

# Modern Physics

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with L<sup>A</sup>T<sub>E</sub>X



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# Modern Physics Chronology

- 1632 Galileo's *Dialogo sopra i due massimi sistemi del mondo* (Dialogue Concerning the Two Chief World Systems) contains the principle that we today call Galilean (or classical) relativity. This principle will become one of the cornerstones of Einstein's relativity.
- 1687 Isaac Newton's *Philosophiæ Naturalis Principia Mathematica* (The Mathematical Principles of Natural Philosophy) lays out his laws of motion. (Fun fact: Newton wrote  $F = p'$ , not  $F = ma$ .)
- 1804 Thomas Young's paper "Experiments and Calculations Relative to Physical Optics" describes an early form of the double-slit experiment that demonstrates the wave nature of light.
- 1861 James Maxwell's paper "On Physical Lines of Force" lays out a set of equations summarizing classical electromagnetism. Maxwell's roughly 20 equations were later combined into 4 by Oliver Heaviside.
- 1887 Albert Michelson and Edward Morley's paper "On the Relative Motion of the Earth and the Luminiferous Ether" describes their failed attempt to detect the Earth's motion through the aether.
- 1889 Johannes Rydberg's paper "Researches sur la constitution des spectres d'émission des éléments chimiques" ("Research on the Constitution of the Emission Spectra of Chemical Elements") gives a formula for the spectral lines of hydrogen and hydrogen-like atoms.
- 1897 In two papers, both entitled "Cathode Rays," J.J. Thomson announces the discovery—and measures the mass and charge—of very light, negatively charged particles that are parts of atoms. (Thomson used the word "corpuscles" for what we now call electrons.)
- 1900 Max Planck proposes quantization of cavity radiation to resolve the ultraviolet catastrophe. (He developed the ideas behind this proposal in a series of papers and talks in 1900 and 1901.)
- 1905 Albert Einstein's paper "Zur Elektrodynamik bewegter Körper" ("On the Electrodynamics of Moving Bodies") introduces his special theory of relativity. Later that year he publishes "Ist die Trägheit eines Körpers von seinem Energieinhalt abhängig?" ("Does the Inertia of a Body Depend Upon Its Energy Content?") which introduces an early form of the relation  $E = mc^2$ .
- 1905 Einstein's paper "Über einem die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Gesichtspunkt" ("On a Heuristic Viewpoint Concerning the Production and Transformation of Light") shows that the quantization of light, earlier proposed by Planck, explains the photoelectric effect.

- 1909 G.I. Taylor's paper "Interference Fringes with Feeble Light" describes performing the double-slit experiment with light of such low intensity that non-overlapping incident regions appear on the back wall, eventually forming an interference pattern.
- 1911 Ernest Rutherford's paper "The Scattering of  $\alpha$  and  $\beta$  Particles by Matter and the Structure of the Atom" proposes a nucleus of positive charge at the core of an atom, based on the gold foil experiments performed by Geiger and Marsden.
- 1912 Henrietta Swan Leavitt publishes "Periods of 25 Variable Stars in the Small Magellanic Cloud," giving a relationship between the oscillation period of Cepheid variable stars and their intrinsic brightness. This relationship was later used by Edwin Hubble to show that other galaxies exist, and later to discover the expansion of the universe. (Leavitt's paper was signed by her supervisor Edward Pickering, with a note that Leavitt had "prepared" the paper.)
- 1913 In a series of papers entitled "On the Constitution of Atoms and Molecules," Niels Bohr proposes his model of the atom, with electrons making discrete jumps between quantized energy levels.
- 1913 Henry Moseley's paper "The High-Frequency Spectra of the Elements" suggests a physical meaning to atomic number.
- 1914 James Franck and Gustav Hertz's paper "Über Zusammenstöße zwischen Elektronen und Molekülen des Quecksilberdampfes und die Ionisierungsspannung desselben" ("On Collisions Between Electrons and Molecules of Mercury Vapor and the Ionization Potential of the Same") shows evidence for quantized atomic energy levels.
- 1914 Robert Millikan's paper "A Direct Determination of  $h$ " reports his careful replication of the photoelectric effect in a vacuum—an experiment that, much to Millikan's chagrin, validated Einstein's explanation
- 1915 In the paper "Die Feldgleichungen der Gravitation" ("The Field Equations of Gravitation"), Einstein proposes his general theory of relativity, which incorporates gravity into the theory of relativity.
- 1915 Emmy Noether proves that every continuous symmetry of a physical system corresponds to a conservation law. (The proof is not published until three years later.)
- 1920 Dyson, Eddington, and Davidson's paper "A Determination of the Deflection of Light by the Sun's Gravitational Field, From Observations Made at the Total Eclipse of 29 May 1919" provides observational verification of Einstein's general theory of relativity.
- 1922 Otto Stern and Walther Gerlach demonstrate quantization of angular momentum in the paper "Der experimentelle Nachweis der Richtungsquintelung im Magnetfeld" ("The Experimental Proof of Directional Quantization in the Magnetic Field"). It was later recognized that the angular momentum they had measured was spin.

- 1923 Arthur Compton's paper "A Quantum Theory of the Scattering of X-Rays by Light Elements" describes changes in wavelength from light scattering off electrons.
- 1923 Edwin Hubble reports in the paper "Cepheids in Spiral Nebulae" measurements of distances to Cepheid variable stars in nebulae. He proves that some nebulae such as Andromeda are outside our galaxy, thus proving for the first time that anything exists outside our galaxy.
- 1924 Louis de Broglie, in his PhD thesis "Recherches sur la théorie des quanta" ("Research on Quantum Theory"), proposes matter waves.
- 1925 Wolfgang Pauli proposes the exclusion principle in the paper "Über den Einfluss der Geschwindigkeitsabhängigkeit der Elektronenmasse auf den Zeeman-Effekt" ("On the Connection Between the Termination of the Electron Groups in the Atom and the Complex Structure of the Spectra").
- 1925 Goudsmit and Uhlenbeck propose spin (intrinsic angular momentum) to explain the Stern-Gerlach results in "Ersetzung der Hypothese vom unmechanischen Zwang durch eine Forderung bezüglich des inneren Verhaltens jedes einzelnen Elektrons" ("Replacement of the Hypothesis of Nonmechanical Connection by an Internal Degree of Freedom of the Electron").
- 1926 Erwin Schrödinger's paper "Quantisierung als Eigenwertproblem" ("Quantization as an Eigenvalue Problem") presents what we now call Schrödinger's equation.
- 1926 Max Born proposes the probabilistic interpretation of wavefunctions in "Zur Quantenmechanik der Stoßvorgänge" ("On the Quantum Mechanics of Collision Processes").
- 1927 Werner Heisenberg proposes the uncertainty principle in "Über den anschaulichen Inhalt der quantentheoretischen Kinematik und Mechanik" ("About the Descriptive Content of Quantum Theoretical Kinematics and Mechanics")
- 1927 Davisson and Germer ("Diffraction of Electrons by a Crystal of Nickel") and G.P. Thomson ("Experiments on the Diffraction of Cathode Rays," published in 1928) independently demonstrate electron diffraction.
- 1928 Paul Dirac's paper "The Quantum Theory of the Electron" expands the theory of quantum mechanics to be compatible with special relativity.
- 1929 In the paper "A Relation Between Distance and Radial Velocity Among Extra-Galactic Nebulae," Edwin Hubble shows that most galaxies are receding from us at speeds proportional to their distances from us. This is now generally considered the observational discovery of the expansion of the universe.
- 1931 Georges Lemaître describes his theory of the "Primeval Atom," now known as the "Big Bang," to explain Hubble's observations: "A Homogeneous Universe of Constant Mass and Increasing Radius Accounting for the Radial Velocity of Extra-Galactic Nebulae."
- 1932 James Chadwick's paper "Existence of a Neutron" announces the discovery of the neutron.

