waves. At some places the waves are in phase, so the amplitudes add to give a larger amplitude and thus brighter spot on the screen, while in some places the waves are out of phase, so the amplitudes subtract and we see a dark spot. There is no such analogue of this in the experiments with the bullets—two bullets in the same spot can't cancel each other out to give less probability of seeing a bullet! In other words, unlike our classic notion of a particle, waves exhibit interference.

Let the ray radiated from hole 1 at the screen be described by the real part of  $\psi_1 = A_1 e^{i\omega t}$ , and the ray radiated from hole 2 be described by  $\psi_2 = A_2 e^{i\omega t}$ , where in general the amplitudes  $A_{1,2}$  are complex. Then,

$$I_1 = |\psi_1|^2 = \psi_1^* \psi_1 = |A_1|^2, \quad I_2 = |\psi_2|^2 = \psi_2^* \psi_2 = |A_2|^2, \quad I_{12} = |\psi_1 + \psi_2|^2.$$

In particular, the intensity with both slits open is related to the intensity with only one slit open by

$$I_{12} = |\psi_1 + \psi_2|^2 = |A_1|^2 + |A_2|^2 + A_1 A_2^* + A_2 A_1^*. \quad (2.29)$$

Let  $\delta$  be the phase difference between  $A_1$  and  $A_2$ , so that the amplitudes are related as,

$$A_1 = |a_1| e^{i\phi_1}, \quad A_2 = |a_2| e^{i(\phi_1 - \delta)}$$

The latter two terms in (2.29) can then be rewritten,

$$A_1 A_2^* + A_1^* A_2 = |a_1| |a_2| \left( e^{i\delta} + e^{-i\delta} \right) = 2|a_1| |a_2| \cos \delta = 2\sqrt{I_1 I_2} \cos \delta.$$

In sum, the total intensity at the detection screen when both slits are open is equal to the sum of the individual intensities from when only one slit is open, plus an “interference term” which depends on the phase difference between the two rays

$$I_{12} = I_1 + I_2 + 2\sqrt{I_1 I_2} \cos \delta,$$

for  $\delta$  the phase difference between the amplitudes of the two rays coming through the slits.

**Back to electrons** Finally, let's do the experiment with electrons. What do we see at the detection screen?

The answer is twofold. First of all, the electrons arrive at the screen in particle-like lumps; we could set up our experiment to click whenever an electron arrives at the screen, and then a click would be heard every time an electron hits the screen—like the indestructible bullets, there is no half-electron arriving at the screen.

So, what is the probability that an electron will arrive at the detection screen some distance  $x$  from the center,  $P_{12}$ ? The answer is that  $P_{12}$  looks just like the curve  $I_{12}$ ! In particular,  $P_{12} \neq P_1 + P_2$  for electrons, but rather, if we count enough electrons, the rate of their arrival at various points on the screen can be predicted by a curve that looks like it's coming from the interference of two waves! Importantly, this same pattern is observed when electrons are shot one at a time at the screen—it has nothing to do with electrons interfering with other electrons; rather the electron's matter wave is interfering with itself!

What if we close one of the slits? Then, we would know for certain that the electron goes through the only open slit, and the interference pattern would be lost. A way to view this result is to say that *the act of measurement of which slit the electron passes through disturbs the electron's path, destroying the interference pattern.*

Electrons arrive in lumps, like particles, but the probability of the arrival of these lumps is like the distribution of intensity of a wave. Electrons behave both like waves, and like particles. The associated wave to the electron is the “matter wave” that we've been discussing throughout this section. In the next section, when we develop the theory of quantum mechanics, we'll be more precise about exactly what these matter waves are, and what they mean.

## 3 Part III: Quantum Mechanics

### 3.1 Quantum Mechanics in 1d

Quantum mechanics as a theory is as beautiful as it is complex. In this section we will discuss the foundations of quantum mechanics: the postulates and their implications. We will restrict ourselves for the time being to one-dimensional cases, extending later into three dimensions. Furthermore, for the remainder of this discussion we will assume that velocities are much smaller than the speed of light, so that we do not need to worry about relativity. (A completely consistent theory of relativistic quantum mechanics is a very rich and interesting subject, but is outside the scope of this course.)

#### 3.1.1 Postulate: Associated to a Particle is a Wavefunction

As we have discussed in some detail, particles behave as waves. In quantum mechanics, these waves are the main object that describe the state of a particle. *Postulate:* Associated to a particle is a *wavefunction*  $\Psi(x, t)$  that describes everything that can be known about the system. The wavefunction is a complex function of space and time that is the ultimate DNA of the particle: it contains all the information about the particle under the influence of whatever forces are acting on the particle.

Quantum mechanics is inherently probabilistic; we do not specify with certainty the location of a particle, but instead assign a probability of finding it between  $x$  and  $x + dx$ . The wavefunction represents the probability amplitude for finding a particle at a particular point in space and time. In particular, the probability that a particle constrained to move along the  $x$ -axis is found in an interval  $dx$  at time  $t$  is given by

$$\boxed{\text{Probability density : } P(x) dx = |\Psi(x, t)|^2 dx = \Psi^* \Psi dx} \quad (3.1)$$

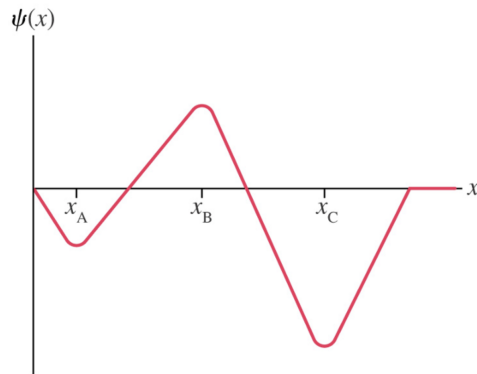
Then, the probability of finding the particle in a spatial interval  $a \leq x \leq b$  is given by

$$\boxed{P(a \leq x \leq b) = \int_a^b P(x) dx = \int_a^b |\Psi|^2 dx}. \quad (3.2)$$

In other words, it's the area under the curve of the probability density. This integral must always result in a number between 0 and 1, where 0 corresponds to 0% probability of the particle being found at that location, and 1 corresponds to 100% probability of the particle being found at that location.

Mathematically this is all well and good, but it is certainly not intuitive. How is it that all we can understand about the location of a particle is the probability of finding it in some location? It seems as if it should be in a certain spot or not, even if it is hard to precisely measure it. Where actually is the particle? One answer is that we truly cannot say until we make sure measurement, at which point we find the particle in a single position (within the precision of the measurement) with probability given by the wavefunction. If we were to repeat the measurement many times, we would expect to get a distribution of measurements that roughly follows the curve of the probability density.

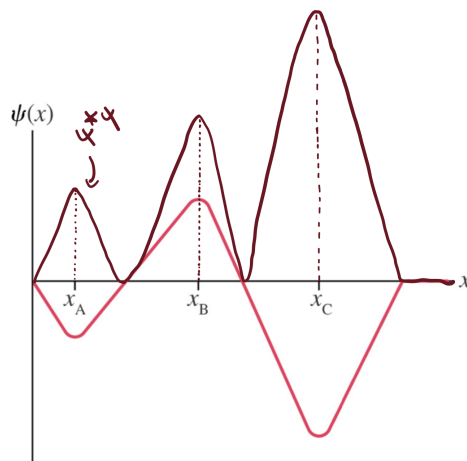
### Clicker Question: Practice with Wavefunctions



Suppose that this is the wavefunction of a neutron. Of the following options, where is the neutron most likely to be found?

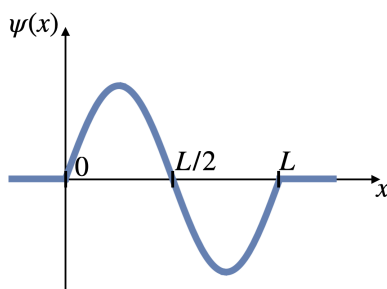
- (a)  $x = x_A$
- (b)  $x = x_B$
- (c)  $x = x_C$
- (d)  $x = 0$

*Solution:* The probability density is given by  $|\psi|^2$ , which looks roughly like the figure dark red line sketched below. The particle is most likely to be found at  $x_C$ , (c).



### Clicker Question: Practice with Wavefunctions

This is the wavefunction of a particle. Where is the particle most likely to be found?



- (a)  $x = L/4$
- (b)  $x = L/2$
- (c)  $x = 3L/4$
- (d)  $x = L/4$  and  $x = 3L/4$

*Solution:*  $\psi$  has the largest equal magnitudes at  $x = L/4$  and  $x = 3L/4$ , so  $\psi^*\psi$  will also be largest at these values. The answer is (d).

### Clicker Question: Dimensions of $\Psi$

What are the dimensions of the wavefunction  $\Psi(x, t)$  in 1 spatial dimension?

*Solution:* The probability  $P = \int |\psi|^2 dx$  has to be equal to a dimensionless number (in order to correspond to actually correspond to a probability!). Since  $dx$  has units of [Length], the integrand  $|\psi|^2$  has to have units of  $[\text{Length}]^{-1}$ , so that  $\psi$  has units of  $[\text{Length}]^{-1/2}$ .

In order for this interpretation of the wavefunction to make sense, it must be true that the *total* probability that we find the particle *somewhere* on the  $x$ -axis is 1: there is 100% probability that we find the particle somewhere on the  $x$ -axis! This is called the *normalization condition*,

$$\text{Normalization: } \int_{-\infty}^{\infty} |\Psi|^2 dx = 1 \quad (3.3)$$

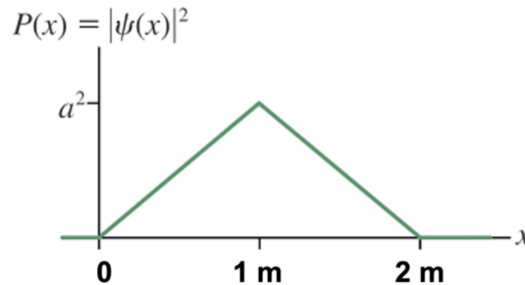
This is a physical condition that the particle must be found somewhere.

While a wavefunction is a mathematical function, it describes a physical object, and so must satisfy some other physical properties. In particular, we also need to require that:

- $\Psi$  must be finite (otherwise we'd get infinite probabilities!).
- $\Psi$  must be a single-valued function of space and time (what would it mean to have two different probabilities assigned to the same point??).

- $\Psi$  must be a continuous function of space and time.
- $\Psi$  must have a continuous derivative as a function of  $x$ , wherever the potential is finite.

### Example Problem: Fun with Wavefunctions



By imposing the normalization condition,

$$\int_{-\infty}^{\infty} |\Psi|^2 dx = 1$$

find the value of the constant  $a^2$  for the above probability density.

*Solution:* The integral is zero except between  $x \in (0, 2m)$ . The easiest way to compute this integral is just to compute the area under the curve, which is the area of the triangle.

$$1 = \frac{1}{2}(2)a^2 = a^2$$

so  $a^2 = 1$ , or  $a = 1$ . (And indeed,  $a$  has units of  $1/\sqrt{\text{meters}}$ ).

Alternatively we can write out the functional form of  $|\Psi|^2$  and explicitly integrate. The slope of the first segment is  $a^2$  with  $y$ -intercept 0, and the slope of the second segment is  $-a^2$ , so the  $y$ -intercept is  $2a^2$ . We can then integrate the piecewise function as,

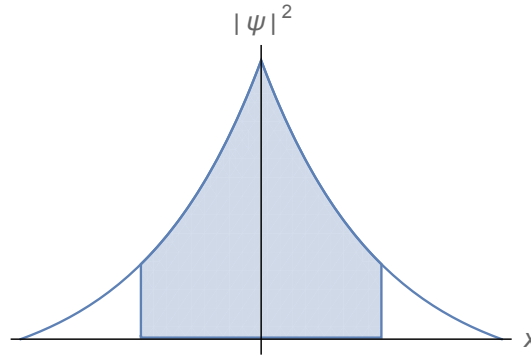
$$\begin{aligned} \int_{-\infty}^{\infty} |\Psi|^2 dx &= \int_0^1 a^2 x dx + \int_1^2 (-a^2 x + 2a^2) dx \\ &= \frac{1}{2}a^2 x^2 \Big|_0^1 + \left( -\frac{1}{2}a^2 x^2 + 2a^2 x \right) \Big|_1^2 \\ &= a^2 \left( \left( \frac{1}{2} - 0 \right) + \left( -\frac{4}{2} + 2(2) + \frac{1}{2} - 2 \right) \right) = a^2 \end{aligned}$$

So that again, we have found

$$a^2 = 1$$

—————End Lecture 14.

### Example Problem: More Fun with Wavefunctions



As an example, consider the following wavefunction (given at  $t = 0$ ),

$$\Psi(x, 0) = C e^{-|\frac{x}{a}|},$$

where  $C$  and  $a$  are real, positive constants.

This is a symmetric wavefunction with diminishing amplitude away from the origin, whose amplitude is a maximum at  $x = 0$ —thus, that's where the probability is a maximum as well, meaning a particle described by this wavefunction is most likely to be found at  $x = 0$ . If the absolute value is confusing, you can write the wavefunction without the absolute value by noting that the  $-|\cdot|$  in the exponent implies that the exponent must be negative for all values of  $x$ , so

$$\Psi(x, 0) = C e^{-|\frac{x}{a}|} = \begin{cases} C e^{-\frac{x}{a}} & x > 0 \\ C e^{\frac{x}{a}} & x < 0 \end{cases}$$

Written in this peicewise way, the exponent is explicitly negative for all values of  $x$ .

1. What is  $C$ ?

*Solution:* In order to determine the constant  $C$ , we must normalize the wavefunction:

$$1 = \int_{-\infty}^{\infty} |\Psi(x, 0)|^2 dx$$

Since this wavefunction is *symmetric* (the same under  $x \rightarrow -x$ ), whenever we're integrating over a symmetric region around the origin the answer will just be equal to twice the integral over the positive  $x$  axis. In this case, we have that

$$\int_{-\infty}^{\infty} |\Psi(x, 0)|^2 = 2 \int_0^{\infty} |\Psi(x, 0)|^2$$

Performing the integral,

$$\begin{aligned} 1 &= 2 \int_0^{\infty} C^2 e^{-2\frac{x}{a}} = 2C^2 \left( -\frac{a}{2} \right) e^{-\frac{2x}{a}} \Big|_0^{\infty} \\ &= 2C^2 \left( -\frac{a}{2} \right) (0 - 1) = C^2 a \quad \Rightarrow \quad C = \frac{1}{\sqrt{a}}. \end{aligned}$$

2. What is the probability that the particle is found within the spatial interval  $-a < x < a$ ?

*Solution:* This probability is the area of the shaded region in the figure between  $-a$  and  $a$ . We compute

$$\begin{aligned} P(-a < x < a) &= \int_{-a}^a |\Psi(x, 0)|^2 dx = 2 \int_0^a |\Psi(x, 0)|^2 dx \\ &= 2 \int_0^a C^2 e^{-2\frac{x}{a}} dx = 2C^2 \left(-\frac{a}{2}\right) (e^{-2} - 1) \\ &= 1 - e^{-2} = 0.865. \end{aligned}$$

where we used  $C^2 a = 1$ . This probability says that there is an 87% chance that we find the particle in a region around zero of  $\pm a$ .

Note that there are some common integrals and derivatives that it would be helpful to practice for this material! I'll list them here, where everywhere below  $\alpha$  is some constant that is independent of  $x$ . Some common (indefinite) integrals are,

$$\begin{aligned} \int x^\alpha dx &= \frac{x^{\alpha+1}}{\alpha+1}, & \int e^{\alpha x} dx &= \frac{e^{\alpha x}}{\alpha} \\ \int \sin(\alpha x) dx &= -\frac{\cos(\alpha x)}{\alpha}, & \int \cos(\alpha x) dx &= \frac{\sin(\alpha x)}{\alpha} \end{aligned}$$

Remember also that a definite integral taken between two bounds is equal to the indefinite integral evaluated at the upper bound, minus the evaluation at the lower bound. For example,

$$\int_a^b e^{\alpha x} dx = \frac{e^x}{\alpha} \Big|_a^b = \frac{1}{\alpha} (e^{\alpha b} - e^{\alpha a})$$

Some common derivatives are,

$$\begin{aligned} \frac{d}{dx} x^\alpha &= \alpha x^{\alpha-1}, & \frac{d}{dx} e^{\alpha x} &= \alpha e^{\alpha x} \\ \frac{d}{dx} \sin(\alpha x) &= \alpha \cos(\alpha x), & \frac{d}{dx} \cos(\alpha x) &= -\alpha \sin(\alpha x) \end{aligned}$$

### 3.1.2 The Schrödinger Equation: Time Evolution of the Wavefunction

In classical mechanics, we wish to find particle trajectories as a function of time, so that we may determine positions  $x(t)$  and momenta  $p(t)$  for all time given initial conditions. In quantum mechanics, the goal is to determine the wavefunction  $\Psi(x, t)$  as a function of time, since this will tell us how spatial probabilities evolve with time. The fundamental question is: if we're given the wavefunction at some instant in time (say  $t = 0$ ), what is the wavefunction at some subsequent time  $t$ ? This is essentially asking for a version of Newton's 2nd law that holds for subatomic systems for which probability densities are the best we can ask for!

The next postulate of quantum mechanics is as follows: the time evolution of the wavefunction  $\Psi(x, t)$  of a particle in the presence of a potential  $U(x)$  is given by the *Schrödinger equation*,

$$\text{Schrödinger equation : } -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + U\Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad (3.4)$$



This is also known as the *time-dependent Schrödinger equation*, since it tell us how the wavefunction evolves with time.

There's a lot to unpack looking at this equation. For one, it's a partial differential equation in  $\Psi$ , which means we should prepare ourselves to take some derivatives. The next notable features is that this equation is a *postulate*: it is assumed. There is no way to derive this equation from the basic principles of physics, because we assume that it is such a basic principle. That said, it has been confirmed time and time again! (Later, we will be able to understand this equation as a kind of averaged conservation of energy equation for a system.)

This equation depends on the potential  $U(x)$  in which the particle is evolving in. This makes sense—the particle's position should certainly depend on the potential! To draw a comparison, think about the classical mechanics scenario where we have a particle whose motion  $x(t)$  we wish to determine from a force  $F = ma$ . The time evolution  $x(t)$  of the position is governed by Newton's second law,

$$F = ma = m \frac{d^2x}{dt^2}$$

The force applied to the particle can be derived from the potential energy in which the particle evolves,  $F = -\frac{dU}{dx}$ , so that the equation of motion for the particle is

$$-\frac{dU}{dx} = m \frac{d^2x}{dt^2}. \quad (3.5)$$

For example, the harmonic oscillator potential  $U = \frac{1}{2}kx^2$  would yield the following force,

$$F = -\frac{d}{dx} \left( \frac{1}{2}kx^2 \right) = -kx$$

where  $k$  is the spring constant. Setting this equal to  $ma$  yields the equation of motion,

$$-kx = m \frac{d^2x}{dt^2} \quad (3.6)$$

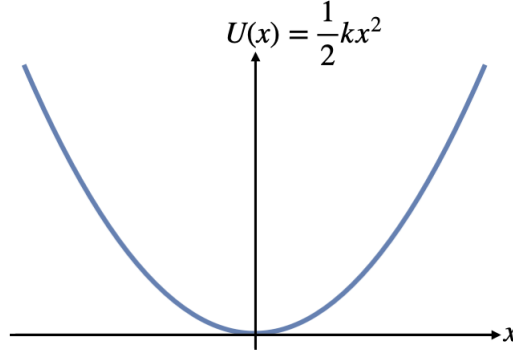
This is a differential equation that allows us to solve for  $x(t)$ . If the particle is at  $x = 0$  at  $t = 0$ , then the solution for the particle's motion for all time is,

$$x(t) = A \sin \left( \sqrt{\frac{k}{m}} t \right)$$

This both solves (3.6) and satisfies the boundary condition: (1) setting  $t = 0$ ,  $\sin(0) = 0$ , so that  $x(0) = 0$ . (2) Differentiating, we explicitly see that

$$m \frac{d^2}{dt^2} x(t) = m \frac{d}{dt} \left( \sqrt{\frac{k}{m}} A \cos \left( \sqrt{\frac{k}{m}} t \right) \right) = -mA \left( \frac{k}{m} \right) \sin \left( \sqrt{\frac{k}{m}} t \right) = -kx(t) \quad \checkmark$$

The idea of the Schrödinger equation is exactly the same—think of (3.4) as the quantum equivalent of (3.5), where now we are solving for the wavefunction rather than the position, and the result will tell us how a probability density evolves with time rather than how the position evolves with time.



**Stationary state solutions to the Schrödinger equation.** So, how do we actually solve this equation? In general it will depend on the character of the potential  $U(x)$  for the system we're asking about. In many cases, the wavefunction is *factorizable* or *separable*: it can be broken up ("factorized" / separated) into a spatial part  $\psi(x)$  that depends only on  $x$  and not on  $t$ , and a time part  $\phi(t)$  that depends only on  $t$  and not on  $x$ , as

$$\Psi(x, t) = \psi(x)\phi(t) \quad (3.7)$$

When this is the case, we can plug into (3.4) and divide both sides by  $\Psi(x, t)$ , leading to

$$-\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \cdot \frac{\partial^2 \psi(x)}{\partial x^2} + U(x) = i\hbar \frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t}$$

The left-hand-side of this equation is *only* a function of  $x$  and is independent of time, while the right-hand-side of this equation is *only* a function of  $t$  and independent of position. Since these two sides are supposed to be equal to each other, this is only possible when they both equal a constant: left-hand-side = right-hand-side = constant. Let us judiciously call this constant  $E$  (since we will soon be able to identify it with the energy of the particle!). Therefore, for separable wavefunctions (3.7), the spatial dependence  $\psi(x)$  satisfies the *time-independent Schrödinger equation* (TISE),

$$\text{TISE:} \quad -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + U(x)\psi(x) = E\psi(x) \quad (3.8)$$

Meanwhile the time dependent part  $\phi(t)$  satisfies the equation,

$$i\hbar \frac{\partial \phi(t)}{\partial t} = E\phi(t).$$

It is straightforward to solve this equation for  $\phi(t)$ , since an exponential function has precisely this property that its derivative is equal to a constant times the exponential we started with. We can summarize the result as follows:

The class of separable solutions to the full Schrödinger equation (3.4) take the form,

$$\text{Stationary states:} \quad \Psi(x, t) = \psi(x)e^{-i\omega t}, \quad E = \hbar\omega \quad (3.9)$$

where  $\psi(x)$  satisfies the time-independent Schrödinger equation (TISE) (3.8).

A comment is in order:

- These are known as *stationary state solutions* because the time-dependence is just a complex phase  $e^{-i\omega t}$ , so that probabilities are time-independent! In particular, since probabilities are computed by taking  $\Psi^*\Psi$ , and  $(e^{-i\omega t})^* = e^{i\omega t}$  we will have

$$P(x) dx = \Psi^*\Psi dx = (e^{i\omega t}\psi^*(x)) (e^{-i\omega t}\psi(x)) = \psi^*(x)\psi(x) \quad \text{is independent of time.}$$

These are an important class of solutions, and we will almost entirely restrict our discussion of quantum mechanical systems to such stationary state solutions.

(*Why?* In classical mechanics we are usually concerned with finding the time dependence,  $x(t)$  for some particle that starts at some position  $x(t=0) = x_0$ . In quantum mechanics, it can be hard enough just to figure out the probability density for *where* the particle might be found, even at  $t=0$ ! So we focus most of our effort in a first course on quantum mechanics on finding the position-dependence of the wavefunction.)

### Clicker Question: Plane waves

A particle moves in a constant potential  $U$ . Suppose this particle has the following plane wave wavefunction,

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

What is the constant  $E$ ? (Hint: Identify  $\psi(x)$  for this wavefunction, and then solve for  $E$  by substituting  $\psi(x)$  into the TISE.)

*Solution:* This is evidently a separable wavefunction, since we can separate out the exponent as,

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

The TISE is,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U\psi = E\psi$$

Substituting  $\psi(x) = Ae^{ikx}$ , and differentiating  $\psi$ ,

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial}{\partial x}(ik)Ae^{ikx} = (ik)^2 Ae^{ikx} = -k^2 \psi(x)$$

we find that

$$-\frac{\hbar^2}{2m}(-k^2 \psi) + U\psi = E\psi$$

An overall factor of  $\psi$  cancels out of each term, so that

$$E = \frac{\hbar^2 k^2}{2m} + U$$

Using the fact that the wavenumber  $k$  is related to the momentum  $p$  of the particle as  $p = \hbar k$ , we can rewrite this as

$$E = \frac{p^2}{2m} + U$$

This is precisely the energy of the particle with momentum  $p$  and potential energy  $U$ ! More generally, the constant  $E$  in the TISE has the interpretation of the energy of the system described by the wavefunction  $\Psi(x, t)$ . So, stationary state solutions to the Schrödinger equation are states with constant energy.

Taking  $U = 0$  in our boxed example, this is a possible wavefunction for a free particle. By

*free particle*, we mean a particle of mass  $m$  and momentum  $p$  constrained to be somewhere on the  $x$ -axis, which is experiencing no external force ( $U = 0$ ), so whose only energy is its kinetic energy,  $E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$ .

—————*End Lecture 15.*

### 3.1.3 Solving the Time-Independent Schrödinger Equation (TISE)

Our general goal is to solve the Schrödinger equation for the wavefunction  $\Psi(x, t)$  of a particle moving in some potential. We will now work through several examples of increasing complexity, considering systems describing some particle moving in a constant, finite potential  $U(x) = U$ . The simplest example is that of a free particle, with potential  $U = 0$ . More generally, we will consider some nonzero but constant  $U$  and ask, what is the wavefunction for a particle moving in a constant potential?

In all cases, the steps we will take to solve for  $\Psi(x, t)$  are as follows.

**Step 1: Restrict to stationary states.** Firstly, let us restrict ourselves to separable stationary state solutions, so that the total wavefunction is

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar}$$

We used that  $\omega = E/\hbar$  for the stationary state solution of energy  $E$ . Then, our goal is to solve for  $\psi(x)$  which satisfies the TISE,

$$\boxed{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U\psi = E\psi}$$

where  $U = 0$  for the free particle.

**Step 2: Substitute an ansatz for  $\psi(x)$  into the TISE to solve for  $E$ .** The TISE is a wave equation, and is in general solved by some superposition of plane wave solutions. The most general type of solution one can write down that will solve the TISE for a constant potential  $U(x) = U$  is

$$\boxed{\psi(x) = Ae^{ikx} + Be^{-ikx} = A' \cos(kx) + B' \sin(kx)} \quad (3.10)$$

where we have parameterized this *ansatz* (meaning “guess”) in terms of two yet-undetermined constants. It is up to you as to whether you prefer to work with the complex exponentials or the cosines and sines; as you showed in the *Practice with waves* example from Part II of this course, they are totally equivalent. (Recall that in that example, you showed that in order to translate between the constants  $A', B'$  and  $A, B$ , you use  $A' = A + B$ ,  $B' = i(A - B)$ .) In these notes, we will do it both ways for practice.

First, let's use the complex exponential form. Here the derivative we need to remember is that  $\frac{d}{dx}e^{\alpha x} = \alpha e^{\alpha x}$ . Then,

$$\begin{aligned} \frac{d}{dx}\psi(x) &= A(ik)e^{ikx} + B(-ik)e^{-ikx} \\ \frac{d^2}{dx^2}\psi(x) &= \frac{d}{dx} \left( A(ik)e^{ikx} + B(-ik)e^{-ikx} \right) = A(ik)^2e^{ikx} + B(-ik)^2e^{-ikx} \\ &= -k^2 \left( A(ik)e^{ikx} + B(-ik)e^{-ikx} \right) = -k^2\psi(x) \end{aligned}$$

where we used that  $i^2 = -1$ . Note that we could have arrived at the same expression using the cosines and sines, by differentiating,

$$\begin{aligned}\frac{d}{dx}\psi(x) &= -A'k \sin(kx) + B'k \cos(kx) \\ \frac{d^2}{dx^2}\psi(x) &= \frac{d}{dx}(-A'k \sin(kx) + B'k \cos(kx)) = A'(-k^2) \cos(kx) + B'(-k^2) \sin(kx) \\ &= -k^2(A' \cos(kx) + B' \sin(kx)) = -k^2\psi(x) \quad \checkmark\end{aligned}$$

Therefore in either case, the TISE simplifies to,

$$\left(\frac{\hbar^2 k^2}{2m} + U\right) \psi = E\psi \quad \Rightarrow \quad E = \frac{\hbar^2 k^2}{2m} + U$$

This expresses the energy  $E$  as a function of the wavenumber  $k$  in the superposition of plane waves. Equivalently, we could use this relation for the energy as a function of  $k$  to solve for  $k$  as a function of  $E$ ,

$$k = \sqrt{\frac{2m(E - U)}{\hbar^2}}$$

The physics of this solution will clearly depend on whether  $E - U$  is positive or negative. There are several possible scenarios:

- $E \geq U$  : then the value under the square root is positive, so that the wavenumber  $k$  is real. Great!
- $U = 0$ : This is a special case of the above. For the free particle with  $U = 0$ , we simply have  $k = \sqrt{2mE/\hbar^2}$ ,

$$\boxed{\text{Energy of a free particle: } E = \frac{\hbar^2 k^2}{2m}} \quad (3.11)$$

or in other words,  $E = p^2/(2m)$ , since  $p = \hbar k$ . As expected!

- $E < U$ : this solution evidently yields an imaginary value of  $k$ , since there is now a minus sign under the square root. This is a little weird...what does an imaginary momentum mean??

Suppose that  $k$  is imaginary ( $E < U$ ), so that  $k = i\hat{k}$  where  $\hat{k}$  is real,

$$k = i\hat{k}, \quad \hat{k} = \sqrt{\frac{2m(U - E)}{\hbar^2}}, \quad E < U$$

Evidently our ansatz for  $\psi$  actually involves growing and decaying exponentials, rather than complex exponentials. We can see this by substituting in to the original ansatz:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} = Ae^{i(i\hat{k})x} + Be^{-i(i\hat{k})x} = Ae^{-\hat{k}x} + Be^{\hat{k}x}$$

This is a perfectly good ansatz for the TISE for a state whose energy  $E$  is less than the constant potential  $U$ . Later we will see some examples where we make use of such solutions.

- There's one more special case, which is that  $U = \infty$ . In a region of space where the potential is infinite, the only way to make sense of the TISE is for the wavefunction to just be zero,

$$\boxed{U = \infty \quad \Rightarrow \quad \psi(x) = 0.}$$

**Warning:** for systems with potentials  $U(x)$  that depend on  $x$ , we will need to try a better ansatz in this step—for example, we might need to add up an infinite number of plane waves (rather than just 2) to allow a more general functional form for  $\psi(x)$ . If you ever need to use an ansatz that differs from (3.10), I will tell you which  $\psi(x)$  to use.

**Step 3: Enforce boundary conditions.** So far in these steps we have assumed a constant potential  $U$  (where  $U = 0$  for a free particle, and  $U = \infty$  in a region where there is no probability to find the particle). More generally, suppose that my potential is divided up into spatial regions where  $U$  takes a different constant value in different regions. For example, a case we will study in more detail soon is the *particle in a box*: a free particle that is restricted to live in some finite range of the  $x$ -axis, with zero probability of being found outside of that region (for example, because it is trapped in a box whose walls correspond to regions with infinite potential energy). This means that the wavefunction is zero outside of the box, but equal to the free particle wavefunction inside the box.

In such a scenario I must enforce that my wavefunction is continuous across the boundary of the box:  $\psi_{\text{outside}}(x) = \psi_{\text{inside}}(x)$  at  $x$  equal to the locations of the walls of the box. Generally, any time I have a piecewise defined wavefunction, I will need to enforce continuity of the wavefunction at the boundaries of different regions.

**Step 4: Normalize the wavefunction.** The final step is to enforce normalizability of the wavefunction, making sure that it is not infinite anywhere and imposing that

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

For our separable wavefunction  $\Psi(x, t) = \psi(x)e^{-i\omega t}$ , this reduces to the condition

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

**The myth of the truly free particle** In the following sections we will apply these steps in various examples. Before we do so, some additional comments regarding the free particle are in order.

We’ve seen that a free particle can have in general a spatial wavefunction of the form,

$$\psi(x) = A' \cos(kx) + B' \sin(kx) \quad (3.12)$$

with energy  $E = \hbar^2 k^2 / (2m)$ . The momentum of a free particle is completely known ( $p = \hbar k$ , so  $\Delta p = 0$ ), but we’ve seen that for such a plane wave the position is completely *unknown* (so  $\Delta x = \infty$ ). This is because the wavefunction (3.12) is periodic over all of space, so that the probability density is totally delocalized over the entire  $x$ -axis.

What this also means, unfortunately, is that the free particle wavefunction is not normalizable. Since  $\psi^* \psi$  is periodic over all of  $x$ , for a free particle the integral of the probability density over all  $x$  is infinity:

$$\int_{-\infty}^{\infty} \psi^* \psi = \infty$$

To fix this problem, we should interpret that the periodic free particle plane wave wavefunction is just an idealized approximation for a real world particle, which must always have a normalizable wavefunction. (This is, of course, why we have spent so much effort building localized

wavepackets.) The idea is that in the real world, a particle can't actually be free over all of space; it must be localized to at least *some* region of space. One way to deal with a more realistic scenario is to put the particle in a box, so that it is free but only in a finite region (say over the length  $L$  of the box), with the wavefunction being zero outside of the box. Then, to normalize the wavefunction we would compute something like

$$\begin{aligned}\int_{-\infty}^{\infty} \psi^* \psi &= \int_{-\infty}^0 \psi_{\text{out}}^* \psi_{\text{out}} + \int_0^L \psi_{\text{in}}^* \psi_{\text{in}} + \int_L^{\infty} \psi_{\text{out}}^* \psi_{\text{out}} \\ &= 0 + \int_0^L \psi_{\text{in}}^* \psi_{\text{in}} + 0\end{aligned}$$

where  $\psi_{\text{in}}$  is equal to (3.12) and  $\psi_{\text{out}} = 0$ . This integral will always be some finite number, since I am only integrating the periodic function over the length of the box. You will see this explicitly in the next example.

### 3.1.4 Particle in a Box

The first truly physical quantum mechanical system we will examine (besides the free particle) is the “particle in a box”, or in other words a particle whose motion is constrained to within a certain region of the  $x$ -axis (say the length  $L$  of a box), but has no forces acting on it within the box.

We can model the walls of the box as regions of infinite potential energy, since then it would require infinite potential energy (impossible!) for the particle to escape the box:

$$U(x) = \begin{cases} \infty & -\infty < x < 0 \\ 0 & 0 < x < L \\ \infty & L < x < \infty \end{cases}$$

Since the potential is piecewise constant, we can use the step-by-step analysis that we introduced in the previous section, solving for the wavefunction in each region. Our goal will be to find the stationary state (constant energy) solutions for the wavefunction of the particle. Let us go step by step. (This is an extremely important quantum mechanical example, so part of your homework for this week will be reproducing these steps!)

**Step 1: Restrict to stationary states.** As instructed, we will restrict to the separable stationary state solutions,

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar}, \quad -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U\psi = E\psi \quad (\text{TISE})$$

We need to solve for the spatial part of the wavefunction,  $\psi(x)$ .

**Step 2: Substitute an ansatz for  $\psi(x)$  into the TISE to solve for  $E$ .** Since  $U$  is split up into three regions of space,  $\psi(x)$  should also be split into three regions.

$$\psi(x) = \begin{cases} \psi_I(x) & \text{satisfying TISE with } U = \infty & -\infty < x < 0 \\ \psi_{II}(x) & \text{satisfying TISE with } U = 0 & 0 < x < L \\ \psi_{III}(x) & \text{satisfying TISE with } U = \infty & L < x < \infty \end{cases}$$

We've learned that when  $U = \infty$ , the wavefunction must be zero, so  $\psi_I(x) = \psi_{III}(x) = 0$ . For the region inside the box, we can use the ansatz  $\psi_{II}(x) = Ae^{ikx} + Be^{-ikx}$ . (Your book uses sines and cosines to solve this problem, so for variety we'll use the complex

exponentials—either method is totally fine.) We found earlier that when we plug this ansatz into the TISE, it satisfies the differential equation with the energy of the particle set equal to

$$E = \frac{\hbar^2 k^2}{2m}$$

Therefore, our ansatz for the spatial part of the wavefunction over all  $x$  is:

$$\psi(x) = \begin{cases} 0 & -\infty < x < 0 \\ Ae^{ikx} + Be^{-ikx} & \text{with } E = \frac{\hbar^2 k^2}{2m} \quad 0 < x < L \\ 0 & L < x < \infty \end{cases}$$

**Step 3: Enforce boundary conditions** In this problem we need to enforce that the wavefunction is continuous across the edges of the box, so that

$$\begin{aligned} \psi_I(0) &= \psi_{II}(0) \\ \psi_{II}(L) &= \psi_{III}(L) \end{aligned}$$

The first equation yields

$$0 = A + B \quad \Rightarrow \quad B = -A$$

where we used that  $e^0 = 1$ . The second equation yields

$$Ae^{ikL} + Be^{-ikL} = 0$$

Substituting for  $B = -A$ ,

$$Ae^{ikL} - Ae^{-ikL} = 0 \quad \Rightarrow \quad e^{ikL} = e^{-ikL}$$

It is only possible that  $e^{i\alpha} = e^{-i\alpha}$  if  $\alpha$  is an integer multiple of  $\pi$ ,  $\alpha = n\pi$ : if  $n$  is an even integer ( $n = 2, 4, \dots$ ) then  $e^{i\pi n} = e^{-i\pi n} = 1$ , and if  $n$  is an odd integer ( $n = 1, 3, \dots$ ) then  $e^{i\pi n} = e^{-i\pi n} = -1$ . Therefore, this second relation constrains  $k$ :

$$kL = n\pi, \quad n = 1, 2, \dots$$

We can summarize the status of our solution as follows. Firstly, substituting for  $B = -A$  yields the following expression for  $\psi_{II}(x)$  inside the box:

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} = A(e^{ikx} - e^{-ikx}) = 2iA \sin(kx)$$

where we used  $\sin(\alpha) = \frac{e^{i\alpha} - e^{-i\alpha}}{2i}$ . Then, we can use the fact that we solved for  $kL = n\pi$  to express the energy of the particle in terms of  $n$ :

Energy levels for particle in a box:  $E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, \dots$

(3.13)

We've added a subscript to  $E_n$  since the energy will depend on the integer  $n$ .