- 1933 Carl Anderson's paper "The Positive Electron" announces the discovery of the positron (from work performed at the same lab as Chadwick's discovery of the neutron).
- 1938 Fission of uranium atoms is observed by Otto Hahn and Fritz
- 1939 Strassman, and explained and confirmed by Lise Meitner and Otto Frisch.
- 1949 The first published Feynman diagram appears in the paper "Space-Time Approach to Quantum Electrodynamics." We can't possibly choose a date when "quantum field theory was invented" but this seems like a nice symbolic milestone.
- 1957 Chien-Shiung Wu's paper "Experimental Test of Parity Conservation in Beta Decay" demonstrates that parity is not an exact symmetry.
- 1961 Claus Jönsson reports a double-slit experiment with electrons in "Elektroneninterferenzen an mehreren künstlich hergestellten Feinspalten" ("Electron Interference at Several Artificially Produced Fine Gaps").
- 1964 Murray Gell-Mann ("A Schematic Model of Baryons and Mesons") and George Zweig ("An SU(3) Model for Strong Interaction Symmetry and its Breaking") independently propose the quark model for hadrons, paving the way for the standard model of particle physics.
- 1964 John Bell's paper "On the Einstein Podolsky Rosen Paradox" demonstrates that quantum mechanics cannot be reconciled with locality.
- 1964 Robert Wilson and Arno Penzias publish "A Measurement Of Excess Antenna Temperature at 4080 Mc/s," reporting measurements of microwave radiation coming to us from all directions. This is now accepted to be the "cosmic microwave background" radiation left over from the early universe.
- 1970 Standard Model of Particle Physics. While there is no one moment when this theory was created, the main pieces that brought it into essentially its current form were developed during this time. Those pieces included a better theoretical understanding of strong forces, and the experimental confirmation of the existence of quarks.
- 1975
- 1980 Vera Rubin and her collaborators publish "Rotational Properties of 21 SC Galaxies With a Large Range of Luminosities and Radii, From NGC 4605 (R=4kpc) to UGC 2885 (R=122kpc)," reporting rotation curves of 21 galaxies that unambiguously showed the existence of dark matter. This paper was the culmination of work Rubin had published for a number of years before this.
- 1981 Alan Guth publishes "Inflationary Universe: A Possible Solution to the Horizon and Flatness Problems," introducing the theory of inflation to explain a number of puzzles in Big Bang cosmology.
- 1992 Radio astronomers Aleksander Wolszczan and Dale Frail's paper "A Planetary System Around the Millisecond Pulsar PSR1257 + 12" announces the first definitive detection of planets outside our solar system. (Thirty years later, over 5000 exoplanets have been confirmed.)

- 1998 Adam Riess and collaborators (“Observational Evidence From Supernovae for an Accelerating Universe and a Cosmological Constant”), and soon after Saul Perlmutter and collaborators (“Measurements of Omega and Lambda from 42 High Redshift Supernovae” in 1999), independently publish supernova measurements showing that the expansion of the universe is accelerating.
- 2012 Detection of the Higgs boson (“Observation of a New Particle in the Search for the Standard Model Higgs Boson with the ATLAS Detector at the LHC”) marks experimental validation of the last piece of the standard model. The paper lists approximately 3000 co-authors.
- 2016 B. P. Abbott et al’s paper “Observation of Gravitational Waves from a Binary Black Hole Merger” announces the 2015 detection of gravitational waves, as predicted by Einstein’s general theory of relativity, by the Laser Interferometer Gravitational-Wave Observatory (LIGO).
- 2021 In a series of papers, Fermilab announces the results of its “Muon g-2” experiment, showing that the measured gyromagnetic ratio (or “g-factor”) of the muon differs from theoretical prediction with a significance of 4.2 sigma. If confirmed, this measurement will be the first-ever experimental failure of the standard model of particle physics.

# Relativity

## Einstein's Postulates

1. **The principle of relativity.** The laws of physics apply in all inertial reference systems.
2. **The universal speed of light.** The speed of light in vacuum is the same for all inertial observers, regardless of the motion of the source.

## Lorentz Transformations

**Galilean transformations.** If we “start the clock” ( $t = 0$ ) at the moment the origins ( $\mathcal{O}$  and  $\bar{\mathcal{O}}$ ) coincide, then at time  $t$ ,  $\bar{\mathcal{O}}$  will be a distance  $vt$  from  $\mathcal{O}$ , and hence

$$x = d + vt$$

where  $d$  is the distance from  $\bar{\mathcal{O}}$  to  $\bar{A}$  at time  $t$ . Classically,  $d = \bar{x}$  and thus constructed the Galilean transformations:

$$\begin{aligned}\bar{x} &= x - vt \\ \bar{y} &= y \\ \bar{z} &= z \\ \bar{t} &= t\end{aligned}$$

**Lorentz transformations.** In relativity, however, there will be a modification for Galilean transformations. As mentioned earlier,  $d$  is the distance from  $\bar{\mathcal{O}}$  to  $\bar{A}$ , with the addition that it is measured by  $S$ .  $\mathcal{O}$  to  $\bar{A}$  measured by  $\bar{S}$ , however, is  $\bar{x}$  and is at rest. Therefore

$$\bar{x} = \gamma d$$

When this is inserted in Galilean Transformations, we obtain the relativistic version:

$$\bar{x} = \gamma(x - vt).$$

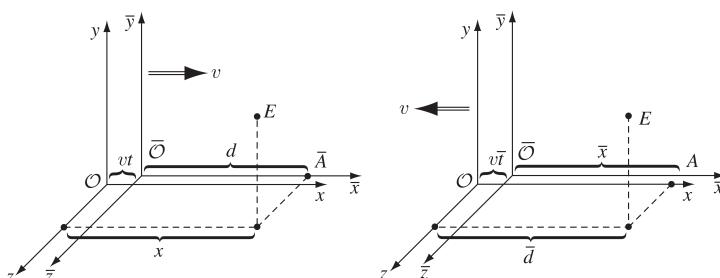


Figure: Reminder that in relativity there is no absolute velocity.  $\bar{S}$  slides along the  $x$  axis at speed  $v$  (with  $S$  being at rest) is the same as  $S$  slides along the  $x$  axis at speed  $-v$  (with  $\bar{S}$  being at rest). Of course that is assuming both systems are inertial.

Of course, we could have run the same argument from the point of view of  $\bar{S}$ . The right diagram looks similar, but in this case it depicts the scene at time  $\bar{t}$ , whereas left diagram showed the scene at time  $t$ . If we assume that  $\bar{S}$  also starts its clock when the origins coincide, then at time  $\bar{t}$ ,  $\mathcal{O}$  will be a distance  $v\bar{t}$  from  $\bar{\mathcal{O}}$ , and therefore

$$\bar{x} = \bar{d} - v\bar{t}$$

Similar as before,  $\bar{d}$  is the distance from  $O$  to  $A$  in  $\bar{S}$ , whereas  $x$  is the distance from  $\mathcal{O}$  to  $A$  in  $S$  and is at rest. Therefore

$$x = \gamma \bar{d}$$

It follows that

$$x = \gamma(\bar{x} + v\bar{t})$$

This last equation obviously be identical to the formula for  $\bar{x}$ , except for a switch in the sign of  $v$ . Nevertheless, this is a useful result, for if we substitute  $\bar{x}$ , and solve for  $\bar{t}$ , we complete the relativistic “dictionary”:

$$\bar{x} = \gamma(x - vt)$$

$$\bar{y} = y$$

$$\bar{z} = z$$

$$\bar{t} = \gamma \left( t - \frac{v}{c^2} x \right)$$

These are the famous Lorentz transformations. The reverse dictionary, which carries you from  $\bar{S}$  back to  $S$ , can be obtained algebraically by solving for Lorentz transformations  $x$  and  $t$ , or, more simply, by switching the sign of  $v$ :

$$x = \gamma(\bar{x} + v\bar{t})$$

$$y = \bar{y}$$

$$z = \bar{z}$$

$$t = \gamma \left( \bar{t} + \frac{v}{c^2} \bar{x} \right)$$

## Relativity Geometry

**The relativity of simultaneity.** Imagine a freight car, traveling at constant speed along a smooth, straight track; someone then switches the lamp on, and the light spreads out in all directions at speed  $c$ . The two events in question occur simultaneously. However, to an observer on the ground these same two events are not simultaneous. For the beam going to the back end has a shorter distance to travel than the one going forward. According to this observer, therefore, event (b) happens before event (a).

Two events that are simultaneous in one inertial system are not, in general, simultaneous in another.

Using Lorentz transformations we could also come to the sam conclusion. Suppose event A occurs at  $x_A = 0$ ,  $t_A = 0$ , and event B occurs at  $x_B = b$ ,  $t_B = 0$ . The two events are simultaneous in  $S$ . But they are

not simultaneous in  $\bar{S}$ , for the Lorentz transformations give  $\bar{x}_A = 0$ ,  $\bar{t}_A = 0$  and  $\bar{x}_B = \gamma x$ ,  $\bar{t}_B = -\gamma(v/c^2)b$ . According to  $\bar{S}$  then, B occurs before A, as before.

**Time dilation.** The time it takes for the light to leave the bulb and strike the floor of the car directly below is

$$\Delta\bar{t} = \frac{h}{c}$$

For an observer, however

$$\Delta t = \frac{\sqrt{h^2 + (v\Delta t)^2}}{c}$$

Solving for  $\Delta t$ , we have

$$\Delta t = \frac{h}{c} \frac{1}{\sqrt{1 - v^2/c^2}}$$

therefore

$$\begin{aligned}\Delta\bar{t} &= \sqrt{1 - v^2/c^2}\Delta t \\ &= \frac{1}{\gamma}\Delta t\end{aligned}$$

This is, by the way, how most textbooks introduce constant gamma in relativity. Gamma defined as

$$\gamma \equiv \frac{1}{\sqrt{1 - v^2/c^2}}$$

To derive using Lorentz transformations, Suppose that at time  $t = 0$  observer S decides to examine all the clocks in  $\bar{S}$ . He finds that they read different times, depending on their location

$$\bar{t} = -\gamma \frac{v}{c^2}x$$

Those to the left of the origin (negative x) are ahead, and those to the right are behind. S focuses his attention on a single clock at rest in the  $\bar{S}$  frame, and watches it over some interval  $\Delta t$ . Because  $\bar{x}$  is fixed, the Reverse Lorentz transformations gives

$$\Delta\bar{t} = \frac{1}{\gamma}\Delta t$$

**Lorentz contraction.** To an observer on the train, the time it takes for light signal to be sent down and back

$$\Delta\bar{t} = 2 \frac{\Delta\bar{x}}{c}$$

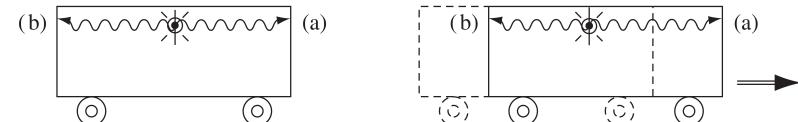
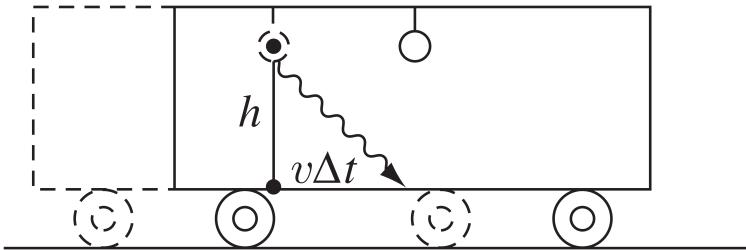


Figure: Train, freight car even



How long does it take the light to make this trip?

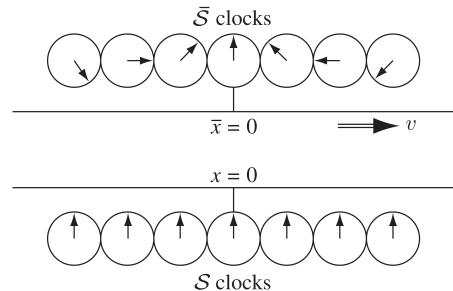


Figure: Clocks that are properly synchronized in one system will not be synchronized when observed from another system

If  $\Delta t_1$  is the time for the light signal to reach the front end, and  $\Delta t_2$  is the return time, then to an observer on the ground

$$\Delta t_1 = \frac{\Delta x + v\Delta t_1}{c} \quad \Delta t_2 = \frac{\Delta x - v\Delta t_2}{c}$$

solving for  $\Delta t_1$  and  $\Delta t_2$

$$\Delta t_1 = \frac{\Delta x}{c-v} \quad \Delta t_2 = \frac{\Delta x}{c+v}$$

So the round-trip time is

$$\Delta t = 2 \frac{\Delta x}{c} \frac{1}{1-v^2/c^2}$$

Applying time dilation formula and solving for  $\Delta x$

$$\Delta \bar{x} = \frac{1}{\sqrt{1-v^2/c^2}} \Delta x = \gamma \Delta x$$

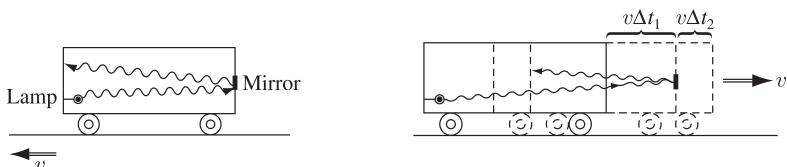


Figure: Railway carriage, if you will

Now, Imagine a stick at rest in  $\bar{S}$ . Its rest length is  $\Delta\bar{x}$ . If an observer in  $S$  were to measure the stick, he would subtract the positions of the two ends at one instant of his time  $t$ . In another word,  $t$  is fixed and Lorentz transformations give

$$\Delta\bar{x} = \gamma\Delta x$$

**Einstein's velocity addition rule.** Suppose a particle moves a distance  $dx$  (in  $S$ ) in a time  $dt$ . Its velocity  $u$  is then

$$u = \frac{dx}{dt}$$

In  $\bar{S}$ , meanwhile, it has moved a distance

$$d\bar{x} = \gamma(dx - vdt)$$

in a time

$$d\bar{t} = \gamma(dt - \frac{v}{c^2}dx)$$

The velocity in  $\bar{S}$  is therefore

$$\bar{u} = \frac{d\bar{x}}{d\bar{t}} = \frac{u - c}{1 - uv/c^2}$$

To recover the more transparent notation, let  $A$  be the particle,  $B$  be  $S$ , and  $C$  be  $\bar{S}$ ; then  $u = v_{AB}$ ,  $\bar{u} = v_{AC}$ , and  $v = v_{CB} = -v_{BC}$ , so

$$v_{AC} = \frac{v_{AB} + v_{BC}}{1 - +(v_{AB}v_{BC}/c^2)}$$

## Structure of Spacetime

**Four-vectors.** The Lorentz transformations take on a simpler appearance when expressed in terms of the quantities

$$x^0 \equiv ct \quad \beta \equiv \frac{v}{c}$$

If, at the same time, we number the  $x, y, z$  coordinates, so that

$$x^1 \equiv x \quad x^2 \equiv y \quad x^3 \equiv z$$

then the Lorentz transformations read

$$\begin{aligned}\bar{x}^0 &= \gamma(x^0 - \beta x^1) \\ \bar{x}^1 &= \gamma(x^1 - \beta x^0) \\ \bar{x}^2 &= x^2 \\ \bar{x}^3 &= x^3\end{aligned}$$