There are two things to note about these energies:

- The smallest energy the particle can have is  $E_{n=1} = \frac{\pi^2 \hbar^2}{2mL^2}$  (it can't have energy 0 without also having zero momentum... that's why  $n$  starts at 1!) The  $n = 1$  state is thus called the ground state, since it's the lowest energy state.



- The energy of the particle gets larger as  $L$  gets smaller—localizing the electron into a smaller box leads to an increase in the electron’s energy.

**Step 4: Normalize the wavefunction.** The final step is to normalize. To do so, we need to impose that the following integral equals 1:

$$\begin{aligned}
 1 &= \int_{-\infty}^{\infty} |\psi(x)|^2 = \int_{-\infty}^0 |\psi_I(x)|^2 + \int_0^L |\psi_{II}(x)|^2 + \int_L^{\infty} |\psi_{III}(x)|^2 \\
 &= 0 + \int_0^L |\psi_{II}(x)|^2 + 0 \\
 &= \int_0^L (2iA \sin(kx))^* (2iA \sin(kx))
 \end{aligned}$$

The only nonzero part comes from the inside of the box. We can compute  $|\psi_{II}(x)|^2$  by taking the complex conjugate of  $\psi_{II}(x)$ ,

$$|\psi_{II}(x)|^2 = (2iA \sin(kx))^* (2iA \sin(kx)) = (-2iA^* \sin(kx)) (2iA \sin(kx)) = 4|A|^2 \sin^2(kx)$$

Therefore, the integral is

$$1 = \int_0^L 4|A|^2 \sin^2(kx)$$

In general, the indefinite integral of  $\sin^2(kx)$  is equal to

$$\int \sin^2(kx) dx = \frac{x}{2} - \frac{\sin(2kx)}{4k}$$

Then,

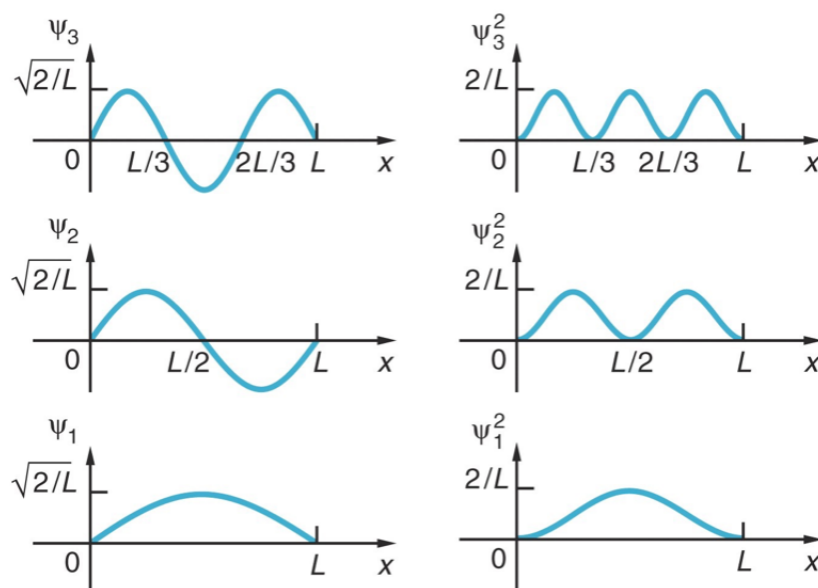
$$\begin{aligned}
 1 &= \int_0^L 4|A|^2 \sin^2(kx) = 4|A|^2 \left( \frac{x}{2} - \frac{\sin(2kx)}{4k} \right) \Big|_0^L \\
 &= 4|A|^2 \left( \frac{L}{2} - \frac{\sin(2kL)}{4k} - 0 + \frac{\sin(0)}{4k} \right) \\
 &= 4|A|^2 \frac{L}{2} \quad \Rightarrow \quad |A|^2 = \frac{1}{2L}
 \end{aligned}$$

where in going to the last line we used  $\sin(0) = 0$ , and that  $2kL = 2n\pi$  is always an even integer multiple of  $\pi$ , so that  $\sin(2kL) = \sin(2n\pi) = 0$  regardless of  $n$ .

We have thus determined the constant  $A$ , up to a possible phase:

$$A = \frac{e^{i\theta}}{\sqrt{2L}} \quad \Leftrightarrow \quad |A|^2 = A^* A = \frac{1}{2L}$$

The ambiguity with the phase factor  $e^{i\theta}$  just comes from the fact that an overall complex phase (such as a factor of  $\pm i$ ) cancels out of the physical probability density  $|\psi|^2$ , since  $(e^{i\theta})^* (e^{i\theta}) = e^{-i\theta+i\theta} = 1$ . We are free to choose any real value of  $\theta$ , since all give the same probability density. Since we determined that  $\psi_2(x) = 2iA \sin(kx)$ , we’ll choose  $A = \frac{-i}{\sqrt{2L}}$  (*i.e.*  $\theta = 3\pi/2$ , since  $e^{3\pi i/2} = -i$ ) so that the  $i$ ’s cancel and  $\psi_2(x)$  is real and positive. (Again, this overall factor of  $-i$  is totally non-physical, you didn’t have to make this choice but we’ll do it for convenience!)



In sum, we have completely solved for the wavefunction describing the particle with energy  $E_n$ . The result is that outside of the box, the wavefunction is zero, while inside the box the wavefunction is,

Wavefunctions for particle in a box:  $\psi_n(x) = \sqrt{\frac{2}{L}} \sin(kx), \quad k = \frac{n\pi}{L}, \quad n = 1, 2, \dots$

(3.14)

We've added an  $n$  subscript to emphasize that it depends on the integer  $n$ .

———End Lecture 16.

**Discussion** We have completed our derivation of the energy levels and wavefunctions for the particle in a box. As we've shown, these are labeled by an integer  $n$ , just like in Bohr's model of Hydrogen! This integer  $n$  is called the quantum number: it labels the quantum state of the particle.

So, what do these wavefunctions look like? These wavefunctions and the associated probability densities are plotted in the figure. Just like an electron in the Bohr model was modeled as a standing wave fitting the circumference of the orbit, the wavefunction for our particle in a box is described by standing waves in the box. The  $n = 1$  quantum state is the lowest energy state, or ground state, and has no nodes; the  $n = 2$  quantum state has 1 node, and so on. In general, the higher energy the state, the more nodes in the wavefunction, with

$$n - 1 = \# \text{ of nodes inside the box.}$$

You can see this yourself by noting that  $\sin(\alpha)$  is zero whenever  $\alpha$  is an integer multiple of  $\pi$ , so that  $\psi_n(x)$  has a zero whenever

$$\frac{n\pi x}{L} = (\text{integer } m) \cdot \pi \quad \Rightarrow \quad x = \frac{mL}{n}, \quad m = 1, 2, 3, \dots$$

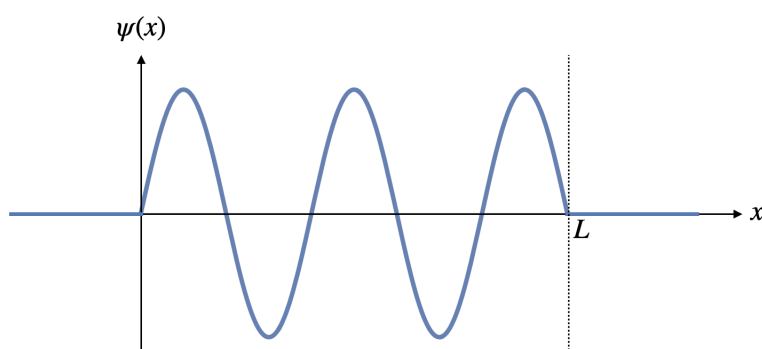
For the  $n = 1$  state, there is no possible integer  $m$  that satisfies this equation for  $0 < x < L$ ; for the  $n = 2$  state there is exactly one possible integer  $m = 1$  that satisfies this equation for

$0 < x < L$ , so there is one node at  $x = \frac{L}{2}$ ; for the  $n = 3$  state there are two possible integers  $m = 1, 2$  that satisfy this equation for  $0 < x < L$ , so that there are nodes at  $x = \frac{L}{3}$  and  $x = \frac{2L}{3}$ ; and so on.

These nodes (zeroes of the wavefunction) correspond to locations where the particle has *zero* probability of being found. For example, if the particle is in the  $n = 2$  excited state, it has zero probability of being found at the exact center of the box! This is very different from a classical particle, where the particle would have equal probability of being found anywhere in the box. You will further explore these wavefunctions on your Homework 7 problem set.

### Clicker Question: Which wavefunction?

Suppose that a particle in a box has the pictured wavefunction. What is the energy of this state?



*Solution:* This wavefunction has 4 nodes inside the box, so corresponds to the  $n = 5$  state. (Recall that the  $n = 1$  state has no nodes inside the box, the  $n = 2$  state has 1 node, etc., so the  $n = 5$  state has 4 nodes inside the box.) Therefore, the energy is

$$E_n = \frac{5^2 \pi^2 \hbar^2}{2mL^2} = \frac{25\pi^2 \hbar^2}{2mL^2}$$

### Example Problem: Electron in a box

Suppose an electron is trapped in a box of length  $a_0$ , and is in an excited state. The electron makes a transition from the 1st excited state ( $n = 2$ ) to the ground state ( $n = 1$ ), emitting a single photon in the process. What is the energy of this photon?

*Solution:* The change in energy levels must be equal to the photon's energy,  $E = hf$ :

$$\Delta E = E_{n=2} - E_{n=1} = \frac{\pi^2 \hbar^2}{2m_e(a_0)^2} (2^2 - 1^2) = \frac{3\pi^2 \hbar^2}{2m_e(a_0)^2}$$

This is the energy of the photon. (The photon's frequency can be derived by setting this quantity equal to  $hf$ .) Substituting for the values of these constants,

$$E = \frac{3\pi^2 \hbar^2}{2m_e a_0^2} = \frac{3\pi^2 (1.055 \times 10^{-34} \text{ J} \cdot \text{s})^2}{2(9.109 \times 10^{-31} \text{ kg})(0.529 \times 10^{-10} \text{ m})^2} = 6.5 \times 10^{-17} \text{ J} = 403 \text{ eV}$$

### Example Problem: Trapped Again!

I trap an electron in a box of length  $L$ , so that  $\Delta x = L$ . In a previous example problem, you computed the minimum uncertainty in the electron's momentum to be,

$$\Delta x \Delta p \geq \frac{\hbar}{2} \Rightarrow \Delta p_{\min} = \frac{\hbar}{2\Delta x} = \frac{\hbar}{2L}$$

If I estimate the minimum energy of the electron based on this uncertainty, what is the energy of the electron? How does it compare to the minimum energy  $E_1$  that we derived for the electron in the box?

*Solution:* We're told to estimate the energy using  $p = \Delta p_{\min}$ , which gives

$$E_{\text{estimate}} = \frac{p^2}{2m_e} \approx \frac{\Delta p_{\min}^2}{2m_e} = \frac{\hbar^2}{8m_e L^2}$$

This gives a pretty decent estimate of the actual minimum energy of the electron in the box,

$$E_1 = \frac{\hbar^2 \pi^2}{2mL^2} = 4\pi^2 E_{\text{estimate}}$$

Not bad!

**Merging the classical and quantum pictures** This example illustrates an stark difference between the quantum mechanical picture and classical picture: quantum mechanically, *the particle cannot have  $E = 0$* . A particle confined to a finite space has to have some minimum energy! The particle moves around in the box with kinetic energy inversely proportional to the length of the 1d box. As we just saw in the last example, this fact is a consequence of the uncertainty principle: because there is some minimum uncertainty in the momentum of the particle, it can't just have  $E = 0$ . Of course, if  $\frac{\hbar^2}{mL^2}$  is very small, then this energy is very small and we wouldn't notice it. The denominator  $mL^2$  has to be very tiny to compete with how small  $\hbar$  is and make this quantum mechanical effect noticeable.

We should also ask at this point how the classical picture could possibly emerge from the periodic probability densities we derived in this section. Classically, we suppose that all we know is that the particle is *somewhere* in the box. Then, the probability that the particle is found at some location in a box of length  $L$  is just a constant (call it  $C$ ) inside the box, and zero outside the box. Normalization informs us that this constant must be equal to  $1/L$ :

$$\text{Classically: } P(x) = C, \quad 1 = \int_{-\infty}^{\infty} P(x) dx = \int_0^L C dx = LC \Rightarrow C = \frac{1}{L}.$$

This is pretty different from the wiggles in the quantum mechanical probability distribution! How are these differences smoothed out in the classical limit? The answer is basically that in the limit that  $n \rightarrow \infty$ , *i.e.* the limit of large quantum number  $n$ , the wiggles in the quantum probability distribution become so fuzzy that you stop seeing them, and the distribution approximates a constant.

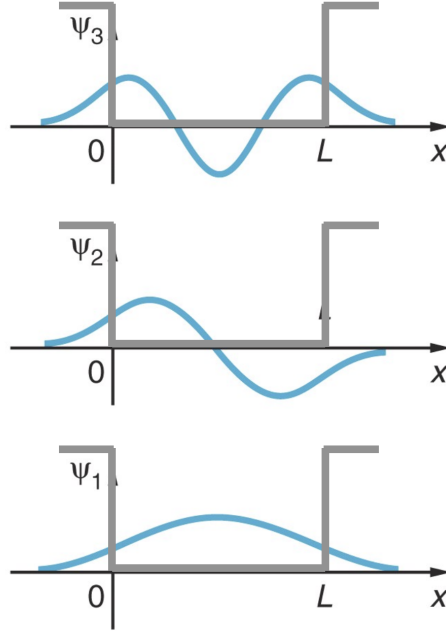


Figure 8: The spatial wavefunctions of the first three energy levels  $n = 1, 2, 3$  for a particle in a finite potential well.

### 3.1.5 Particle in a Finite Potential Well

Of course, there are no truly infinite potentials in the real world. Next up, we'll consider a more realistic example than an infinite potential well: a finite potential well. By this, we mean a free particle that is trapped in some potential well where the potential energy of the walls  $U$  is large compared to the kinetic energy  $E = \frac{p^2}{2m}$  of the particle, but not infinite.

Classically, in this scenario the particle is stuck: as long as its kinetic energy  $E < U$ , it doesn't have enough energy to make it over the walls. Quantum mechanically, we'll see a different story emerge: a particle that classically doesn't have enough energy to leave the box quantum mechanically could "leak" outside of the walls of a finite potential.

So, consider a particle in a 1-dimensional potential well, where the potential is a constant  $U > 0$  outside of the well, and  $U = 0$  from  $0 < x < L$ , where the particle has energy  $E < U$  such that classically it would be trapped inside the well. What are the possible wavefunctions and corresponding energies of the particle? This is a somewhat more mathematically involved example than the case of a particle in an infinite potential well, since in that case the particle's wavefunction is just zero outside of the well, while here since  $U$  is finite the particle's wavefunction is nonzero over all of  $x$ . Here we will sketch the idea of the solution.

- Firstly, we note that there are three distinct areas relevant to this problem: the area to the left of the well with finite potential  $U$ ; the area inside the box where  $U = 0$ ; and the area to the right of the well which again has finite potential  $U$ .
- Inside the well, we already know the correct ansatz to substitute into the TISE:

$$\psi_{\text{in}}(x) = Ae^{ikx} + Be^{-ikx} \quad 0 < x < L$$

where the wavenumber is fixed by the TISE in terms of the energy,

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

- Outside the well, the particle's energy satisfies  $E < U$ . Recall that when we solved the TISE in section 1.3, we found that in such a region, our ansatz should actually take the form of growing and decaying exponentials, rather than complex exponentials:

$$\begin{aligned}\psi_{\text{left}}(x) &= A_L e^{\hat{k}x} + B_L e^{-\hat{k}x} & x < 0 \\ \psi_{\text{right}}(x) &= A_R e^{\hat{k}x} + B_R e^{-\hat{k}x} & x > L\end{aligned}$$

We saw in section 1.3 that such a function satisfies the TISE for  $E < U$ , with

$$\hat{k} = \sqrt{\frac{2m(U - E)}{\hbar^2}}$$

- Our total wavefunction now has 6 unknown constants,  $A, B, A_L, B_L, A_R, B_R$ . These constants can be determined by imposing continuity and normalizability of the wavefunction. For example, continuity of the wavefunction implies that  $\psi_{\text{left}}(0) = \psi_{\text{in}}(0)$  and  $\psi_{\text{in}}(L) = \psi_{\text{right}}(L)$ . What does normalizability imply?

#### Clicker Question: The wavefunction outside a finite well

To the left of the finite potential well, the solution to the TISE is

$$\psi_{\text{left}}(x) = A_L e^{\hat{k}x} + B_L e^{-\hat{k}x}$$

Considering the fact that the wavefunction must be normalized, which of the following is true?

- (a)  $A_L = 0$
- (b)  $B_L = 0$
- (c)  $A_L = B_L$
- (d)  $A_L = -B_L$

*Solution:* In order to be normalizable, the wavefunction cannot be infinite anywhere. Remember, this is not allowed, since an infinite wavefunction implies infinite probability! Since we are on the left hand side of the well, we have to consider the ansatz in the region  $-\infty < x < 0$ . As  $x \rightarrow -\infty$ ,  $e^{-\hat{k}x} \rightarrow e^{+\infty} \rightarrow \infty$ , which is not allowed. Therefore,  $B_L = 0$ . The answer is (b).

A similar analysis can be applied to the ansatz to the right of the well, fixing one more constant. Then, imposing  $1 = \int_{-\infty}^{\infty} |\psi|^2 dx$  fixes yet another constant.