Or, in matrix form:

$$\begin{pmatrix} \bar{x}^0 \\ \bar{x}^1 \\ \bar{x}^2 \\ \bar{x}^3 \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma\beta & 0 & 0 \\ -\gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \end{pmatrix}$$

Letting Greek indices run from 0 to 3, this can be distilled into a single equation:

$$\bar{x}^\mu = \sum_{v=0}^3 \Lambda_v^\mu x^v$$

where  $\Lambda$  is the Lorentz transformation matrix in (the superscript  $\mu$  labels the row, the subscript  $v$  labels the column). (3-d) vector defined as any set of three components that transform under rotations the same way ( $x, y, z$ ) do; by extension, we now define a 4-vector as any set of four components that transform in the same manner as  $(x_0, x_1, x_2, x_3)$  under Lorentz transformations:

$$\bar{a}^\mu = \sum_{v=0}^3 \Lambda_v^\mu a^v$$

There is a 4-vector analog to the dot product, but it's not just the sum of the products of like components; rather, the zeroth components have a minus sign

$$\mathbf{A} \cdot \mathbf{B} = -a^0 b^0 + a^1 b^1 + a^2 b^2 + a^3 b^3$$

It has the same value in all inertial systems; just as the ordinary dot product is invariant (unchanged) under rotations, this combination is invariant under Lorentz transformations.

It is convenient to introduce the covariant vector  $a^\mu$ , which differs from the contravariant  $a^\mu$  only in the sign of the zeroth

$$a^\mu = (a_0, a_1, a_2, a_3) \equiv (-a^0, a^1, a^2, a^3)$$

Upper indices designate contravariant vectors; lower indices are for covariant vectors. Raising or lowering the temporal index costs a minus sign; raising or lowering a spatial index changes nothing. Formally,

$$a_\mu = \sum_{v=0}^3 g_{\mu v} a^v \quad q \equiv \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The scalar product can now be written with the summation symbol

$$\sum_{\mu=0}^3 a^\mu b_\mu$$

or, more compactly still

$$a^\mu b_\mu$$

This is called the Einstein summation convention, after its inventor, who regarded it as one of his most important contributions. Of course, we could just as well take care of the minus sign by switching to covariant  $b$

$$a^\mu b_\mu = a_\mu b^\mu = -a^0 b^0 + a^1 b^1 + a^2 b^2 + a^3 b^3$$

**The invariant interval.** The scalar product of a 4-vector with itself,

$$a^\mu a_\mu = -(a^0)^2 + (a^1)^2 + (a^2)^2 + (a^3)^2$$

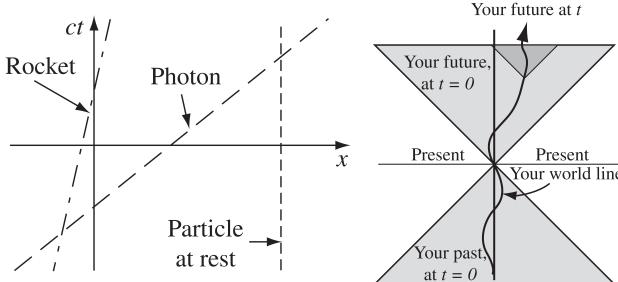


Figure: Minkowski diagrams

can be positive (if the “spatial” terms dominate) or negative (if the “temporal” term dominates) or zero:

- If  $a^\mu a_\mu > 0$ ,  $a^\mu$  is called **spacelike**
- If  $a^\mu a_\mu < 0$ ,  $a^\mu$  is called **timelike**
- If  $a^\mu a_\mu = 0$ ,  $a^\mu$  is called **lightlike**

Suppose event A occurs at  $(x_A^0, x_A^1, x_A^2, x_A^3)$  and event B at  $(x_B^0, x_B^1, x_B^2, x_B^3)$ . The difference

$$\Delta x^\mu \equiv x_A^\mu - x_B^\mu$$

is the displacement 4-vector. The scalar product of  $\Delta x^\mu$  with itself is called the invariant interval between two events:

$$\begin{aligned} I &\equiv (\Delta x)^\mu (\Delta x)_\mu = -(\Delta x^0)^2 + (\Delta x^1)^2 + (\Delta x^2)^2 + (\Delta x^3)^2 \\ &= -c^2 t^4 + d^2 \end{aligned}$$

If the displacement between two events is timelike ( $I < 0$ ), there exists an inertial system (accessible by Lorentz transformation) in which they occur at the same point. On the other hand, if the displacement is spacelike ( $I > 0$ ), then there exists a system in which the two events occur at the same time. And if the displacement is lightlike ( $I = 0$ ), then the two events could be connected by a light signal.

**Space-time diagrams.** On such a Minkowski diagrams, position plotted horizontally and time (or, better,  $x^0 = ct$ ) vertically. Velocity is then given by the reciprocal of the slope. A particle at rest is represented by a vertical line; a photon, traveling at the speed of light, is described by a 45° line; and a rocket going at some intermediate speed follows a line of slope  $c/v = 1/\beta$ .

The trajectory of a particle on a Minkowski diagram is called a world line. Because no material object can travel faster than light, your world line can never have a slope less than 1. Accordingly, your motion is restricted to the wedge-shaped region bounded by the two 45° lines. We call this your “future,” in the sense that it is the locus of all points accessible to you. as time goes on, and you move along your chosen world line, your options progressively narrow. Meanwhile, the backward wedge represents your “past,” in the sense that it is the locus of all points from which you might have come. As for the rest, this is the generalized “present.” There’s no way you can influence any

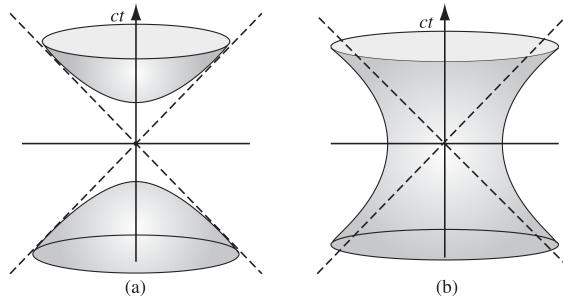


Figure: Hypercones

event in the present; it's a vast expanse of spacetime that is absolutely inaccessible to you. If we include a  $y$  axis coming out of the page, the “wedges” become cones—and, with an undrawable  $z$  axis, hypercones. Because their boundaries are the trajectories of light rays, we call them the forward light cone and the backward light cone. Your future, in other words, lies within your forward light cone, your past within your backward light cone.

Under Lorentz transformations, the interval  $I$  is preserved, and the locus of all points with a given value of  $I$  is a hyperbola—or, if we include the  $y$  axis, a hyperboloid of revolution. When the displacement is timelike, it's a “hyperboloid of two sheets”; when the displacement is spacelike, it's a “hyperboloid of one sheet.” When you perform a Lorentz transformation, the coordinates  $(x, t)$  of a given event will change to  $(\bar{x}, \bar{t})$ , but these new coordinates will lie on the same hyperbola as  $(x, t)$ . No amount of transformation will carry it, say, from the upper sheet of the timelike hyperboloid to the lower sheet, or to a spacelike hyperboloid.

If the displacement 4-vector between two events is timelike, their ordering is absolute; if the interval is spacelike, their ordering depends on the inertial system from which they are observed. In terms of the space-time diagram, an event on the upper sheet of a timelike hyperboloid definitely occurred after  $(0, 0)$ , and one on the lower sheet certainly occurred before; but an event on a spacelike hyperboloid occurred at positive  $t$ , or negative  $t$ , depending on your reference frame. Conclusion: The displacement between causally related events is always timelike, and their temporal ordering is the same for all inertial observers.

Here's some neat summary

Timelike separation	Spacelike separation	Lightlike separation
$I < 0$ $a^\mu a_\mu < 0$ The two events may or may not have a causal connection.	$I > 0$ $a^\mu a_\mu > 0$ The two events cannot have a causal connection.	$I = 0$ $a^\mu a_\mu = 0$ The two events may or may not have a causal connection.(citation needed!)

All observers will agree about the order in which the two events occurred.	Different observers will disagree about the order in which the two events occurred.	Different observers will disagree about the distance between them and the time between them, but everyone will agree that the distance equals the time multiplied by c. (source incomplete!)
There will be one reference frame in which the two events happened at the same place.	There will be one reference frame in which the two events happened at the same time.	

## Proper Time and Proper Velocity

As you progress along your world line, your watch runs slow; while the clock on the wall ticks off an interval  $dt$ , your watch only advances  $d\tau$ :

$$d\tau = \sqrt{1 - u^2/c^2} dt$$

The time  $\tau$  your watch registers (or, more generally, the time associated with the moving object) is called proper time. I'll use  $u$  for the velocity of a particular object—you, in this instance—and reserve  $v$  for the relative velocity of two inertial systems. The velocity

$$\mathbf{u} = \frac{d\mathbf{l}}{dt}$$

relative to ground (displacement divided by the time), both  $d\mathbf{l}$  and  $dt$  are to be measured by the ground observer. However there is also distance covered per unit proper time

$$\boldsymbol{\eta} \equiv \frac{d\mathbf{l}}{d\tau}$$

This hybrid quantity (distance measured on the ground, over time measured by *you*) is called proper velocity.

$$\boldsymbol{\eta} = \frac{1}{\sqrt{1 - u^2/c^2}} \mathbf{u}$$

$\eta$  is the spatial part of a 4-vector

$$\eta \equiv \frac{dx^\mu}{d\tau}$$

whose zeroth component is

$$\eta^0 = \frac{dx^0}{d\tau} = \frac{d}{d\tau} ct = \frac{c}{\sqrt{1 - u^2/c^2}}$$

Thus, for instance, when you go from system  $S$  to system  $\bar{S}$ , moving at speed  $v$  along the common  $x\bar{x}$  axis,

$$\begin{aligned}\bar{\eta}^0 &= \gamma(\eta^0 - \beta\eta^1) \\ \bar{\eta}^1 &= \gamma(\eta^1 - \beta\eta^0) \\ \bar{\eta}^2 &= \eta^2 \\ \bar{\eta}^3 &= \eta^3\end{aligned}$$

More generally

$$\bar{\eta}^\mu = \Lambda_v^\mu \eta^v$$

$\eta^\mu$  is called the proper velocity 4-vector, or simply the 4-velocity. By contrast, the transformation rule for ordinary velocities  $\mathbf{u}$  is quite cumbersome. The reason for the added complexity is plain: we're obliged to transform both the numerator  $d\mathbf{l}$  and the denominator  $dt$ , whereas for proper velocity, the denominator  $d\tau$  is invariant, so the ratio inherits the transformation rule of the numerator alone.

$$\begin{aligned}\bar{u}_x &= \frac{d\bar{x}}{d\bar{t}} = \frac{u_x - v}{1 - vu_x/c^2} \\ \bar{u}_y &= \frac{d\bar{y}}{d\bar{t}} = \frac{u_y}{\gamma(1 - vu_x/c^2)} \\ \bar{u}_z &= \frac{d\bar{z}}{d\bar{t}} = \frac{u_z}{\gamma(1 - vu_x/c^2)}\end{aligned}$$

**Relativistic Energy and Momentum.** Relativistic momentum of an object of mass  $m$  traveling at (ordinary) velocity  $\mathbf{u}$

$$p \equiv m\eta = \frac{m\mathbf{u}}{\sqrt{1 - u^2/c^2}}$$

Relativistic momentum is the spatial part of a 4-vector

$$p^\mu \equiv m\eta^\mu$$

with temporal component

$$p^0 = \frac{mc}{\sqrt{1 - u^2/c^2}}$$

Einstein identified  $p^0c$  as relativistic energy

$$E \equiv \frac{mc^2}{\sqrt{1 - u^2/c^2}}$$

Notice that the relativistic energy is nonzero even when the object is stationary; we call this rest energy:

$$E_{\text{rest}} \equiv mc^2$$

The remainder, which is attributable to the motion, is kinetic energy

$$E_{\text{kin}} \equiv E - mc^2 = mc^2 \left( \frac{1}{\sqrt{1 - u^2/c^2}} - 1 \right)$$

So far, this is all just notation. The physics resides in the experimental fact:

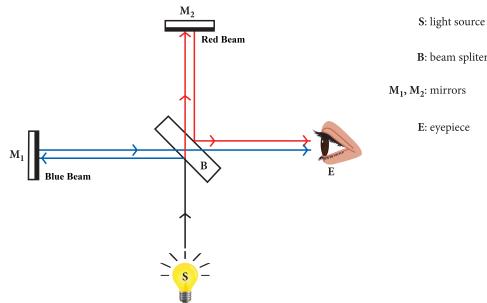


Figure 1: Michelson-Morley Experiment

In every closed system, the total relativistic energy and momentum are conserved.

Mass, however, is not conserved. Specifically , mass is invariant but not conserved; energy is conserved but not invariant; electric charge is both conserved and invariant; velocity is neither conserved nor invariant. Note the distinction between an invariant quantity (same value in all inertial systems) and a conserved quantity (same value before and after some process).

The scalar product of  $p^\mu$  with itself is

$$p^\mu p_\mu = -(p^0)^2 + (\mathbf{p} \cdot \mathbf{p}) = -m^2 c^2$$

In terms of the relativistic energy and momentum

$$E^2 - p^2 c^2 = m^2 c^4$$

For massless and relativistic particle

$$E = pc$$

**Michelson-Morley Experiment.** You already know the story of aether wind and how this experiment disprove that model, so i'll omit that and focus on this experiment itself. The Michelson interferometer is represented in Figure 1. Light from a single source reaches a half-silvered mirror and splits into two beams traveling at right angles to each other. The beams reach mirrors that send them back to the splitter, where they travel together to an eyepiece. There are three possibilities that determine whether or not the two beams arrive in phase at the end of the eyepiece:

1. If the two paths are identical in length, and the two beams travel identical speeds, then the two beams are in phase, and the interference is constructive.
2. If the two paths are different lengths, then the beams may therefore arrive out of phase.
3. If the two paths are identical lengths but are traveled at different speeds, then the two beams may be out of phase.