For more details, I recommend checking out the video <https://www.youtube.com/watch?v=rX8fbYaSf70>. The result of this analysis is pictured in the figure. Some comments:

- The surprising conclusion is that there is a probability that the particle is found outside of the box! Classically the particle is trapped, but quantum mechanically we might find the particle outside of the box, since the potential is finite so some probability density leaks through the walls.
- Now, there is a cap on how many energy levels before the particle is no longer trapped:  $n = 1, 2, \dots, N$ . Any higher energy and the particle would just be free in all space.

### 3.1.6 Superposition and Schrödinger's Cat

Before we move on to other examples of quantum systems, consider the following thought experiment. Suppose I know that an electron is localized *either* in a small area around  $x = x_1$ , or in a small area around  $x = x_2$ . What does the wavefunction for the electron look like?

If we know that the electron is localized around an small length (say  $L$ ) around  $x = x_1$ , we can model the wavefunction for this electron by the particle-in-a-box wavefunction: nonzero from  $x_1 - L/2 < x < x_1 + L/2$ , and zero everywhere else. Call this wavefunction  $\Psi_1$ . On the other hand, if we know that the electron is localized around  $x_2$ , we can model the wavefunction  $\Psi_2$  by the particle-in-a-box wavefunction that is nonzero from  $x_2 - L/2 < x < x_2 + L/2$  and zero everywhere else. If the electron might be in *either* box, so that there is equal probability of finding the electron either near  $x_1$  or  $x_2$ , we model the total wavefunction as the sum of the different possibilities:

$$\Psi_{\text{tot}} = \Psi_1 + \Psi_2 \quad \Rightarrow \quad P(x)dx = |\Psi_{\text{tot}}|^2 dx$$

This is called the principle of *superposition*: if there are multiple states that the system could be in, the total wavefunction is the sum of all of these possibilities. I don't actually know what box the particle is found in until I make a measurement, at which time I measure the particle either in box 1 or box 2. Until then, all I know is the probability that if I made a measurement, I would find the electron either in box 1 or box 2.

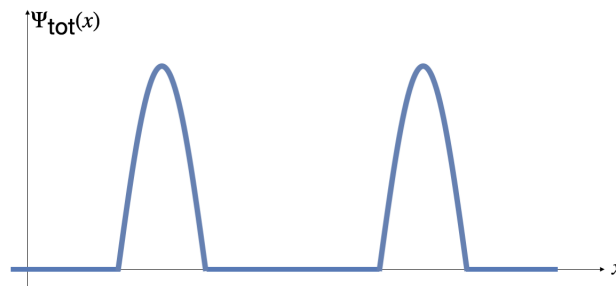


Figure 9: The wavefunction for a particle that could either be found in the ground state of box 1 (centered around  $x_1$ ) or in the ground state of  $x_2$  (centered around  $x_2$ ).

This idea of superposition should be familiar from our discussion of the double slit experiment. In that case, there was more than one possible path that the electron could take to reach its final destination on the viewing screen, and so the probability of finding the electron at some place on the screen was expressed in terms of a wavefunction that represents the sum of the two different possibilities:

$$\Psi_{\text{tot}} = \Psi_1 + \Psi_2 \quad \Rightarrow \quad P(x)dx = |\Psi_{\text{tot}}|^2 dx$$

where  $\Psi_1$  here represented the wavefunction for the electron going through slit 1 (with slit 2 closed), and  $\Psi_2$  represented the wavefunction for the electron going through slit 2 (with slit 1

closed). Again: if there are many possible paths the system could take, the total wavefunction for the system is the sum of all of these possibilities.

This is the concept often motivated by the example of Schrödinger’s cat, a famous thought experiment. It begins by placing a cat in a closed box with a radioactive particle. That particle, which is described by quantum mechanics, is left for some time after which it will have decayed with some probability. If the particle does decay, the radiation will kill the cat. If it doesn’t, the cat will live. Since there are two possible states the system can be in, the wavefunction of the cat has the schematic form

$$\Psi = \psi_{\text{alive}} + \psi_{\text{dead}}$$

When we open the box to “measure” the state of the system, the cat will be found to be either alive or dead. But until we measure it, one can think of the cat as both alive and dead!

———*End Lecture 17.*

### 3.1.7 Quantum Harmonic Oscillator

We now consider a slightly more complicated system: a particle of mass  $m$  attached to a spring with spring constant  $k_{\text{spring}}$ , related to the angular frequency  $\omega$  of the simple harmonic motion as  $k_{\text{spring}} = m\omega^2$ . We already reviewed the classical harmonic oscillator around (3.5); the potential is a parabola, of the form  $U(x) = \frac{1}{2}k_{\text{spring}}x^2 = \frac{1}{2}m\omega^2x^2$ , leading to a restoring spring force  $F = -k_{\text{spring}}x$  on the particle. The motion of the particle is sinusoidal:  $x(t) = A \sin(\sqrt{k_{\text{spring}}/m}t) = A \sin(\omega t)$ .

This problem arises frequently in physics, since around any stable equilibrium for a potential energy function  $U(x)$  we can approximate the function with a parabola, and the motion for small displacements from equilibrium is sinusoidal.

We will now consider the quantum mechanical system of a harmonic oscillator. In other words, we ask what the possible wavefunctions are for a particle of mass  $m$  in a potential  $U = \frac{1}{2}m\omega^2x^2$ ? We will look for stationary state solutions of definite energy,

$$\Psi(x, t) = \psi(x)e^{-iEt/\hbar}$$

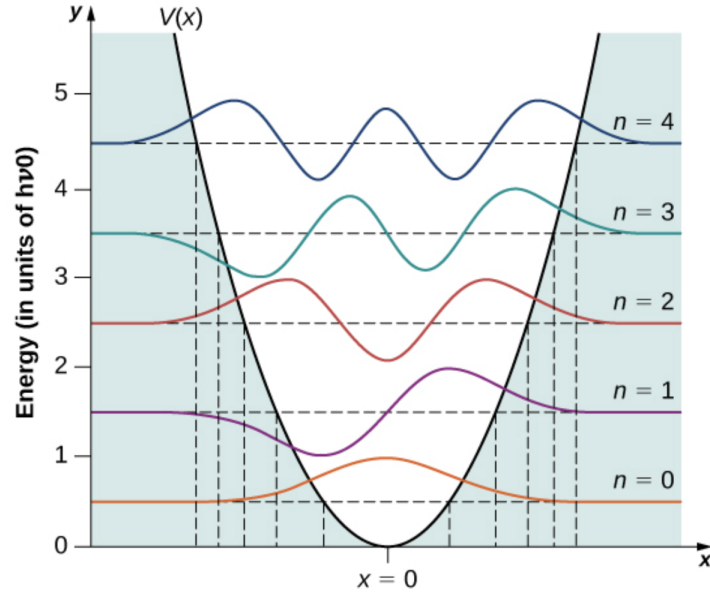
where  $E$  is the energy of the stationary state solution. Therefore, we are searching for the spatial wavefunctions  $\psi(x)$  that solve the TISE with the harmonic operator potential,

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi \quad (3.15)$$

This is clearly a somewhat more involved example than particle in a box, since now the potential is not constant;  $U(x)$  depends on  $x$ . Therefore, our plane wave ansatz  $Ae^{ikx} + Be^{-ikx}$  will *not* solve this equation. (You can check this! substitute that ansatz into (3.15) and you will see there is no way to solve the resulting equation for a constant energy  $E$ .) The reason  $Ae^{ikx} + Be^{-ikx}$  was a good ansatz for a particle in a constant potential is that its second derivative is proportional to itself, so that  $\psi$  canceled out of every term. Now, we need an ansatz for  $\psi(x)$  such that its second derivative is both proportional to  $\psi(x)$ , *and* pulls down a factor of  $x^2$  that can cancel the  $x^2$  in the potential term.

In these lectures we will not find the most general possible solution for  $\psi(x)$ . Instead, we will review the results.





- Just like the particle in a box wavefunctions, the possible wavefunctions that solve (3.15) are quantized, labeled by an integer  $n$  which ranges from  $n = 0, 1, 2, \dots, \infty$ . (NOTE: in the particle-in-a-box solution the integer  $n$  started at 0, but for the quantum harmonic oscillator  $n$  starts at 1.)
- The energies of the stationary states are given by

$$\boxed{\text{Energy levels for QHO: } E_n = \left(n + \frac{1}{2}\right) \hbar\omega, \quad n = 0, 1, 2, \dots} \quad (3.16)$$

where again, in this section  $\omega$  refers to the angular frequency of the classical oscillation, related to the spring constant as  $\omega = \sqrt{\frac{k_{\text{spring}}}{m}}$ . Therefore, there is still a minimum nonzero energy for this quantum system: this ground state energy is  $E_0 = \frac{1}{2}\hbar\omega$ .

- The ground state wavefunction is of the form

$$\psi_0(x) = Ae^{-bx^2}, \quad n = 0$$

On your Homework 8, you will show by plugging this wavefunction into the TISE (3.15) that it indeed satisfies the TISE, with energy  $E_0 = \frac{1}{2}\hbar\omega$ .  $b$  is a real constant that you will determine on this homework.

(Note: you might recognize  $\psi_0(x)$  as a Gaussian function! Recall from our previous Math Break on waves that a function that looks like  $e^{-x^2}$  can be obtained by summing up an infinity of plane waves with different values of  $k$ . This is precisely the type of wavefunction that we also previously noted saturates the uncertainty principle, *i.e.* for which  $\Delta x \Delta p = \frac{\hbar}{2}$ .)

### Example Problem: Normalizing the QHO ground state wavefunction

For practice, let's determine the constant  $A$  in the quantum harmonic oscillator ground state wavefunction,  $\psi_0(x) = Ae^{-bx^2}$ . This can be done by normalizing,

$$1 = \int_{-\infty}^{\infty} |\psi_0(x)|^2 dx = |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx$$

where we used the fact that the constant  $b$  is real, so  $b^* = b$ . This is a Gaussian integral, whose general solution is given as

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$$

Taking  $\alpha = 2b$  in this formula, we therefore have

$$1 = |A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx = |A|^2 \sqrt{\frac{\pi}{2b}} \Rightarrow |A| = \left(\frac{2b}{\pi}\right)^{1/4}.$$

- Since the potential energy function is an even function of  $x$  (symmetric about  $x \rightarrow -x$ , since it depends only on  $x^2$ ), we expect that the probability density for this system should also be an even function of  $x$ . Therefore, the solutions for the wavefunction should be either even or odd functions. This is indeed true: the ground state  $n = 0$  is an even function of  $x$ , the first excited state  $n = 1$  an odd function, and so on. The general form of the  $n$ 'th level wavefunction looks something like

$$\psi_n(x) = (\text{even or odd polynomial in } x)e^{-bx^2}$$

- Much like the particle-in-a-box wavefunctions, the ground state has no nodes, the first excited state has one node, the second excited state has two nodes, *etc.*
- Finally, we note that the wavefunctions go to zero at  $x \rightarrow -\infty$  and  $x \rightarrow +\infty$ , so that they are normalizable.

### Example Problem: Excited states of the QHO

A quantum harmonic oscillator has energy  $E = \frac{7}{2}\hbar\omega$ .

- (a) What is the value of  $n$  for this state?

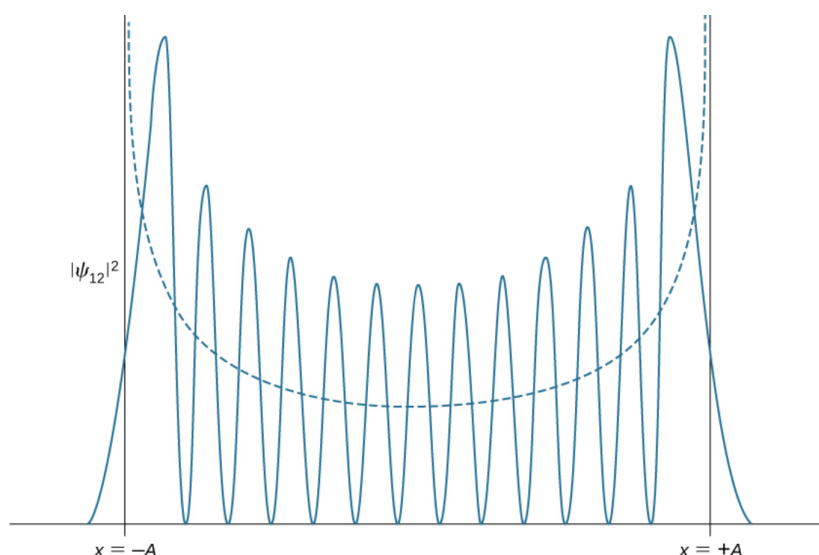
*Solution:* We can compare with  $E = \hbar\omega(n + 1/2)$ , so see that  $n = 3$  for this energy (since  $3 + 1/2 = 7/2$ ).

- (b) Suppose a particle makes a transition from this state to the ground state, emitting a single photon in the process. What is the energy of this photon?

*Solution:* The change in energy between the  $n = 3$  state and the  $n = 0$  ground state is equal to the energy of the photon,

$$\Delta E = E_{\text{photon}} = E_3 - E_0 = \frac{7}{2}\hbar\omega - \frac{1}{2}\hbar\omega = 3\hbar\omega$$

One useful application of this quantum mechanical system is known as *Vibrational spectroscopy*. The idea is that photons (typically in the infrared range of wavelengths) can excite



molecules to higher vibrational energy levels. Since the potential energy of a molecular bond looks like the harmonic oscillator potential, one can use the results from this section to understand the energy levels of the molecules. Chemists use this technique to classify molecules based on their absorption wavelengths and bond energies.

—————End Lecture 18.

What do these probability densities look like at large  $n$ ? We expect that in the limit that  $n \rightarrow \infty$ , the quantum mechanical system should look classical. In the figure, we plot the probability density  $|\psi_n(x)|^2$  for a large value of  $n$ , overlapping it with the classical probability density. We can note from this picture that classically, the particle is more likely to be found near the turning points of the simple harmonic motion, where it is moving slower. In the quantum system, however, this is only true in the large  $n$  limit. Indeed, in the large  $n$  limit the quantum picture blurs into the classical one.

### 3.1.8 Expectation Values of Quantum Operators

As we've seen throughout this section, the position of a particle cannot be determined exactly. The same thing applies to all other *observables*, *i.e.* properties of the particle that you can measure—momentum, kinetic energy, potential energy, *etc.* So, how do we calculate the averages and uncertainties of various physical observables?

Observables in quantum mechanics have to be treated completely differently than in classical mechanics, since we cannot measure their exact values. In quantum mechanics, all observables become *operators*. An operator is an object that acts on the wavefunction and gives another function as a result. An example would be multiplying by some number; the number 3 is an operator which acts on the wavefunction  $\Psi(x, t)$  to give  $3\Psi(x, t)$ . Another example is taking a derivative; the operator  $\frac{d}{dx}$  acts on the wavefunction to give  $\frac{d\Psi(x, t)}{dx}$ . Think of the operator as an information extractor for your state.

The next postulate of quantum mechanics is: To every physical observable  $Q$ , we associate a linear quantum *operator*, which we denote (with a hat) by  $\hat{Q}$ .<sup>11</sup>

<sup>11</sup>There are some math footnotes that constrain the type of operators we can consider, which you will learn about if you take PHYS 320—in particular quantum operators must be *linear* and *Hermitian*.

There are two main operators we will discuss in this part of the course, associated to position and momentum:

- The position operator,  $\hat{x}$ , which just acts via normal multiplication. In other words,

$$\hat{x}\Psi(x, t) = x\Psi(x, t) \quad \leftrightarrow \quad \boxed{\hat{x} = x \quad \text{position operator}} \quad (3.17)$$

- The momentum operator,  $\hat{p}$ , which acts as  $-i\hbar$  times a derivative in position:

$$\hat{p}\Psi(x, t) = -i\hbar \frac{d}{dx} \Psi(x, t) \quad \leftrightarrow \quad \boxed{\hat{p} = -i\hbar \frac{d}{dx} \quad \text{momentum operator}} \quad (3.18)$$

### Clicker Question: Momentum operator

What is the result of acting with the momentum operator on the wavefunction  $\psi(x) = Ae^{-ikx}$ . In other words, what is  $\hat{p}\psi(x)$ ?

- (a)  $+\hbar k$
- (b)  $-\hbar k$
- (c)  $+\hbar k\psi(x)$
- (d)  $-\hbar k\psi(x)$

*Solution:* We need to compute

$$\hat{p}\psi(x) = -i\hbar \frac{d}{dx} Ae^{-ikx} = -i\hbar A(-ik)e^{-ikx} = -\hbar k\psi(x)$$

The answer is (d).

From these two operators, we may construct most other observables, but just replacing our classical dynamical variables  $x, p$  with the quantum operators  $\hat{x}, \hat{p}$ . For example, the kinetic energy operator is given by replacing the  $p$  in  $p^2/(2m)$  with the operator  $\hat{p}$ :

$$\hat{K} = \frac{\hat{p}^2}{2m} = (-i\hbar)^2 \frac{1}{2m} \frac{d^2}{dx^2} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$$

The potential energy operator is given by just replacing the potential as a function of  $x$ ,  $U(x)$ , with the potential as a function of the operator  $\hat{x}$ ,  $U(\hat{x})$ . Then, the *total energy* operator, which we will denote by  $\hat{H}$ , is given by the sum of  $\hat{K}$  and  $U(\hat{x})$ :

$$\boxed{\hat{H} = \frac{\hat{p}^2}{2m} + U(\hat{x}) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(\hat{x}) \quad \text{Total energy operator}} \quad (3.19)$$

So, how can we use our wavefunctions to gain information about our observables? The main goal we wish to achieve is to find the averages of physical observables. Given the wavefunction, we should be able to calculate those averages. How to do this is another postulate:

The *expectation value*, or average, of an observable  $Q$  at time  $t$  is given by,

$$\text{Expectation value:} \quad \langle Q \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{Q} \Psi dx \quad (3.20)$$

The notation “ $\langle Q \rangle$ ” denotes the average of  $Q$ —it’s called an expectation value because it’s the “expected value”. Keep in mind that the order in which the terms are written in this equation are important: for example, if  $\hat{Q}$  is a differential operator, it acts on  $\Psi$  in this equation, not  $\Psi^*$ .

### Example Problem: Particle in a box, Revisited

Find the expectation value  $\langle x \rangle$  for the ground state of the particle-in-a-box.

*Hint:* Before computing integrals, can you argue the answer based on symmetry?

*Solution:* The probability density for the particle in a box is symmetric about the middle of the box. Therefore, taken on average we would expect to find the particle in the center of the box, at  $x = L/2$ .