Now suppose the Earth is traveling along the horizontal axis from  $M_1$  to  $B$ . The aether model predicts that for part of the trip the blue beam

is going faster, and for part of the trip the red beam is going faster. But these two effects do not fully cancel out, and even if the two path lengths are identical, the beams will arrive out of phase.

After measuring the type of interference they observed, they rotated the entire apparatus. A uniform rotation does not change the geometry of the experiment; whatever phase change was caused by differences in path length is still exactly the same as it was. But a phase change caused by differences in speed, due to orientation with respect to the aether wind, will change.

So the experiment was not to see whether the two beams constructively or destructively interfered on the wall, since such interference might have multiple causes. Rather, they looked to see how the interference pattern changed as they rotated the device.

The result is, as you know it, their experiment found no evidence at all that the two beams had traveled at different speeds. Michelson wrote in a letter that the result was “decidedly negative.” Even allowing for measurement errors, his experiment seemed to show that “the relative velocity [of the Earth and the aether] is less than one sixth of the Earth’s velocity.”

## Appendix

**Relativistic kinematics.** For first example, we will discuss relativistic collision. In relativity an isolated system always conserves both momentum and energy.

Two lumps of clay, each of (rest) mass  $m$ , collide head-on at  $3/5c$ . They stick together. Question: what is the mass ( $M$ ) of the composite lump?

In this case conservation of momentum is trivial: zero before, zero after. The energy of each lump prior to the collision is

$$\frac{mc^2}{\sqrt{1 - (3/5)^2}} = \frac{4}{5}mc^2$$

and the energy of the composite lump after the collision is  $Mc^2$  (since it's at rest). So conservation of energy says

$$\frac{4}{5}mc^2 + \frac{4}{5}mc^2 = Mc^2$$

and hence

$$M = \frac{5}{2}m$$

Thus collision mass is greater than the sum of the initial masses, because mass was not conserved in this collision; kinetic energy was converted into rest energy, so the mass increased.

**Pair creation.** Next example will discuss pair creation.

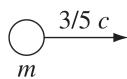
A pion at rest decays into a muon and a neutrino. Find the energy of the outgoing muon, in terms of the two masses,  $m_\pi$  and  $m_\mu$  (assume  $m_\nu = 0$ )

In this case,

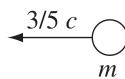
$$\begin{aligned} E_{\text{before}} &= m_\pi c^2 & \mathbf{p}_{\text{before}} &= 0 \\ E_{\text{after}} &= E_\mu + E_\nu & \mathbf{p}_{\text{after}} &= \mathbf{p}_\mu + \mathbf{p}_\nu \end{aligned}$$

Conservation of momentum requires that  $\mathbf{p}_v = -\mathbf{p}_\mu$ . Conservation of energy says that

$$E_\mu + E_\nu = m_\pi c^2$$



(before)



(after)

Figure: Inelastic collision, which (Classically) defined as a collision in which energy is not conserved, but momentum does.

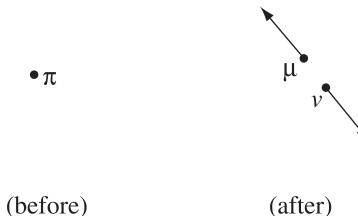


Figure: Pair Creation

Now,  $E_v = |\mathbf{p}_v|c$  and  $|\mathbf{p}_\mu| = \sqrt{E_\mu^2 - m_\mu^2 c^4}/c$ . So,

$$\begin{aligned} E_\mu + \sqrt{E_\mu^2 - m_\mu^2 c^4} &= m_\pi c^2 \\ \sqrt{E_\mu^2 - m_\mu^2 c^4} &= m_\pi c^2 - E_\mu \\ E_\mu^2 - m_\mu^2 c^4 &= E_\mu^2 + m_\pi^2 c^4 - 2E_\mu m_\pi c^2 \\ 2E_\mu m_\pi c^2 &= (m_\pi^2 + m_\mu^2)c^4 \\ E_\mu &= \frac{(m_\pi^2 + m_\mu^2)c^2}{2m_\pi} \end{aligned}$$

We call the collision elastic if kinetic energy is conserved. In such a case the rest energy (being the total minus the kinetic) is also conserved, and therefore so too is the mass. In practice, this means that the same particles come out as went in.

**Compton scattering.** Those two examples were inelastic processes; the next one is elastic.

A photon of energy  $E_0$  “bounces” off an electron, initially at rest. Find the energy  $E$  of the outgoing photon, as a function of the scattering angle  $\theta$

Conservation of momentum in the “vertical” direction gives  $p_e \sin \phi = p_p \sin \theta$ . Since  $p_p = E/c$

$$\sin \phi = \frac{E}{cp_e} \sin \theta$$

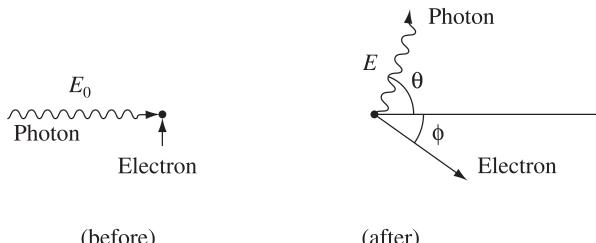


Figure: Pair Creation

Conservation of momentum in the “horizontal” direction gives

$$\begin{aligned}\frac{E_0}{c} &= p_p \cos \theta + p_e \cos \phi \\ &= \frac{E}{c} \cos \theta + p_e \sqrt{1 - \left(\frac{E}{cp_e} \sin \theta\right)^2} \\ (E_0 - E \cos \theta)^2 &= p_e^2 c^2 - E^2 \sin^2 \theta \\ p_e^2 c^2 &= E_0^2 + E^2 \cos^2 \theta - 2EE_0 \cos \theta + E_0^2 \sin^2 \theta \\ &= E^2 + E_0^2 - 2EE_0 \cos \theta\end{aligned}$$

where  $\cos \phi$  obtained from Phytagorean identity. Finally, conservation of energy says that

$$\begin{aligned}E_0 + mc^2 &= E + E_e \\ &= E + \sqrt{m^2 c^4 + p_e^2 c^2} \\ &= E + \sqrt{m^2 c^4 + E^2 + E_0^2 - 2EE_0 \cos \theta}\end{aligned}$$

Next, we solve for  $E$

$$(E_0 - E)^2 = E^2 + E_0^2 + m^2 c^4 + E_0^2 - 2EE_0 \cos \theta$$

expanding the term in parenthesis

$$\begin{aligned}E^2 + E_0^2 + m^2 c^4 - 2EE_0 - 2Emc^2 + 2E_0 mc^2 \\ = E^2 + E_0^2 + m^2 c^4 + E_0^2 - 2EE_0 \cos \theta\end{aligned}$$

The first three terms cancel, thus

$$-2EE_0 - 2Emc^2 + 2E_0 mc^2 = -2EE_0 \cos \theta$$

Finally,

$$\begin{aligned}\frac{mc^2}{E} - \frac{mc^2}{E_0} - 1 &= -\cos \theta \\ \frac{E}{mc^2} &= \frac{1}{1 - \cos \theta + mc^2/E_0} \\ E &= \frac{1}{(1 - \cos \theta)/mc^2 + 1/E_0}\end{aligned}$$

The answer looks nicer when expressed in terms of photon wavelength

$$E = hv = \frac{h\lambda}{c}$$

Then,

$$\begin{aligned}\frac{hc}{\lambda} &= \frac{1}{(1 - \cos \theta)/mc^2 + \lambda_0/hc} \\ \frac{\lambda}{hc} &= \frac{1}{mc^2}(1 - \cos \theta) + \frac{\lambda_0}{hc}\end{aligned}$$

So

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

The quantity  $(h/mc)$  is called the Compton wavelength of the electron.

# Quantum Mechanics

## Orthodox Interpretation of Quantum Mechanics

From Young's experiment, we saw bright bands (lots of light) and dark bands (no light). The patch is being hit by light waves from both slits, out of phase with each other, causing destructive interference. The explanation relies on the fact that light waves spread out through space, traveling through both slits at once.

The one photon at a time double-slit experiment result however suggest that photon is a particle that able to interfere with itself. The interference pattern has a clear mathematical implication: a wave is spreading out from the two slits and then interfering with itself. But, what is waving? The classical answer is that an electric field and a magnetic field are both oscillating, and a high amplitude of the wave corresponds to high strengths of these two fields. But that answer would never lead to an individual spot at one point on the back wall. In 1926, Max Born proposed that the wave represents probabilities. A photon is a particle that hits the back wall in a particular spot, but associated with that particle is a wave that determines the probabilities of measuring that photon at various positions.

The orthodox interpretation (Copenhagen interpretation) says that the particle exists as a wave, spread out throughout space, until the moment you measure it. At that moment the wave "collapses" into a state of being in one particular place.

## Photoelectric Effect

Consider two metal plates in a vacuum. Plate B is large and is bent around Plate A. Voltage source sets up a potential difference such that  $V_A > V_B$ . Due to potential difference, electrons on Plate A are certainly not going to jump to Plate B. Now suppose that we shine a beam of ultraviolet light onto Plate A. Such a beam can transfer energy to electrons in the metal, and an electron that absorbs enough energy will escape from the metal entirely.

The required energy  $w$  for an electron to initially escape Plate A depends on how tightly bound the electron is to its atom, and on how close it is to the surface. After escaping Plate A, the electron will need to fight the electric field; the required kinetic energy for a charge  $e$  to cross a voltage gap  $V$  is  $eV$ . Thus, total energy required for an electron to escape Plate A and reach Plate B is

$$E_{A \rightarrow B} = w + eV$$

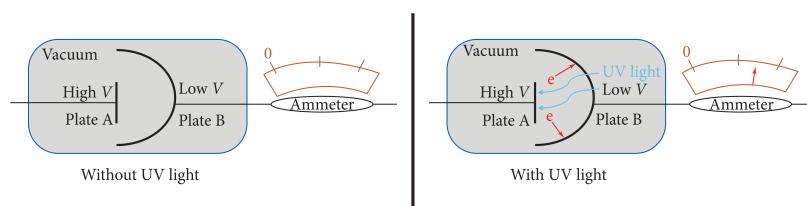


Figure: Photoelectric experiment

Only the ones with  $K \geq Ve$  make it to Plate B; if the maximum kinetic energy of any escaped electron is below  $eV$  then the current stops completely. So by increasing the potential gap until we find the potential difference that stops all current  $V_0$ , we can calculate the maximum kinetic energy with which any electron leaves Plate A

$$K_{\max} = eV_0$$

We will show the result of the experiment, and the we will compare how classical electrodynamics versus quantum mechanics prediction; which, as you know, classical electrodynamics got some wrong.

1. Intensity of the light proportional to the resulting current.
2.  $K_{\max}$  is independent of the light intensity.
3.  $K_{\max}$  is a function of frequency: electrons liberated by high-frequency light have more kinetic energy than electrons liberated by low-frequency light. Furthermore, there is a cutoff frequency; in which light below this frequency liberates no electrons.
4. No time lag is observed, no matter how low the intensity of the radiation.

Classically, the energy of that wave is a function of its intensity, which is to say, of the amplitude. The amount electron liberated, thus current, therefore proportional to that wave energy, thus intensity. Classical electrodynamics, however, only able to correctly predict that first item. Wrong classical electrodynamics are as follow:  $K_{\max}$  increase at higher intensities; frequency of the light have no effect on  $K_{\max}$ ; and a dim light should take a while to impart enough energy to liberate an electron, so there should be a measurable time lag before any current is detected.

Quantum mechanics, however, able correctly predict and explain the experiment. For the first item, according to quantum mechanics, a higher intensity beam has more photons per second, so more electrons get knocked out.

There is a minimum possible value of  $w$ , for the electrons nearest the surface and most lightly bound to their atoms. That value,  $w_0$ , is called the work function of the material on Plate A. The electrons that are easiest to knock free require a total energy  $w_0 + eV$  to reach Plate B. If  $h\nu$  is lower than  $w_0 + eV$  then no electrons cross the gap to Plate B. This explains the cutoff frequency that is seen in experiment but is impossible to explain classically. For the lack of time lag, quantum mechanics explains that some electrons get hit by a photon and instantly receive energy  $h\nu$ , while others aren't hit and receive zero energy; so as soon as photons strike Plate A, electrons are liberated.

## Atomic Models

**Thomson's model.** In 1897, J. J. Thomson showed that atoms contain electrons, negatively charged particles much smaller and lighter than the atoms themselves. Since atoms are generally neutral, there had to be something to cancel that negative charge, and to account for most of the mass of the atoms. In 1904, Thomson proposed that the electrons in an atom were embedded in a uniform spherical distribution

of positive charge; this description is called the plum pudding model of the atom because the electrons are distributed in the atom like raisins in a plum pudding.

**Rutherford's model.** That model was conclusively disproven in 1911 when Ernest Rutherford fired high-energy alpha particles at a thin gold foil. Electrons are too light to significantly deflect alpha particles, so any observed deflection resulted from interactions with the positive charges in the atom. Rutherford observed some alpha particles recoiled at angles greater than 90 degrees, which would have been essentially impossible in Thomson's model.

Rutherford concluded that instead of being embedded in a diffuse medium of positive charge, the electrons must orbit about a tiny ball of positive charge that he called the nucleus. An alpha particle that happens to strike almost exactly next to this small, dense nucleus experiences a large force and can recoil at a large angle.

But Rutherford's model faced two important problems. The first problem is stability. As you know, any orbiting object has a centripetal acceleration, thus lose energy and rapidly spiral into the nucleus. In fact, Maxwell's equations predict that a Rutherford-style hydrogen atom should last about  $10^{-12}$  s. The second problem is atomic spectra.

**Bohr's Model.** Bohr's model described electrons orbiting a nucleus in circular orbits have quantized orbit and angular momentum equal to  $nh/(2\pi)$ . Electrons can jump discontinuously between allowed orbits. Such a jump will emit or absorb a photon whose energy is precisely the difference between the energies of those two orbits. Bohr's rule for quantized angular momentum quantized energy

$$E_n = -\frac{m_e e^4}{24(\pi \epsilon_0)^2 \hbar^2} \frac{1}{n^2} = -\frac{1}{n^2} \text{Ry}$$

and quantized radius

$$r = \frac{\pi \epsilon_0 \hbar^2}{m_e e^2} n^2 = a_0 n^2$$

with  $\hbar = h/(2\pi)$ . The energy unit "rydberg" (Ry) is roughly equal to 13.6 eV. The distance  $a_0$ , called the "Bohr radius," is about half an angstrom, or  $5 \times 10^{-11}$  m.