We can see this explicitly by performing the integral,

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^* \hat{x} \Psi dx$$

where for the ground state of a particle in a box,

$$\Psi_1(x, t) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) e^{-iE_1 t/\hbar}, \quad 0 \leq x \leq L$$

and  $\Psi_1(x, t)$  is zero outside the box. Substituting into the first equation, the time dependence will cancel (as usual for a stationary state). Since  $\hat{x} = x$  doesn’t do anything to the wavefunction except multiply it, this expression simplifies to,

$$\langle x \rangle = \int_0^L x \psi_1(x)^* \psi_1(x) dx = \frac{2}{L} \int_0^L x \sin^2\left(\frac{\pi x}{L}\right) dx$$

The integral evaluates to  $\frac{L^2}{4}$  (you can check for example by substituting into Wolfram Alpha—in general, I would give you at least the indefinite form of these sorts of integrals on homeworks/quizzes if you needed them). Then, the expectation value is

$$\langle x \rangle = \frac{2}{L} \frac{L^2}{4} = \frac{L}{2}$$

As expected, the answer is the middle of the box.

Notice that if  $\hat{Q}$  is just a function of  $\hat{x}$  and no other operators, then since  $\hat{x}$  acts multiplicatively (it doesn’t do anything to the wavefunction it’s acting on except multiply it, this expression simplifies,

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

For example,  $\langle x \rangle$  is essentially computing the weighted average of the position: it’s summing up all the possibilities of where the particle is, times the probability that the particle would be found there.

A useful quantity that we can compute from the expectation values of an operator is the *uncertainty* of the operator, which we denote by  $\Delta Q$ :

$$\boxed{\text{Uncertainty of } Q : \quad \Delta Q = \sqrt{\langle Q^2 \rangle - \langle Q \rangle^2}} \quad (3.21)$$

In other words, compute the expectation value of  $Q^2$  by computing  $\int \Psi^* \hat{Q}^2 \Psi$  and subtract the square of the expectation value of  $Q$ , so that the square root of this whole quantity yields the uncertainty. This definition formalizes our notion of uncertainty that we have been referencing in the Heisenberg uncertainty principle. You can verify that with this definition of uncertainty,

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

is always satisfied.

### Example Problem: Particle in a box, Revisited again

Find the value of  $\langle x^2 \rangle$  for the ground state of the particle-in-a-box. Using the previous result for  $\langle x \rangle$ , find the uncertainty in position,  $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ .

*Solution:*

Let's do the integral. The setup is the same as the last example problem, except replacing  $x \rightarrow x^2$ , so that we end up with

$$\langle x^2 \rangle = \int_0^L x^2 \psi_1(x)^* \psi_1(x) dx = \frac{2}{L} \int_0^L x^2 \sin^2 \left( \frac{\pi x}{L} \right) dx$$

Now, this integral evaluates to

$$\int_0^L x^2 \sin^2 \left( \frac{\pi x}{L} \right) dx = \frac{1}{12} L^3 \left( 2 - \frac{3}{\pi^2} \right)$$

Then,

$$\langle x^2 \rangle = L^2 \left( \frac{1}{3} - \frac{1}{2\pi^2} \right)$$

Combining with our previous answer of  $\langle x \rangle$ , we obtain

$$\begin{aligned} \Delta x &= \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \\ &= \sqrt{L^2 \left( \frac{1}{3} - \frac{1}{2\pi^2} \right) - \left( \frac{L}{2} \right)^2} = L \sqrt{\frac{1}{12} - \frac{1}{2\pi^2}} = 0.18L \end{aligned}$$

This should be interpreted as the standard deviation in our probability density for the particle's position, which is a statistical measure of the uncertainty in the position of the particle due to the fact that the position is determined probabilistically.

**Fuzzy vs sharp observables** Sometimes it happens that acting with an operator on the wavefunction gives back a constant times the function again:

$$\hat{Q}\Psi = Q_0\Psi, \quad Q_0 \text{ a constant}$$

When this is the case, we say that the observable is “sharp”: this is because in precisely this case there is a 100% chance that measuring  $\hat{Q}$  will yield the value  $Q_0$ ! In particular, you can check that when this is the case, the uncertainty in that observable is zero, so the observable is precisely determined:

$$\boxed{\text{Sharp observable: } \hat{Q}\Psi = Q_0\Psi \quad \Rightarrow \quad \Delta Q = 0} \quad (3.22)$$

I can make 100 measurements of  $\hat{Q}$  and will always get back the answer  $Q_0$ .

On the other hand, if this is *not* true, so that  $\hat{Q}\Psi \neq Q_0\Psi$  for some constant  $Q_0$ , the observable is “fuzzy”: the uncertainty is greater than zero, and there are several possibilities for what measurement of  $\hat{Q}$  will return. The best we can do is calculate the probabilities of each measurement outcome.

### Clicker Question: More on Momentum

Recall that in the previous clicker question, you found that for  $\psi(x) = Ae^{-ikx}$ ,

$$\hat{p}\psi(x) = -\hbar k\psi(x)$$

What does this tell you about the momentum observable for this wavefunction?

- (a) It is sharp
- (b) It is fuzzy
- (c) Can't say

This equation is of the form

$$\hat{p}\psi(x) = p_0\psi(x), \quad p_0 = \text{constant} = -\hbar k$$

Therefore, momentum is a sharp observable, (a). A particle with this wavefunction has a well-defined momentum.

You already knew this from our discussion of the free particle—plane waves like this one have definite a wavenumber, which correspond to definite values of momentum! There is no uncertainty in the momentum of the free particle with this wavefunction. Here, you have learned how to formally check that momentum is definite for a free particle, and furthermore you’ve learned to interpret the relation  $p = \hbar k$  as the magnitude of the particle’s momentum, with the particle moving to the left (hence the minus sign). Therefore in general, the plane wave  $Ae^{-ikx}$  corresponds to a left-moving free particle with magnitude of momentum  $\hbar k$ , and the plane wave  $Ae^{ikx}$  corresponds to a right-moving free particle with magnitude of momentum  $\hbar k$ . The general free particle solution is a superposition of these left-moving and right-moving pieces.

**Re-interpreting the Schrödinger equation** With our new knowledge of operators, uncertainty, and fuzzy versus sharp observables, let us take another look back at the time-independent Schrödinger equation,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + U(x)\psi(x) = E\psi(x)$$

We can now recognize that the left-hand-side of this equation is just

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + U(x)\psi(x) = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right) \psi(x) = \hat{H}\psi(x)$$

Then, the TISE can be rewritten

$$\boxed{\text{TISE, rewritten: } \hat{H}\psi(x) = E\psi(x)} \quad (3.23)$$

This is precisely the equation that a sharp variable satisfies: acting with the total energy operator  $\hat{H}$  on the wavefunction gives back a constant (the energy of the state!) times the wavefunction. This affirms what we already knew: stationary states that satisfy the time-independent Schrödinger equation have constant, definite energies, given by the  $E$  that shows up on the right-hand-side of the TISE. Furthermore, it allows us to reinterpret the TISE as not just some complicated differential equation, but as the condition a wavefunction must satisfy to have a definite value of the energy. *All* wavefunctions with definite, “sharp” energy must satisfy the TISE for precisely this reason.

———End Lecture 19.

### 3.1.9 Tunneling and Reflection

Our analysis of the TISE for in regions of constant potential can be equally well applied to the problem of particles being sent at a potential barrier. Consider the problem of sending a free particle towards a barrier of height  $U$ . We’ll ask: what is the probability that the particle gets transmitted through the barrier?

Classically, when a particle or beam of particles is incident on a barrier, there are two scenarios: if the energy  $E$  of the particle is bigger than the barrier potential  $U$ , the particle just goes over the barrier (gets transmitted). Meanwhile, if the energy of the particle is *smaller* than the barrier potential, the particle is stuck on one side of the barrier—it gets reflected.

What happens for a quantum mechanical barrier? As we’ve learned, when the potential is finite, no region is inaccessible to the particle—the wavefunction will be nonzero. As we saw in the case of the finite potential well, the wavefunction is nonzero in the classically forbidden region of finite potential outside the well, so that the particle could be found outside of an area that classically it wouldn’t have had the energy to jump outside of.

For example, let’s take the case of a square barrier of height  $U$  extended from  $x = 0$  to  $x = L$ , and send in a particle from the left towards the barrier. As we’ve already analyzed, the wavefunction of the free particle to the left and right of the barrier (where  $U = 0$ ) is given by a sum of complex exponentials, while the wavefunction inside the barrier region where  $E < U$  is given by a combination of growing and decaying exponentials.

$$\begin{aligned} \psi_L(x) &= Ae^{ikx} + Be^{-ikx}, & x \leq 0 \\ \psi_{\text{in}}(x) &= Ce^{-\beta x} + De^{\beta x}, & 0 < x < L \\ \psi_R(x) &= Fe^{ikx} + Ge^{-ikx}, & x \geq 0 \end{aligned}$$

where  $k$  and  $\beta$  are given by,

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \quad \beta = \sqrt{\frac{2m(U - E)}{\hbar^2}}$$



In this section, we are calling  $\beta = \hat{k}$  the variable that we had previously been using in a region with  $E < U$ , to match onto the notation that the book uses for quantum tunneling.  $A, B, C, D, F, G$  are all constants that need to be determined by imposing the usual conditions: continuity of the wavefunction and its derivative at the boundaries  $x = 0$  and  $x = L$ .

With these expressions, we can compute the probability that a particle incident on the barrier from the left is reflected by it, called the *reflection coefficient*  $R$ ,

$$R = \frac{|B|^2}{|A|^2} = \text{probability that incident particle is reflected}$$

This expression comes from the fact that  $A$  is interpreted as a wave incident on the barrier from the left (moving to the right), and  $B$  is interpreted as a wave reflected from the barrier and moving from right to left. Similarly, the probability that a particle incident on the barrier from the left is transmitted *through* the barrier, and penetrates to emerge on the other side, is given by the *transmission coefficient*  $T$ ,

$$T = \frac{|F|^2}{|A|^2} = \text{probability that incident particle is transmitted}$$

Since a particle incident on the barrier should either be reflected or transmitted, we must have that

$$R + T = 1.$$

Your book derives what  $T$  is by imposing the continuity conditions. Here, we will just review the result: for a square barrier of length  $L$ , the transmission coefficient  $T$  is,

$$T = \left( 1 + \frac{U^2}{4E(U-E)} \sinh^2(\beta L) \right)^{-1} \quad (3.24)$$

Then,  $R = 1 - T$ , since what's not transmitted is reflected. Note that this expression is completely equivalent to the expression given in your textbook,

$$T = (\cosh^2(\beta L) + (\gamma/2)^2 \sinh^2(\beta L))^{-1}, \quad (\gamma/2)^2 = \frac{1}{4} \left( \frac{1-E/U}{E/U} + \frac{E/U}{1-E/U} - 2 \right)$$

I just think the boxed presentation is a bit nicer.

Quantum tunneling has many interesting applications, and I encourage you to read the end of Section 7.6 in your book about some of these!

—————End Lecture 20.

## 3.2 Quantum Mechanics in 3d and Atomic Structure

### 3.2.1 The 3d Schrödinger Equation

We will now learn to extend the Schrödinger equation and its solutions from examples in one spatial dimension  $x$ , to three spatial dimensions  $(x, y, z)$ . We will start with Cartesian coordinates, generalizing the 1d particle in a box to the 3d particle in a box. This formalism will provide us a starting point to study the Hydrogen atom, for which we will switch to spherical coordinates. A key feature that we will find in more than 1 dimension is that we will need more

quantum numbers  $n$  to specify the state of the system: since now there are three degrees of freedom, we will need 3 different quantum numbers  $n_i$ .

The generalization of the probability density is straightforward: The probability that a particle in 3 spatial dimensions is found in an interval of  $(x + dx, y + dy, z + dz)$  at time  $t$  is,

$$\text{Probability density: } P(x, y, z) dx dy dz = |\Psi(x, y, z, t)|^2 dx dy dz \quad (3.25)$$

so that the probability of finding the particle in some spatial integral is given by integrating the probability density over that spatial integral. Of course now, to normalize the wavefunction we will have to integrate this probability density over *all* space,

$$1 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\Psi(x, y, z, t)|^2 dx dy dz$$

Next, let's discuss the generalization of stationary states to three dimensions. Stationary state solutions will take precisely the same form as in 1 dimension,

$$\Psi(x, y, z, t) = \psi(x, y, z) e^{-iEt/\hbar}$$

where now the spatial part of the wavefunction depends on all three coordinates  $x, y, z$ , and satisfies the 3d TISE:

$$\text{TISE: } -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(x, y, z) + U(x, y, z) \psi(x, y, z) = E \psi(x, y, z) \quad (3.26)$$

All we have done is replaced the  $\partial^2/\partial x^2$  with Laplacian operator in 3d,  $\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ , and recognized that both  $\psi$  and the potential  $U$  are in principle functions of all three coordinates.

In particular, the TISE can still be written as the “sharp” condition for the energy,  $\hat{H}\psi = E\psi$ , where now the kinetic energy operator is

$$\hat{K} = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$$

and we have three components of momentum:

$$\hat{p}_x = -i\hbar \frac{d}{dx}, \quad \hat{p}_y = -i\hbar \frac{d}{dy}, \quad \hat{p}_z = -i\hbar \frac{d}{dz} \quad (3.27)$$

### 3.2.2 Particle in a 3d Box

We need to do a bit more work to solve this TISE in three dimensions. Let's focus on the particle-in-a-box example, where now the particle resides in a 3-dimensional box with sides of length  $L_x, L_y, L_z$ . Inside the box the potential is zero, and outside the box the potential is infinite. *Note: below I will go into more detail as to how these solutions are derived than we will cover in lecture. What is important is understanding how to interpret the final solutions for the wavefunctions and energy levels.*

Inside the box, the particle is free, and we need to solve the TISE with  $U(x, y, z) = 0$ . Since  $x, y, z$  are independent of one another, we'll look for separable solutions of the form

$$\psi(x, y, z) = \psi_x(x) \psi_y(y) \psi_z(z).$$

We can play the same trick we did before when we looked for separable solutions: substituting back into the master TISE (with  $U = 0$ ) and dividing throughout by  $\psi = \psi_x\psi_y\psi_z$ , we find

$$-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi_x(x)\psi_y(y)\psi_z(z) = E\psi_x(x)\psi_y(y)\psi_z(z)$$

$$-\frac{\hbar^2}{2m} \left( \frac{1}{\psi_x(x)} \frac{\partial^2 \psi_x(x)}{\partial x^2} + \frac{1}{\psi_y(y)} \frac{\partial^2 \psi_y(y)}{\partial y^2} + \frac{1}{\psi_z(z)} \frac{\partial^2 \psi_z(z)}{\partial z^2} \right) = E.$$

$E$  is a constant, and each of the terms on the left hand side of this equation depend only on one of the three dimensions. Thus, this equation can only be true if *each* term is a constant for all  $x, y, z$ . Call these three constants  $E_{x,y,z}$ :

$$\boxed{\begin{aligned} -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_x(x)}{\partial x^2} &= E_x \psi_x(x), \\ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_y(y)}{\partial y^2} &= E_y \psi_y(y), \\ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_z(z)}{\partial z^2} &= E_z \psi_z(z), \\ E_x + E_y + E_z &= E = \text{constant energy} \end{aligned}} \quad (3.28)$$

These equations are the ones we need to solve to get stationary state solutions to the Schrödinger equation for a particle in 3d in a region where the potential is zero. Each of these equations looks just like the TISE for a particle in a 1d box! Therefore, the 3d particle in a box wavefunction just factors into three copies of the 1d particle in a box wavefunction, one factor for each dimension.

Let's do this explicitly for a particle in a 3d box with sides of different lengths  $L_1, L_2, L_3$ . Each of these three equations is identical to the TISE for a particle in a 1d box, and our entire discussion from the last section applies. The solutions look like

$$\psi_x(x) = A_x \sin(k_x x), \quad \psi_y(y) = A_y \sin(k_y y), \quad \psi_z(z) = A_z \sin(k_z z). \quad (3.29)$$

As usual, the fact that there are no cosine terms follows from imposing the boundary conditions that

$$\psi_x(x=0) = 0, \quad \psi_y(y=0) = 0, \quad \psi_z(z=0) = 0.$$

The  $k_i$ 's are related to the  $E_i$ 's by plugging the ansatz wavefunctions (3.29) into the differential equations they must satisfy, (3.28), resulting in

$$E_x = \frac{\hbar^2 k_x^2}{2m}, \quad E_y = \frac{\hbar^2 k_y^2}{2m}, \quad E_z = \frac{\hbar^2 k_z^2}{2m}, \quad E = E_x + E_y + E_z.$$

Then, the  $k_i$ 's are further constrained by applying the boundary conditions

$$\psi_x(x=L_x) = 0, \quad \psi_y(y=L_y) = 0, \quad \psi_z(z=L_z) = 0.$$

Therefore, the arguments of the sines must be an integer multiple of  $\pi$  when  $(x, y, z) = (L_x, L_y, L_z)$ , which results in the quantization conditions

$$k_x = \frac{n_x \pi}{L_x}, \quad k_y = \frac{n_y \pi}{L_y}, \quad k_z = \frac{n_z \pi}{L_z}, \quad n_x, n_y, n_z = 1, 2, 3, \dots$$

The possible wavefunctions are labeled by three independent quantum numbers,  $n_1, n_2, n_3$ . These integers run from 1 to  $\infty$ , and do *not* have to be the same—they are all independent of each other.

The last thing to do is normalize these wavefunctions. Just as in the 1d case, this will result in the following values for the normalization constants,

$$A_x = \sqrt{\frac{2}{L_x}}, \quad A_y = \sqrt{\frac{2}{L_y}}, \quad A_z = \sqrt{\frac{2}{L_z}}.$$

Finally, we'll summarize our answer for the possible energies and wavefunctions of a particle in a 3d box with sides of lengths  $L_x, L_y, L_z$ :

$$\boxed{\begin{aligned} \psi(x, y, z)_{n_x n_y n_z} &= \sqrt{\frac{2}{L_x}} \cdot \sqrt{\frac{2}{L_y}} \cdot \sqrt{\frac{2}{L_z}} \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right) \sin\left(\frac{n_z \pi z}{L_z}\right) \\ E_{n_x n_y n_z} &= \frac{\pi^2 \hbar^2}{2m} \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right), \quad n_x = 1, 2, \dots; \quad n_y = 1, 2, \dots \quad n_z = 1, 2, \dots \end{aligned}} \quad (3.30)$$

The energy is again quantized, and brought to you by three (independent!) integers  $n_x, n_y, n_z$ . We've put the subscript  $n_x n_y n_z$  on the wavefunctions and energies to remind ourselves of this fact. Note that as we anticipated, since we are in three spatial dimensions there are precisely three quantum numbers labeling the solution. The total time-dependent wavefunction for the particle is then given by

$$\Psi(x, y, z, t) = \psi(x, y, z)_{n_x n_y n_z} e^{-iE_{n_x n_y n_z} t / \hbar},$$

for  $E_{n_x n_y n_z}$  the total energy of the particle.

**Energy spectrum and degeneracy** These solutions look just like three copies of the 1d solutions. However, there is one important feature evident in 3d that is not present in 1d. To see this feature, let's compute the states corresponding to the first 3 energy levels for the case of a symmetric box (a cube):  $L_x = L_y = L_z \equiv L$ ,

$$E = \frac{\pi^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2), \quad n_x = 1, 2, \dots; \quad n_y = 1, 2, \dots \quad n_z = 1, 2, \dots$$

The lowest energy corresponds to all of  $n_x = n_y = n_z = 1$ ,

$$E_{111} = \frac{\pi^2 \hbar^2}{2mL^2} (1^2 + 1^2 + 1^2) = \frac{3\pi^2 \hbar^2}{2mL^2}.$$

Thus,  $n_x = n_y = n_z = 1$  is the ground state of this system, and  $E_{111}$  is the ground state energy. The corresponding wavefunction is  $\psi_{111}$ , given by substituting for  $n_x = n_y = n_z = 1$  and  $L_x = L_y = L_z = L$  in (3.30).

When we come to the first excited state, we notice something interesting: there are actually 3 *different* sets of integers  $(n_x, n_y, n_z)$  that will give us the *same* next highest energy. When only one of  $(n_x, n_y, n_z)$  is 2 and the others are still 1, the energy is

$$E_{112} = E_{121} = E_{211} = \frac{\pi^2 \hbar^2}{2mL^2} (1^2 + 1^2 + 2^2) = \frac{6\pi^2 \hbar^2}{2mL^2} = 2E_{111}.$$

The next highest energy level is twice the ground state energy, but *three different states with different quantum numbers have the same energy!* In particular, even though the energies of

these three states are the same, the wavefunctions are different:

$$\begin{aligned}\psi_{112} &= \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{2\pi z}{L}\right) \\ \psi_{121} &= \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right) \\ \psi_{211} &= \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right)\end{aligned}$$

They are truly three unique states. This phenomenon of *different* states having the *same* energies, and thus all belonging to the same energy level, is called *degeneracy*. We have therefore shown that the first excited state of a particle in a 3d symmetric box (a cube) is 3-fold degenerate.

Let's try the next highest energy level. The next highest energy will correspond to 2 of the  $n_i$ 's being equal to 2, and one of them being equal to 1. (This energy is smaller than having one  $n_i$  equal to 3 and the others equal to 1—you can verify that that's a higher energy level.) Now there are three possibilities with the same energy:

$$E_{122} = E_{221} = E_{212} = \frac{\pi^2 \hbar^2}{2mL^2} (1^2 + 2^2 + 2^2) = \frac{9\pi^2 \hbar^2}{2mL^2} = 3E_{111}.$$

This second excited state (third energy level) has three times the ground state energy, and is again 3-fold degenerate since three unique states  $\psi_{122}, \psi_{221}, \psi_{212}$  have the same energy.

When an energy level is degenerate, it means that we can't tell by measuring the energy of the particle which quantum state it is in. For instance, If I measure the energy of the particle to be  $\frac{6\pi^2 \hbar^2}{2mL^2}$ , then I don't know whether the particle is in the (112), (121) or (211) quantum state.

### Clicker Question: Degeneracy in a 3d cube

A particle is in a 3d box with sides of length  $L$ , and is measured to have an energy

$$E = \frac{11\pi^2 \hbar^2}{2mL^2}.$$

How many different quantum states of the particle could this measurement correspond to?

- (a) 1
- (b) 2
- (c) 3
- (d) 4

*Solution:* The formula for the energies of a symmetric box is

$$E_{n_x n_y n_z} = \frac{\pi^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2)$$

So we need to check, which combinations of integers give  $n_x^2 + n_y^2 + n_z^2 = 11$ ? The answer is that we can have  $n_x^2 + n_y^2 + n_z^2 = 11$  for one of the integers being 3, and the others being 1. Thus, there are three possibilities: (1, 1, 3); (1, 3, 1); (3, 1, 1), and the answer is (c).

We did this exercise for a particle in a symmetric box, meaning a box with equal length sides  $L_x = L_y = L_z = L$ . We can lift the degeneracy by breaking the symmetry between  $x, y$ , and  $z$ . In other words, If I make one side, say  $L_z$ , different from the other two, then I will find that I have *less* degeneracy in the energy levels. This is an exercise I work in detail in the “A degenerate box” problem-solving video [https://youtu.be/lPS\\_Iv6srsrw](https://youtu.be/lPS_Iv6srsrw)—check it out for more details!

### Example Problem: Degeneracy in a 3d box

Suppose a particle is in a box with  $(x, y, z)$  dimensions  $L \times 2L \times 3L$ . Write down the normalized wavefunction for the 1st excited state. What is the degeneracy of this state?

*Solution:* Inside the box, the spatial wavefunction for the state with quantum numbers  $n_x, n_y, n_z$  is,

$$\psi(x, y, z) = \sqrt{\frac{2}{L}} \cdot \sqrt{\frac{2}{2L}} \sqrt{\frac{2}{3L}} \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{2L}\right) \sin\left(\frac{n_z \pi z}{3L}\right)$$

where we substituted  $L_x = L$ ,  $L_y = 2L$ , and  $L_z = 3L$ . The energy of this state is,

$$E_{n_x n_y n_z} = \frac{\pi^2 \hbar^2}{2m} \left( \frac{n_x^2}{L^2} + \frac{n_y^2}{(2L)^2} + \frac{n_z^2}{(3L)^2} \right) = \frac{\pi^2 \hbar^2}{2mL^2} \left( n_x^2 + \frac{n_y^2}{4} + \frac{n_z^2}{9} \right)$$

The smallest possible energy (the ground state) occurs when  $n_x, n_y$ , and  $n_z$  are their minimum possible values,  $n_x = n_y = n_z = 1$ . The first excited state is the state with next highest energy. This will occur when we take  $n_z = 2$  while keeping  $n_x = n_y = 1$ , since  $2^2/9$  is smaller than either  $2^2$  or  $2^2/4$ . Then,  $(n_x, n_y, n_z) = (1, 1, 2)$  represents the first excited state: the smallest energy jump from the ground state. There is no degeneracy for this first excited state, since there is no other combination of the quantum numbers  $n_x, n_y, n_z$  which leads to the same energy. For example, the state  $(1, 2, 1)$  has larger energy than the state  $(1, 1, 2)$ .

Thus, substituting for  $(n_x, n_y, n_z) = (1, 1, 2)$  allows us to write the wavefunction for the first excited state of this box:

$$\psi(x, y, z) = \sqrt{\frac{2}{L}} \cdot \sqrt{\frac{2}{2L}} \sqrt{\frac{2}{3L}} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{2L}\right) \sin\left(\frac{2\pi z}{3L}\right)$$

It has energy

$$E_{112} = \frac{\pi^2 \hbar^2}{2mL^2} \left( 1^2 + \frac{1^2}{4} + \frac{2^2}{9} \right) = \frac{61\pi^2 \hbar^2}{72mL^2}$$

and no degeneracy—the degeneracy of the symmetric box was completely lifted by making the three sides have unequal lengths.

### 3.2.3 The Hydrogen Atom and the Radial Wave Equation

The next quantum mechanics problem we wish to tackle is the hydrogen atom. The Bohr model was a semiclassical model for describing the electron-proton bound state, but finally we know enough quantum mechanics to study the full quantum mechanical solution for this bound state system.

Recall that the hydrogen atom consists of an electron in a central potential,

$$U(r) = -\frac{kZe^2}{r}$$

By central potential, I mean that this potential only depends on the radial distance  $r$  from the center of mass of the 2-body system. In this section, we will study the form of solutions to the Schrödinger equation for particles in central potentials. Since the potential just depends on  $r$ , it will be simplest to do this in spherical coordinates rather than in Cartesian coordinates; everything will depend on  $r^2 = x^2 + y^2 + z^2$ ,

$$(x, y, z) \longrightarrow (r, \theta, \phi) : \quad x = r \sin \theta \cos \phi, \quad y = r \sin \theta \sin \phi, \quad z = r \cos \theta$$

Our goal will be looking for stationary states of the TISE for the hydrogen potential. So, what changes?

———End Lecture 21.

Firstly, let's take a look at the TISE. We can look at the TISE as  $\hat{H}\Psi = E\Psi$ . Now,  $\hat{H}$  involves the Laplacian (3d gradient operator) in spherical coordinates:

$$\begin{aligned} \hat{H} &= -\frac{\hbar^2}{2m} \nabla^2 + U(r) \\ \nabla^2 &= \frac{\partial^2}{\partial r^2} + \left(\frac{2}{r}\right) \frac{\partial}{\partial r} + \frac{1}{r^2} \left[ \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \csc^2 \theta \frac{\partial^2}{\partial \phi^2} \right]. \end{aligned} \quad (3.31)$$

The wavefunction in spherical coordinates depends on  $r, \theta, \phi$ , and  $t$ . We will look for stationary state wavefunctions that are separable in  $r, \theta, \phi$ :

Stationary states in spherical coordinates:  $\Psi(\vec{r}, t) = R(r)\Theta(\theta)\Phi(\phi)e^{-iEt/\hbar}$

Here we are calling  $R(r)$  the part of the spatial wavefunction that depends only on  $r$ ;  $\Theta(\theta)$  is the part that depends only on  $\theta$ ; and  $\Phi(\phi)$  is the part that depends only on  $\phi$ . As usual,  $E$  is the constant energy of the stationary state, to be determined. So, we need to solve the equation:

$$-\frac{\hbar^2}{2m} \nabla^2 [R(r)\Theta(\theta)\Phi(\phi)] + U(r) [R(r)\Theta(\theta)\Phi(\phi)] = E [R(r)\Theta(\theta)\Phi(\phi)]$$

where  $\nabla^2$  is the differential operator in (3.31), and we are interested in the case  $U(r) = -ke^2/r$  for the case of an electron in the Hydrogen atom.

This equation looks quite complicated, but actually simplifies significantly, using the same sort of tricks we employed to solve the TISE for particle-in-a-box. Here we will just review the solution:

- Much as the 3d particle in a box solutions were labeled by 3 integers, the solutions are labeled by three integers:  $n, \ell$  and  $m_\ell$ . We will call  $n$  the *principal quantum number*;  $\ell$  the *orbital quantum number*, or *angular momentum quantum number*; and  $m_\ell$  the *magnetic quantum number*, or *angular momentum projection quantum number*. (We will explain the meanings of these quantum numbers in the next section.)
- The three quantum number  $n, \ell, m_\ell$  are constrained; they do not take all possible values of integers. Note that this is different from particle-in-a-box: for that system we found that the three integers  $n_x, n_y, n_z$  were independent of each other, while in the Hydrogen atom the integers  $n, \ell, m_\ell$  are not totally independent. In particular:

- The principal quantum number  $n$  can be any positive integer:  $n = 1, 2, 3, \dots, \infty$ .
- The orbital quantum number  $\ell$  runs from 0 to  $n - 1$ :  $\ell = 0, 1, 2, \dots, n - 1$ .
- The magnetic quantum number  $m_\ell$  runs from  $-\ell$  to  $\ell$ :  $m_\ell = -\ell, -\ell + 1, \dots, \ell - 1, \ell$ .  
So in other words,  $m_\ell$  runs over the values  $0, \pm 1, \pm 2, \dots, \pm \ell$ .

**Clicker Question: The magnetic quantum number**

If the value of the orbital quantum number  $\ell$  is 4, how many possibilities are there for the magnetic quantum number  $m_\ell$ ?

- (a) 4
- (b) 5
- (c) 7
- (d) 9

*Solution:* If  $\ell = 4$ , then  $m_\ell$  can equal 0,  $\pm 1$ ,  $\pm 2$ ,  $\pm 3$ , or  $\pm 4$ . This is 9 possibilities, so the answer is (d).

- The angular parts of the solutions,  $\Theta(\theta)\Phi(\phi)$ , are called *spherical harmonics*, and are labeled by two of the integers,  $\ell$  and  $m_\ell$ :

$$\Theta(\theta)\Phi(\phi) = Y_\ell^{m_\ell}(\theta, \phi) = \text{“spherical harmonics”} \quad (3.32)$$

- The radial part of the wavefunction,  $R(r)$ , is labeled by the integers  $n$  and  $\ell$ , and satisfies the radial wave equation,

$$-\frac{\hbar^2}{2m} \left[ \frac{d^2 R_{n\ell}(r)}{dr^2} + \frac{2}{r} \frac{dR_{n\ell}(r)}{dr} \right] + \left( \frac{\hbar^2 \ell(\ell+1)}{2mr^2} - \frac{ke^2}{r} \right) R_{n\ell}(r) = E_n R_{n\ell}(r). \quad (3.33)$$

we’ve put the  $n\ell$  subscript on  $R_{n\ell}(r)$  to remind ourselves that the radial wavefunction depends on both  $n$  and  $\ell$ , and we’ve put the  $n$  subscript on  $E_n$  to remind ourselves and the energy levels  $E_n$  depend on this integer  $n$ . We will come back to the energies of these states momentarily.

herefore, we label our spatial wavefunctions as,

$$\text{Hydrogen atom wavefunctions: } \psi_{n\ell m_\ell}(r, \theta, \phi) = R_{n\ell}(r) Y_\ell^{m_\ell}(\theta, \phi) \quad (3.34)$$

The time dependent wavefunction is given by multiplying with the usual factor of  $e^{-iE_n t/\hbar}$ .

**Energy levels and degeneracies** The bound state energy levels of the hydrogen atom can be derived by solving for  $R_{n\ell}(r)$  in the radial wave equation, (3.33). We will only quote the result:

$$\text{Energy levels of Hydrogen: } E_n = -\frac{ke^2}{2a_0} \frac{1}{n^2} = -(13.6 \text{ eV}) \frac{1}{n^2} \quad (3.35)$$

**These are precisely the energy levels predicted by the Bohr model of hydrogen!** Solving the full quantum mechanical system of an electron in a central Coulomb potential yields the same answer for the possible energies of the electron as Bohr found in his semi-classical model!

Since the energies  $E_n$  depend on only one quantum number  $n$ , but the wavefunctions also depend on the other two quantum  $\ell$  and  $m_\ell$ , there will be degeneracies: any time multiple different wavefunctions have the same value of  $n$ , they are degenerate.



### Example Problem: Degeneracies in the hydrogen atom

An electron in the hydrogen atom has energy  $E = -\frac{13.6\text{eV}}{9}$ . List all the possible wavefunctions that could correspond to the state with this energy. What is the total degeneracy?

*Solution:* This electron is in the  $n = 3$  state, so we need to list the possible values of the other quantum numbers.

- Since  $\ell$  can run from 0 to  $n - 1$ , the possible values of  $\ell$  are 0, 1, 2.
- For each value of  $\ell$ , we need to count the possible values of  $m_\ell = 0, \pm 1, \dots, \pm \ell$ . For  $\ell = 0$ , the only possibility is 0. For  $\ell = 1$ , there are three possibilities, 0,  $-1$ ,  $+1$ . For  $\ell = 2$ , there are five possibilities: 0,  $-1$ ,  $+1$ ,  $-2$ ,  $+2$ .

Therefore, the possible wavefunctions are labeled as:

$$\psi_{n,\ell,m_\ell} = \{\psi_{3,0,0}; \psi_{3,1,0}; \psi_{3,1,-1}; \psi_{3,1,1}; \\ \psi_{3,2,0}; \psi_{3,2,-1}; \psi_{3,2,1}; \psi_{3,2,-2}; \psi_{3,2,2}\}$$

and the total degeneracy of this energy level is 9. Each of these 9 wavefunctions represents a *distinct* wavefunction with the same energy  $E_3$ .

In general, special names are given for the states labeled by different  $n$  and  $\ell$ . States corresponding to a particular  $n$  are said to form “shells”.  $n = 1$  is known as the K shell,  $n = 2$  is the L shell,  $n = 3$  is the M shell,  $n = 4$  is the N shell, and so on. Then,  $\ell = 0$  is the s subshell,  $\ell = 1$  is the p subshell,  $\ell = 2$  is the d subshell,  $\ell = 3$  is the f subshell,  $\ell = 4$  is the g subshell, and so on.

**Normalization and Probability Density** Before we study some of the actual wavefunctions corresponding to these energy levels, let’s discuss how to compute probabilities and expectation values. We will focus on computing probabilities that the electron is found in some range of radii, and expectation values that involve only the radial distance of the electron to the origin.

In spherical coordinates the volume element is

$$dV = r^2 \sin \theta \, dr \, d\theta \, d\phi$$

Thus, the probability density for stationary states of the Hydrogen atom is

$$P(r, \theta, \phi) \, dV = |\psi_{n\ell m_\ell}(\vec{r}, t)|^2 r^2 \sin \theta \, dr \, d\theta \, d\phi = (|R_{n\ell}(r)|^2 r^2 dr) (|Y_\ell^{m_\ell}(\theta, \phi)|^2 \sin \theta \, d\theta \, d\phi)$$

For example, let’s say that I want to know the probability that the electron will be found at a distance between  $r$  and  $r + dr$  from the nucleus: in other words, I want to integrate over all of  $\theta$  and  $\phi$ ,

$$P(r) \, dr = \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} P(r, \theta, \phi) \, dV = |R_{n\ell}(r)|^2 r^2 dr \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} |Y_\ell^{m_\ell}(\theta, \phi)|^2 \sin \theta \, d\theta \, d\phi$$

A fact about the spherical harmonics given in your book is that they are normalized and orthonormal, such that the integral above over the full range  $\theta$  and  $\phi$  just gives 1. Therefore,

the the probability that the electron will be found at a distance between  $r$  and  $r + dr$  from the nucleus, which we'll call the *radial probability density*, is

$$\boxed{\text{Radial probability density: } P(r) dr = r^2 |R_{n\ell}(r)|^2 dr} \quad (3.36)$$

To make sure the radial wavefunction is normalized, we'd need to check that integrating the radial probability density over the full range of  $r$  from 0 to  $\infty$  yields one—this is the condition that the electron has to be found at *some* distance  $r$ .

$$1 = \int_0^\infty P(r) dr = \int_0^\infty r^2 |R_{n\ell}(r)|^2 dr.$$

With this condition, and the normalized spherical harmonics, the integral over all space of the full  $P(r, \theta, \phi) dV$  is 1. Then given the normalized electron's radial wavefunction, the probability of finding the electron between radii  $r_1$  and  $r_2$  is

$$\boxed{\text{Radial probability: } P(r_1 < r < r_2) = \int_{r_1}^{r_2} r^2 |R_{n\ell}(r)|^2 dr} \quad (3.37)$$

The expectation value of an operator  $\hat{Q}$  which is a function of  $r$  and independent of  $\theta$  and  $\phi$ ,  $\hat{Q}(r)$ , is then given by

$$\boxed{\langle \hat{Q}(r) \rangle = \int_0^\infty \hat{Q}(r) P(r) dr = \int_0^\infty \hat{Q}(r) r^2 |R_{n\ell}(r)|^2 dr} \quad (3.38)$$

**The ground state of Hydrogen** Let's take a moment and look at the first couple of energy levels. Actually solving the differential equations for the wavefunctions is beyond the scope of this class, but we will still examine what the wavefunctions look like.

The ground state (also called the  $1s$  state) has quantum numbers ( $n = 1, \ell = 0, m_\ell = 0$ ), and is the only state with  $n = 1$ . Therefore, it is not degenerate. The energy is

$$E_1 = -\frac{ke^2}{2a_0} = -13.6 \text{ eV}.$$

The radial wavefunction for  $n = 1$  is given by

$$R_{n\ell}(r) = R_{10}(r) = \frac{2}{a_0^{3/2}} e^{-r/a_0}.$$

and the angular part of the wavefunction is actually just a constant, given by

$$Y_0^0 = \frac{1}{\sqrt{\pi}}.$$

Thus, the ground state of hydrogen has a spatial wavefunction

$$\psi_{n\ell m_\ell}(r, \theta, \phi) = \psi_{100}(r, \theta, \phi) = R_{10}(r) Y_0^0 = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \quad (\text{ground state of hydrogen})$$

We'll comment on a few aspects of this wavefunction. Firstly, note that it is spherically symmetric: it doesn't depend at all on  $\theta, \phi$ . Since it's spherically symmetric, this means that the likelihood of finding the electron at some location around the proton is the *same* for all  $\theta, \phi$ , and only depends on the radial separation between the electron and the nucleus. In other words, there is an equal probability of finding the electron in the ground state of hydrogen anywhere around the proton at a given distance of  $r$ .

So, where is the electron most likely to be found in the ground state of hydrogen?

### Example Problem: The ground state of hydrogen

An electron is in the 1s (ground) state of Hydrogen, with radial wavefunction

$$R_{10}(r) = \frac{2}{a_0^{3/2}} e^{-r/a_0}.$$

- (a) What is the *average* location of the electron in this state?
- (b) What is the *most likely* radial distance from the proton that we'll find the electron?

*Solution:* First, let's make the distinction between *average* and *most likely*. Average means that we should make many measurements of the electron's distance from the proton, and then compute the average of all of these measurements. This is what's computed with the expectation value,  $\langle r \rangle$ . On the other hand, *most likely* means that the value that appears most frequently if we make many measurements (the mode).

There is clearly a difference between the two: for example, consider the first excited state of particle in a box. The average position of the particle is  $\langle x \rangle = \frac{L}{2}$  in the center of the box—this is true since the probability density is symmetric about the center of the box. However, the most likely values are at either  $L/4$  or  $3L/4$ ; these are the locations where the probability density is at a maximum, so if we make many measurements we expect to see these locations most frequently. The most likely value cannot possibly be  $L/2$ , since actually there is zero probability of finding the electron in the exact center of the box for this state!

For both parts of this problem, we require the radial probability density:

$$P(r) dr = r^2 |R_{10}|^2 = \frac{4r^2}{a_0^3} e^{-2r/a_0}.$$

For part (a), we ask what's the *average* location of the electron in this state? In other words, compute

$$\langle r \rangle = \int_0^\infty r P(r) dr = \int_0^\infty \frac{4r^3}{a_0^3} e^{-2r/a_0} dr.$$

This is an integral of the form

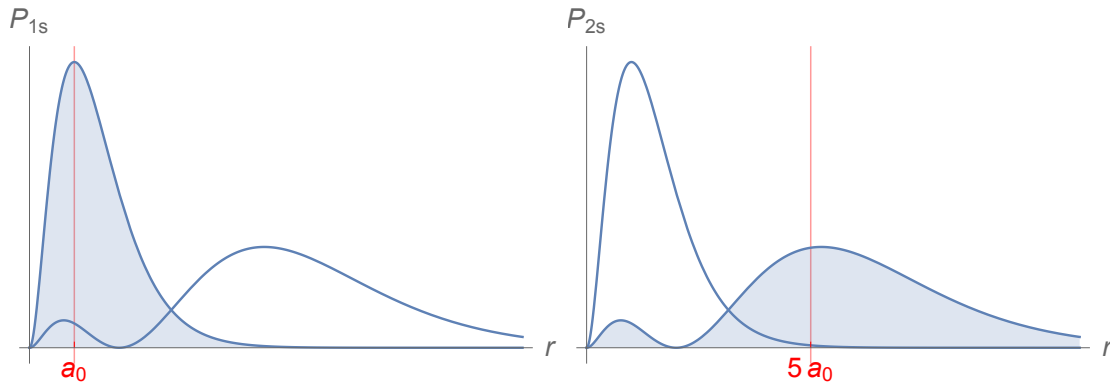
$$\int_0^\infty z^n e^{-z} dz = n!$$

Substituting  $z = 2r/a_0$ ,  $dz = 2dr/a_0$ , we find

$$\langle r \rangle = \frac{a_0}{4} \int_0^\infty z^3 e^{-z} dz = \frac{3!}{4} a_0 = \frac{3}{2} a_0.$$

The average location of the electron is at a distance of  $r = \frac{3}{2} a_0$  from the origin, with equal probability of finding the electron at any angle in  $\theta, \phi$ .

For part (b): What about the *most likely* radial distance? The most likely location  $r_0$



is the location for which the probability density is a maximum, *i.e.*

$$\begin{aligned}\frac{dP(r_0)}{dr} = 0 &\Leftrightarrow \left( \frac{8r_0}{a_0^3} + \frac{4r_0^2}{a_0^3} \cdot \frac{-2}{a_0} \right) e^{-2r_0/a_0} = 0 \\ \frac{8r_0}{a_0^3} e^{-2r_0/a_0} \left( 1 - \frac{r_0}{a_0} \right) &= 0 \\ \Rightarrow r_0 &= a_0.\end{aligned}$$

So the most likely position where we're going to find the electron is the Bohr radius! This is why Bohr's model was so successful, even though it didn't incorporate probabilities: most of the time, we're going to find the electron in Hydrogen at the Bohr radius, even if we'd get some variation from repeated measurements.

**The first excited states** The first excited state has  $n = 2$ , so that the possible values of the other quantum numbers are  $\ell = 0, 1$ , and  $m_\ell = 0, \pm\ell$ . Thus, the possibilities are  $(n, \ell, m_\ell) = (2, 0, 0); (2, 1, 0); (2, 1, 1); (2, 1, -1)$ . This level is therefore 4-fold degenerate. All of these degenerate states have energy

$$E_n = -\frac{ke^2}{2a_0} \frac{1}{2^2} = -\frac{13.6}{4} \text{ eV}.$$

We've plotted the 1s radial probability density, as well as the 2s radial probability density, in the figure. Both of these states are spherically symmetric. In the 2s state, the electron is most likely to be found at a distance of about  $5a_0$  (the highest peak), 5 times farther from the nucleus than the electron in the ground state. The other first excited states, the 2p states with  $\ell = 1$  and  $m_\ell = 0, \pm 1$ , do not have spherically symmetric probability distributions.

—————*End Lecture 22.*

### Clicker Question: A superposition of hydrogen stationary states

An electron in the hydrogen atom is in a state that is a superposition of 2p states with different  $m_\ell$  quantum numbers,

$$\psi_{\text{electron}} = \frac{1}{\sqrt{2}} (\psi_{2,1,1} + \psi_{2,1,-1}).$$

What is the energy of the electron?

(a)  $\frac{-13.6 \text{ eV}}{4}$

(b)  $\frac{-13.6 \text{ eV}}{2}$

(c) The electron doesn't have a definite energy (it is fuzzy).

*Solution:* Both  $\psi_{2,1,1}$  and  $\psi_{2,1,-1}$  are stationary state wavefunctions of the hydrogen atom with the *same* energy, since both have  $n = 2$ :

$$E_2 = \frac{-13.6 \text{ eV}}{2^2} = \frac{-13.6 \text{ eV}}{4}.$$

Therefore, the superposition of these two states is also a stationary state with energy  $E_2$ . This follows from the linearity of the Schrodinger equation.

We can also show this explicitly. We can schematically write the TISE for the wavefunction as

$$\begin{aligned} \hat{H}\psi_{\text{electron}} &= E\psi_{\text{electron}} \\ \hat{H} \frac{1}{\sqrt{2}} (\psi_{2,1,1} + \psi_{2,1,-1}) &= \frac{1}{\sqrt{2}} (\hat{H}\psi_{2,1,1} + \hat{H}\psi_{2,1,-1}) = \frac{1}{\sqrt{2}} (E_2\psi_{2,1,1} + E_2\psi_{2,1,-1}) \\ &= E_2 \left[ \frac{1}{\sqrt{2}} (\psi_{2,1,1} + \psi_{2,1,-1}) \right] \\ &\Rightarrow E = E_2. \end{aligned}$$

and indeed the energy of this state is a sharp observable, with value equal to  $E_2$ .

### 3.2.4 Angular Momentum in Hydrogen

The quantization of angular momentum was crucial to the Bohr model. So, what are the allowed values of angular momentum for these states?

The answer is that we should interpret the quantum numbers  $\ell$  and  $m_\ell$  in terms of the angular momentum of the electron. The statement is both the total magnitude of angular momentum  $L = |\vec{L}|$ , and the  $z$ -component of angular momentum  $L_z$ , are quantized:

Angular momentum quantization: $L = \sqrt{\ell(\ell+1)}\hbar, \quad L_z = m_\ell\hbar$	(3.39)
--	--------

As an example, consider the four degenerate states in the first excited energy level,  $(2, 0, 0)$ ;

$(2, 1, 0); (2, 1, -1); (2, 1, 1).$

$$\begin{aligned}(2, 0, 0) : \quad L &= 0, \quad L_z = 0 \\(2, 1, 0) : \quad L &= \sqrt{2}\hbar, \quad L_z = 0 \\(2, 1, -1) : \quad L &= \sqrt{2}\hbar, \quad L_z = -\hbar \\(2, 1, 1) : \quad L &= \sqrt{2}\hbar, \quad L_z = \hbar\end{aligned}$$

Some comments:

- Since the information about angular momentum is contained entirely in the  $\ell$  and  $m_\ell$  quantum numbers, this reflects a property of the spherical harmonics  $Y_\ell^{m_\ell}(\theta, \phi)$ .
- Angular momentum is a vector quantity, with components  $L_x, L_y, L_z$ . Perhaps surprisingly, we can only simultaneously know both  $L$  and ONE of  $L_x, L_y, L_z$ , which by convention we take to be  $L_z$ . What about the other components of angular momentum?

Quantum mechanically, it is not possible to know all three components at once! Why not? Suppose that  $\vec{L}$  was precisely known, so that we knew all components  $L_x, L_y, L_z$ , and say for example that  $L_y = L_z = 0$ . Since  $\vec{L} = \vec{r} \times \vec{p}$ , this implies that the electron must be in the  $x - y$  plane; we would know with certainty that the electron was at  $z = 0$ , so that  $\Delta z = 0$ . But: if  $\Delta z = 0$ , then by the uncertainty principle  $\Delta p_z = \infty$ , we would have no idea what the electron's  $z$ -component of momentum was. However, since the energy of the electron contains the kinetic energy  $K \supset p_z^2/(2m)$ , this would imply that the electron's energy was also uncertain. But this is a contradiction: an electron in a stationary state of hydrogen by construction has a definite value of energy  $E$ ! Therefore, it is not possible that we could have pinpointed the direction of the angular momentum completely; if we had, then this would have implied an uncertainty in the electron's energy.

- However, we do know something about the directionality of the angular momentum; since we know the total magnitude and the  $z$ -component, we know the angle  $\theta$  that  $\vec{L}$  makes with the  $z$ -axis:

$$\boxed{\cos \theta = \frac{L_z}{L} = \frac{m_\ell}{\sqrt{\ell(\ell+1)}}} \quad (3.40)$$

Since  $L_z$  and  $L$  are quantized, this means that the angle  $\theta$  is also quantized.

For instance, consider the four degenerate states in the first excited energy level. The angles they make to the  $z$ -axis are:

$$\begin{aligned}(2, 0, 0) : \quad L &= 0, \quad L_z = 0 \\(2, 1, 0) : \quad L &= \sqrt{2}\hbar, \quad L_z = 0 \quad \Rightarrow \quad \theta = 90^\circ \\(2, 1, -1) : \quad L &= \sqrt{2}\hbar, \quad L_z = -\hbar \quad \Rightarrow \quad \theta = 135^\circ \\(2, 1, 1) : \quad L &= \sqrt{2}\hbar, \quad L_z = \hbar \quad \Rightarrow \quad \theta = 45^\circ\end{aligned}$$

The first has no angular momentum, but the others all do, pointed at different angles  $\theta$  relative to the  $z$ -axis.

- How does the quantized angular momentum of the electron compare to the predictions of the Bohr model? Bohr predicted that  $L = \hbar \cdot \text{integer}$ , whereas we have found that the stationary orbits have  $L = \hbar\sqrt{\ell(\ell+1)}$ . Therefore the correct comparison to make is between  $L_{\text{Bohr}} = \hbar\ell$ , and the true  $L = \hbar\sqrt{\ell(\ell+1)}$ . We can check:

$\ell$	1	2	3	4	...	100	200	...
$L_{\text{Bohr}}/\hbar = \ell$	1	2	3	4	...	100	200	...
$L/\hbar = \sqrt{\ell(\ell+1)}$	1.4	2.4	3.5	4.5	...	100.5	200.5	...

For small values of  $\ell$  the percent difference between Bohr's estimate and the true quantum mechanical answer is on the order of 30%, but this gets better and better for larger  $\ell$ , dropping for example to 0.2% at  $\ell = 200$ . So, Bohr was certainly on the right track qualitatively, but not necessarily quantitatively, at least for small values of  $\ell$ !

We have interpreted the quantum numbers  $\ell$  and  $m_\ell$  in terms of the angular momentum of the electron. The deeper reason why we can do this is because the magnitude of the total angular momentum  $L$  and  $z$ -component of momentum  $L_z$  are *sharp observables*, taking definite values in states labeled by  $\ell$  and  $m_\ell$ . The operators that correspond to these observables, written in spherical coordinates, are as follows:

$$\hat{L}^2 = -\hbar^2 \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \csc^2 \theta \frac{\partial^2}{\partial \phi^2} \right) \quad (3.41)$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi} \quad (3.42)$$

These definitions follow from the usual definitions in Cartesian coordinates. For example, starting with  $L_z = (\vec{r} \times \vec{p})_z = (xp_y - yp_x)$ , and then substituting the definitions of the momentum operators  $p_x = -i\hbar \frac{\partial}{\partial x}$ ,  $p_y = -i\hbar \frac{\partial}{\partial y}$ , and then changing from Cartesian to spherical coordinates.

The hydrogen stationary state wavefunctions satisfy the following conditions:

$$\hat{L}_z \psi_{n\ell m_\ell} = (m_\ell \hbar) \psi_{n\ell m_\ell}, \quad \hat{L}^2 \psi_{n\ell m_\ell} = (\ell(\ell+1)\hbar^2) \psi_{n\ell m_\ell}$$

Formally, these equations reflect the statement that  $L$  and  $L_z$  are sharp observables for these states.

### 3.2.5 Magnetic Dipole Moment

A charged particle moving in a circular orbit (like the electron in Hydrogen!) results in a magnetic field; therefore we expect that the hydrogen atom produces a magnetic field, and interacts with other magnetic fields. In this section, we'll discuss the magnetic properties of the hydrogen.

Magnetic effects involving the particle are described in terms of what's known as the magnetic dipole moment of the orbiting charge, which is proportional to the particle's angular momentum  $\vec{L}$ ,

$$\vec{\mu} = \frac{q}{2m} \vec{L}$$

For an electron in the Hydrogen atom, we've learned that its angular momentum in the  $z$ -direction is quantized, so the  $z$ -component of the magnetic dipole moment is also quantized!

$$\mu_z = -\frac{e}{2m_e} L_z = -\frac{e\hbar}{2m_e} m_\ell \equiv -\mu_B m_\ell.$$

The minus sign is because the charge of the electron is negative.  $\mu_B$  is a constant known as the Bohr magneton,  $\mu_B = 9.274 \times 10^{-24} \text{ J/T} = 5.8 \times 10^{-5} \text{ eV/T}$ . Similarly, since the magnitude of

angular momentum is quantized, the magnitude of the magnetic moment is quantized, also in units of the Bohr magneton:

$$|\vec{\mu}| = \mu = \frac{e}{2m_e} L = \frac{e\hbar}{2m_e} \sqrt{\ell(\ell+1)} = \mu_B \sqrt{\ell(\ell+1)}$$

To summarize,

$$\boxed{\mu_z = -\mu_B m_\ell, \quad \mu = \mu_B \sqrt{\ell(\ell+1)}, \quad \mu_B = \frac{e\hbar}{2m_e} = 9.274 \times 10^{-24} \text{ J/T}} \quad (3.43)$$

Since the hydrogen atom has a magnetic field, we expect it to interact with an external magnetic field, in the same way that two magnetics interact with each other. If we apply an external magnetic field to the atom, then the atom experiences a torque,

$$\vec{\tau} = \vec{\mu} \times \vec{B}.$$

The energy of a magnetic dipole in an external magnetic field  $\vec{B}$  depends on its orientation, as the dipole will do work to re-orient itself against the torque of the applied field. This potential energy is

$$U = -\vec{\mu} \cdot \vec{B}.$$

For instance, if I apply a magnetic field in the  $z$ -direction to my atom, this dot product only picks up the  $z$ -component of the magnetic moment, so that the rotational symmetry of this expression is broken and the energy due to this interaction is,

$$U = \mu_B m_\ell B_z$$

Then, the *total* energy of the electron becomes the sum of this magnetic energy, plus the energy it had in the absence of the magnetic field,  $E_n$ . This breaks part of the degeneracy of the energy levels, and causes the energies to shift by

$$\Delta E = \mu_B m_\ell B_z.$$

This is called the *Zeeman effect*. The idea is that by applying a magnetic field, we get the electron in each  $(n, \ell, m_\ell)$  state to identify itself! Now, the energies depend both on  $n$  and  $m_\ell$ , which splits some of the degeneracy of the energy levels. (Since energy still does not depend on  $\ell$ , it doesn't lift the whole degeneracy—it lifts the  $(2\ell+1)$ -fold degeneracy of a state with a given  $\ell$  and  $2\ell+1$  possible values of  $m_\ell$ .)

### Example Problem: The Zeeman effect

The transition from the 2p ( $m_\ell = 0$ ) to 1s states emits a photon of wavelength  $121.569 \text{ nm}$ . What is the wavelength of the photon emitted from the transition 2p ( $m_\ell = -1$ ) to 1s, given a magnetic field of 8 Tesla in the  $z$ -direction?

*Solution:*

The energy levels split according to  $\Delta E = \mu_B m_\ell B_z$ , so there is no change in the  $m_\ell = 0$  energy level. The photon in the first transition satisfies

$$\Delta E = hf = \frac{hc}{\lambda} = E_2 - E_1$$

where  $\lambda$  is the observed wavelength of the photon, and the difference in energy levels is unaffected by the magnetic field. We can manifestly check that this equation is satisfied



for the numbers given:

$$\frac{1240.8 \text{ eV} \cdot \text{nm}}{121.569 \text{ nm}} = 10.2 \text{ eV}, \quad -(13.6 \text{ eV}) \left( \frac{1}{2^2} - \frac{1}{1^2} \right) = 10.2 \text{ eV} \checkmark$$

We are next asked to consider a transition from  $m_\ell = -1$  to  $1s$ , given a magnetic field of 8 Tesla. The magnetic field splits the  $E_2$  energy level,

$$E_2 \rightarrow E_2^{(\ell)} = E_2 + \mu_B m_\ell B_z$$

Plugging in the numbers, this corresponds to an energy of

$$\begin{aligned} E_2^{(m_\ell=-1)} &= -\frac{(13.6 \text{ eV})}{2^2} + (9.274 \times 10^{-24} \text{ J/T})(-1)(8 \text{ T}) \frac{1 \text{ eV}}{1.6 \times 10^{-19} \text{ J}} \\ &= -3.4 \text{ eV} - 4.6 \times 10^{-3} \text{ eV} \end{aligned}$$

The wavelength of the photon is then

$$\lambda = \frac{hc}{E_2^{(-1)} - E_1} = 121.592 \text{ nm}$$

This is a very small difference in wavelength from the energy level without the splitting!

—————End Lecture 23.

I've included the following example problem in the lecture notes, try it at home before going through the solution!

### Example Problem: More on the Zeeman effect

An electron in the hydrogen atom is in the state,

$$\psi_{n\ell m_\ell} = \frac{1}{8\sqrt{\pi a_0^3}} \frac{r}{a_0} e^{-r/(2a_0)} \sin \theta e^{i\phi}$$

By how much does the energy of this state change in the presence of a magnetic field of magnitude  $B_z = 1$  Tesla?

*Solution:* The energy splitting depends on the quantum number  $m_\ell$ , so first we need to figure out what  $m_\ell$  is for this state. We can obtain this using the relation between the  $z$ -component of angular momentum operator  $\hat{L}_z$  and its sharp observable:

$$\hat{L}_z \psi_{n\ell m_\ell} = (\hbar m_\ell) \psi_{n\ell m_\ell}, \quad \hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$$

Applying the operator to the wavefunction, we arrive at

$$-i\hbar \frac{\partial}{\partial \phi} \left( \frac{1}{8\sqrt{\pi a_0^3}} \frac{r}{a_0} e^{-r/(2a_0)} \sin \theta e^{i\phi} \right) = -i\hbar \frac{1}{8\sqrt{\pi a_0^3}} \frac{r}{a_0} e^{-r/(2a_0)} \sin \theta \frac{\partial}{\partial \phi} e^{i\phi} = \hbar \psi_{n\ell m}$$

since the derivative only acts on  $e^{i\phi}$  to bring down a factor of  $i$ . Therefore, we have that

$$\hat{L}_z \psi_{n\ell m_\ell} = \hbar \psi_{n\ell m_\ell} \Rightarrow m_\ell = 1.$$

This electron is in a state with  $m_\ell = 1$ . Having obtained  $m_\ell = 1$ , we can substitute into the energy splitting formula:

$$\Delta E = \mu_B m_\ell B_z = (5.8 \times 10^{-5} \text{ eV/T})(1)(1 \text{ T}) = 5.8 \times 10^{-5} \text{ eV}$$

This is how much the energy of this state will change in the presence of a magnetic field.

### 3.2.6 Spin

There's one more set of quantum numbers that label a state of the hydrogen atom, related to what's called the *spin* of the electron. In addition to the usual angular momentum, it turns out that electrons have an intrinsic angular momentum known as spin. The properties of this spin angular momentum are much like those of the angular momentum associated to a charge that's rotating about its axis. However, this is just a useful analogy—there isn't a real sense in which the electron is literally spinning. The existence of spin angular momentum can be inferred from experiments, which indicate that there's a component to the angular momentum of the electron that can't be accounted for by the orbital angular momentum  $L$  alone.

Much like the electron in Hydrogen has a definite magnitude of orbital angular momentum  $L$  and definite  $z$ -component of orbital angular momentum  $L_z$ , it has a definite magnitude of spin angular momentum  $S$  and definite  $z$ -component of spin angular momentum  $S_z$ , resulting in two new quantum numbers  $s$  and  $m_s$ :

$$\begin{aligned} L &= \hbar\sqrt{\ell(\ell+1)} & \Leftrightarrow & S = \hbar\sqrt{s(s+1)} \\ L_z &= \hbar m_\ell & \Leftrightarrow & S_z = \hbar m_s. \end{aligned}$$

It turns out that *all* electrons have spin  $s = \frac{1}{2}$ , and  $m_s$  either equal to  $+\frac{1}{2}$  (commonly called “up”, or denoted  $\uparrow$ ) or  $-\frac{1}{2}$  (commonly called “down”, or denoted  $\downarrow$ ). Therefore, the electron in the hydrogen atom has

$$S = \hbar\sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)} = \frac{\sqrt{3}}{2}\hbar \quad (\text{spin of an electron})$$

and  $m_s = \pm\frac{1}{2}$ . **Any measurement involving the spin of the electron only measures two possible spins: up or down.** What this means for our hydrogen wavefunctions is that there's one more quantum number  $m_s$  that takes one of two values coming from the fact that the electron can either be spin up or spin down, so there's an extra factor of 2 in the degeneracy of each energy level.

#### Clicker Question: Spin in the hydrogen atom

Given that an electron is in a 2p ( $n = 2, \ell = 1$ ) orbital of hydrogen, how many possibilities are there for the four quantum numbers?

*Solution:* Without accounting for spin, we can have  $m_\ell = 0, \pm 1$ , so there would be 3 possibilities. Accounting for spin leads to an extra factor of 2, since for each value of

$(n, \ell, m_\ell)$ , we can have  $m_s = \pm \frac{1}{2}$ . The answer is 6, corresponding to the states:

$$(n, \ell, m_\ell, m_s) = (2, 1, 0, +\frac{1}{2}); (2, 1, 0, -\frac{1}{2}); (2, 1, 1, +\frac{1}{2}); \\ (2, 1, 1, -\frac{1}{2}); (2, 1, -1, +\frac{1}{2}); (2, 1, -1, -\frac{1}{2})$$

The electron's spin gives rise to a magnetic dipole moment, with twice the prefactor of the orbital angular momentum magnetic moment:

$$\vec{\mu}_s = -2 \frac{e}{2m_e} \vec{S}$$

Then, the  $z$ -component of the spin magnetic moment is

$$(\mu_s)_z = - \left( \frac{e}{m_e} \right) m_s \hbar$$

This leads to further energy splitting, even when  $m_\ell = 0$ :

$$\Delta E = 2\mu_B B_z m_s \quad (3.44)$$

The Stern-Gerlach experiment provides experimental evidents that electrons have spin angular momentum – see your book for more information about this experiment.

———End Lecture 24.

### 3.2.7 Pauli Exclusion and the Periodic Table

When you think about how you differentiate particles from each other, you probably have in mind that you can tell them apart, or that they are *distinguishable*. By distinguishable, we mean particles with different characteristics; I can label particle 1 as particle 1, and track where it goes, differentiating it from some other particle 2, like different billiard balls on a pool table.

However, it turns out that all the different types of fundamental particles in nature are actually *indistinguishable*, or *identical*, to particles of the same type. All electrons (for instance) with the same quantum numbers are indistinguishable from each other. For example, say I collide two spin-up electrons with one another, so that after the collision the two electrons scatter, with one ending up at position  $x_A$  and the other at position  $x_B$ . Because all electrons with the same quantum numbers are identical to each other, I can't tell *which* of the 2 electrons ends up at  $x_A$ , and which ends up at  $x_B$ —I can't paint a label onto them to figure out which is which. All I can say is that *an* electron ends up at spot  $x_A$ , and *an* electron ends up at spot  $x_B$ . All the information at our disposal to label an electron is encapsulated by its quantum numbers (for example  $n, \ell, m_\ell, m_s$  for an electron in hydrogen), so two electrons with the same sets of quantum numbers are completely indistinguishable from one another.

This fact has implications for the types of wavefunctions that can describe fundamental particles. In particular: suppose we wish to write the multi-particle wavefunction  $\psi(x_A, x_B)$  that describes two particles, an electron who might be found at  $x_A$  and an electron who might be found at  $x_B$ . (We haven't carefully discussed how to write a wavefunction for multi-particle systems, but the basic idea (as you might guess) is that the total 2-particle wavefunction splits into a wavefunction for the first particle times a wavefunction for the second particle,  $\psi(x_A, x_B) = \psi_1(x_A)\psi_2(x_B)$ ). The wavefunction yields the probability density,

$P(x_A, x_B) = |\psi(x_A, x_B)|^2$ . The fact that the two electrons are indistinguishable implies that the probability of finding electron 1 at  $x_A$  and electron 2 at  $x_B$  must be **equal** to the probability of finding electron 2 at  $x_A$  and electron 1 at  $x_B$ ; in other words,

$$P(x_A, x_B) = P(x_B, x_A). \quad (3.45)$$

This of course would not have to be true if the particles were not identical.

Since  $P(x_A, x_B) = |\psi(x_A, x_B)|^2$ , this condition (3.45) says that  $|\psi(x_A, x_B)|^2 = |\psi(x_B, x_A)|^2$ , or in other words,

For any identical 2-particle wavefunction:  $\psi(x_A, x_B) = \pm\psi(x_B, x_A)$

(3.46)

We conclude that indistinguishable particles come in one of two types: particles whose wavefunctions are symmetric under exchange, *i.e.* satisfying  $\psi(x_A, x_B) = +\psi(x_B, x_A)$ , and those that are antisymmetric under exchange, satisfying  $\psi(x_A, x_B) = -\psi(x_B, x_A)$ . We call the former types of particles *bosons*, and the latter *fermions*. It is an experimental fact that electrons are fermions; their wavefunctions are antisymmetric under exchange of two particles. Other examples of fermions include quarks, neutrinos, and the composite protons. Photons are examples of bosons; other examples of bosons include gluons, and the Higgs particle.

In fact, there is a theorem called the *spin-statistics theorem* which proves that all particles with half-integer spin (like the electron, with spin 1/2) are fermions, and all particles with integer spin (like photons, with spin 0) are bosons. (Discussing this relation in more detail, however, is beyond the scope of this course.)

An immediate consequence of the fact that fermions (like electrons) have antisymmetric wavefunctions is that if a system includes two identical fermions, they cannot be in the same place: since  $\psi_f(x_A, x_B) = -\psi_f(x_B, x_A)$ , setting  $x_A = x_B$  implies that  $\psi_f(x_A, x_A) = -\psi_f(x_A, x_A)$ , which is only possible if the wavefunction is equal to 0 so that there is zero probability of finding the two identical fermions in the same location. Fermions are antisocial particles (they need their space!) while bosons are social (as many as they like can occupy the same space at the same time). This fact that we can't find two identical fermions in the same location is called the *Pauli exclusion principle*. More generally stated, the Pauli exclusion principle states that no two identical fermions can simultaneously occupy the same quantum state. It has important implications for electronic configurations in atoms.

**Electronic configurations in atoms** So far we have focused our discussion on the hydrogen atom, which is a single electron system. To talk about other types of atoms, we need to talk about multi-electron systems of multiple electrons in a Coulomb potential, with various atomic  $Z$ -factors governing how much positive charge is in the nucleus of the atom. To do so, we can approximate the electrons in multi-electron atoms as being labeled by the same quantum numbers used for hydrogen –  $(n, \ell, m_\ell, m_s)$  – except now multiple electrons can inhabit multiple different stationary states. (This approximation is basically assuming that the electrons don't interact strongly with each other, so that each one sees the Coulomb potential from the nucleus and can inhabit  $(n, \ell, m_\ell, m_s)$  stationary states accordingly.) The ground state of the atom corresponds to electrons filling subshells with the least amount of energy first, while excited states correspond to electrons filling subshells with higher energies.

Using the Pauli exclusion principle, we can explain how the electrons in multi-electron atoms in their ground state fill energy levels. Pauli exclusion implies that when electrons fill atomic shells, only one electron can occupy each state: no two electrons in an atom can have the same set of quantum numbers. For example, the 1s state can hold 2 electrons  $(1, 0, 0, \pm\frac{1}{2})$ ,

the 2s state can hold 2 electrons  $(2, 0, 0, \pm\frac{1}{2})$ , the 2p state can hold 6 electrons  $(2, 1, 0, \pm\frac{1}{2})$ ;  $(2, 1, 1, \pm\frac{1}{2})$ ;  $(2, 1, -1, \pm\frac{1}{2})$ , etc.

Let's start simple, with Helium. Helium has two electrons. The lowest available energy level is the  $n = 1$  shell, and the first possible  $\ell$  value is  $\ell = 0$ , so these 2 electrons will both occupy the 1s subshell in the ground state. Both electrons are allowed to have  $n = 1, \ell = 0, m_\ell = 0$  because they can have different spin quantum numbers: one will be spin up with  $m_s = 1/2$ , and one will be spin down with  $m_s = -1/2$ . The ground state of Helium is labeled as  $1s^2$ , to indicate that both electrons are in the 1s subshell.

Next up, Lithium, which has three electrons. The lowest available energy level,  $n = 1$ , only has two spots with unique quantum numbers:  $(n = 1, \ell = 0, m_\ell = 0, m_s = 1/2)$  and  $(n = 1, \ell = 0, m_\ell = 0, m_s = -1/2)$ . Thus, one of the three electrons will have to be in a higher energy level, with  $(n = 2, \ell = 0, m_\ell = 0, m_s = \pm 1/2)$ . Since this electronic configuration has two electrons in the 1s subshell and one in the 2s subshell, it's labeled  $1s^2 2s^1$ .

And so on. What happens once there are enough electrons to start filling the 2p subshell? Take for instance Carbon, which has 6 electrons. The ground state of Carbon will have two electrons in the 1s subshell  $(n = 1, \ell = 0, m_\ell = 0, m_s = \pm\frac{1}{2})$ , two in the 2s subshell  $(n = 2, \ell = 0, m_\ell = 0, m_s = \pm\frac{1}{2})$ , and then two more somewhere in the 2p subshell. The degeneracy of the 2p subshell is 6, since the possible quantum numbers are  $(n = 2, \ell = 1, m_\ell = 0 \text{ or } \pm 1, m_s = \pm\frac{1}{2})$  for a total of 6 possibilities. It turns out that electrons like to fill orbitals with unpaired spins, rather than orbitals with paired spins (this is called *Hund's rule*), so the two electrons will fill out orbitals with different  $m_\ell$  values.

The chemical properties of different types of atoms depend a lot on how many electrons are paired / unpaired in energy levels. For example, Hydrogen has a single electron in its 1s subshell, so the shell is not full. This lone electron tends to be easily shared with other atoms (in order to fill / empty the shell), so hydrogen is chemically active. Whereas helium has a fully filled 1s shell, so helium atoms tend to not share electrons easily with other atoms, and helium is a chemically inactive (or inert) type of atom.

—————End Lecture 25.

### Example Problem: Electrons in a box

4 electrons are placed in a 3d box, with sides of lengths  $L_1 = L_2 = 6 \text{ nm}$ , and  $L_3 = 5 \text{ nm}$ . Assume they do not interact with each other, and occupy the lowest possible energy states.

- (a) Find the total energy of this system (don't forget about spin!)
- (b) By how much does this total energy change if a magnetic field of magnitude  $10T$  is turned on in the  $z$ -direction?

*Solution:* Recall that the energy levels are given by

$$E_{n_x n_y n_z} = \frac{\pi^2 \hbar^2}{2m_e} \left( \frac{n_x^2}{L_1^2} + \frac{n_y^2}{L_2^2} + \frac{n_z^2}{L_3^2} \right)$$

Substituting for the given values of  $L_{1,2,3}$ ,

$$E_{n_x n_y n_z} = \frac{\pi^2 \hbar^2}{2m_e} \left( \frac{n_x^2}{36 nm^2} + \frac{n_y^2}{36 nm^2} + \frac{n_z^2}{25 nm^2} \right)$$

The ground state energy level is  $(n_x, n_y, n_z) = (1, 1, 1)$ . Including spin degrees of freedom  $m_s = \pm \frac{1}{2}$ , the degeneracy of this energy level is 2: one electron can be in  $(1, 1, 1)$  with spin up, and the other in  $(1, 1, 1)$  with spin down.

The first excited state is  $(n_x, n_y, n_z) = (2, 1, 1) = (1, 2, 1)$ . Therefore the degeneracy of this energy level is 4: 2 electrons can be in the  $(2, 1, 1)$  state (one of spin up, one of spin down), and two can be in the  $(1, 2, 1)$  state.

Therefore, of the four electrons, two electrons occupy the ground state, and two occupy the first excited state, one in the  $(2, 1, 1)$  state with one spin (either up or down) and one in the  $(1, 2, 1)$  state with the same spin (by Hund's rule).

$$E_{\text{total}} = 2E_{111} + E_{211} + E_{121} = 0.2 \text{ eV}.$$

To answer part (b), we use that in the presence of a magnetic field, each electron's energy gets shifted by

$$\Delta E = 2\mu_B B_z m_s$$

The two electrons in the ground state have opposite spins, so their energy shifts cancel:

$$2E_{111} \rightarrow (E_{111} + \mu_B B_z) + (E_{111} - \mu_B B_z) = 2E_{111}$$

The two electrons in the first excited state, however, have the same spin, since there was room for two electrons of the same spin but different other quantum numbers in this energy level. Their shift is:

$$E_{211} + E_{121} \rightarrow (E_{211} + \Delta E) + (E_{121} + \Delta E) = E_{211} + E_{121} + 2\Delta E$$

Therefore, the total shift is,

$$2\Delta E = 2(2 \cdot 5.8 \times 10^{-5} \text{ eV/T} \cdot 10T \cdot \frac{1}{2}) = 1.16 \times 10^{-3} \text{ eV}.$$

Is this a shift up or down? If we are asking about the *ground state* after the shift, then this will be a shift down, since that will yield the smallest possible energy configuration of the four electrons upon application of the magnetic field.

### 3.2.8 Lasers

Lasers operate off of the principle of *stimulated emission*. Suppose a system is prepared in an excited state, at an energy  $E_n$ . In order to drop down to the ground state, the system would emit a photon of energy  $E_n - E_1$ , for  $E_1$  the ground state energy. If we bombard the system with a photon of precisely this energy difference, we actually get out *two* photons of this energy. If we prepare a system in such a metastable state and bombard with photons of precisely the right energies, this leads to a chain reaction that outputs many identical photons. The output is a beam of high intensity, monochromatic, coherent light—extremely useful in applications!