Negative sign in the energy formula caused by potential energy; which defined to be 0 when the electron is infinitely far away from the nucleus. Potential energy increases as you move away from the nucleus, which makes the potential energy negative at all finite distances. If the total energy  $E = U + K$  is positive, the electron has enough energy to leave the atom completely, so for any orbiting electron  $E$  will be negative.

An electron dropping from level  $n_2$  to level  $n_1$  will emit photons with the frequencies predicted by the Rydberg formula. The Lyman series comes from electrons dropping from any of the higher levels into the ground state or  $n = 1$ , the Balmer series comes from electrons dropping from higher levels into  $n = 2$ , the Paschen series comes from electrons dropping from higher levels into  $n = 3$ , the Brackett series

comes from electrons dropping from higher levels into  $n = 4$ , the Pfund series comes from electrons dropping from higher levels into  $n = 4$ .

## Atomic Spectra

If you run a large electrical current through a tube filled with gas, the current gives energy to the atoms of that gas. The atoms then release that energy as electromagnetic radiation. If you put that radiation through a prism you find that it is not a uniform rainbow of colors. These colored lines are called “emission lines.” Each element emits a unique pattern known as its “emission spectrum.” The spatial frequencies of the emission lines of hydrogen are given by

$$f = \frac{1}{\lambda} = R_H \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Here  $n_1$  can be any positive integer and  $n_2$  can be any integer larger than  $n_1$ . Rydberg constant for hydrogen  $R_H = 1.10 \times 10^7 \text{ m}^{-1}$ . The frequency (defined as one over the oscillation period  $T$ ) of each line is  $\nu = cf$ .

## Matter Waves

Every particle has an associated “matter wave” with wavelength  $\lambda = h/p$ . Sometimes people use “de Broglie relations” in the plural: the  $\lambda = h/p$ , and also the equation  $E = h\nu$  relating the total relativistic energy of a particle to its frequency. Note that the first involves a wavelength in space, the second a frequency in time.

## Wavefunctions

A particle moves through space as a wave that exists simultaneously throughout an extended region. Knowing the wavefunction does not in general allow you to predict the outcomes of measurements of the particle, instead it allows you to predict the probabilities of different measurements.

**Probability.** For a discrete universe, is the probability of finding the particle at  $x$  is

$$P(x) = |\psi(x)|^2$$

For a continuous distribution

$$P(a \leq x \leq b) = \int_a^b |\psi|^2 dx$$

the integral gives the probability of finding the particle between those two points. Notice that it's not probability, but a probability density.

**Normalization.** A distribution in which all the probabilities add up to 1 is said to be “normalized.”

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

Any valid probability distribution must be normalized.

**Expectation values.** In statistics the average you expect to get from measuring the same thing many times is called the “expectation value” of that measurement. For discrete universe

$$\langle x \rangle = \sum_x x P(x)$$

for continuous universe

$$x = \int_{-\infty}^{\infty} x |\psi|^2 dx$$

applies to any discrete normalized probability distribution  $P(x)$

## Schrödinger's Equations

**Energy Eigenstates.** If a particle's wavefunction  $\psi$  is an “energy eigenstate” (also called “energy eigenfunction”), then the particle has a definite energy. That is, there is a 100 % chance of finding that particular energy, and zero chance of finding any other. That particular energy is called the “eigenvalue” of that “eigenstate.”

**Energy Probabilities.** Suppose a system has energy eigenstates  $\psi_1, \psi_2, \dots$ , with associated eigenvalues  $E_1, E_2, \dots$ . If the system's wavefunction is

$$\psi(x) = c_1 \psi_1 + c_2 \psi_2 + \dots$$

then the probability of measuring energy  $E_n$  is  $|c_n|^2$ .

**In one dimension.** If a particle with mass  $m$  is in a potential energy field  $U(x)$ , its energy eigenstates are the solutions to the time-independent Schrödinger equation,

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

The solution to this equation is not one function  $\psi(x)$  but many different functions, each corresponding to a different value of the constant  $E$ . Each such solution is an eigenfunction, representing the state of the system with definite energy  $E$  (its eigenvalue). What the time-independent Schrödinger equation tells you is which of those possible wavefunctions are energy eigenstates, not what the wavefunction can be. In fact, the wavefunction of any particle can be anything, as long as it everywhere continuous, everywhere differentiable, and properly normalized.

The time-dependent Schrödinger equation in 1D

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

Solving Schrödinger's equation we are able to derive both the time-independent equation and the rule for time evolution of wavefunction.

**In three dimensions.** The time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x) + U(x)\psi(x) = E\psi(x)$$

The time-dependent Schrödinger equation

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

## Time Evolution

Suppose at time  $t = 0$  a particle is in energy eigenstate  $\psi(x, 0)$  with energy eigenvalue  $E_n$ . That is,

$$\Psi(x, 0) = \psi_n(x)$$

Assuming the potential energy field doesn't change, the particle's wavefunction at any later time  $t$  will be given by

$$\Psi(x, t) = \psi_n(x)e^{-iE_nt/\hbar}$$

Every continuous, differentiable, normalizable function can be written as a sum of energy eigenstates. So no matter what your initial wavefunction  $\psi(x, 0)$  is, you can write it in the form

$$\psi(x) \sum_n^\infty C_n \psi_n(x)$$

its time evolution is then

$$\Psi(x, t) = \sum_n^\infty C_n \psi_n(x)e^{-iE_nt/\hbar}$$

If  $\Psi(x, 0) = \psi_n(x)$  is an energy eigenstate with eigenvalue  $E_n$ , then

$$\Psi(x, t) = \psi_n(x)e^{-iE_nt/\hbar}$$

For a sum or integral over energy eigenstates, apply this rule to each individual eigenstate.

## Fourier Transforms and Momentum

The momentum eigenstate is

$$\psi(x) = Ce^{ikx}$$

with eigenvalue

$$p = \hbar k$$

Note that it is the same as the eigenstates of energy of a free particle, but energy eigenstates depend on the forces acting on a particle: that is, they depend on the potential energy function. In the first place, we get the eigenstates of the free particle by solving Schrödinger equation with  $U(x) = 0$ . Momentum eigenstates and eigenvalues, by contrast, are always the same.

Rewrite  $\psi(x)$  using a Fourier transform, the probability of finding a particle's momentum between  $p = \hbar k_1$  and  $p = \hbar k_2$

$$\int_{k_1}^{k_2} |\hat{\psi}(k)|^2 dk$$

Unlike its energy equivalent, momentum uses single integral. The functions  $e^{ix}$  and  $e^{-ix}$  are eigenstates of momentum, and they are also eigenstates of energy for a free particle.

Fourier transforms

$$\begin{aligned}\psi(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\psi}(k) e^{ikx} dk \\ \hat{\psi}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx\end{aligned}$$

The constants in front of these formulas are chosen so that if the position distribution is properly normalized then the momentum distribution is too, and vice versa.

## The Heisenberg Uncertainty Principle

Consider a large number of particles, all prepared with identical wavefunctions  $\psi(x)$ . A quantity  $Q$  is measured for all these particles. The uncertainty  $\Delta Q$  is defined as the standard deviation of those measurements (sometimes written  $\sigma Q$ ). The formula for standard deviation inside

$$\sigma Q = \sqrt{\frac{1}{N} \sum_N (\langle x \rangle x_n)^2}$$

The general relationship between position and momentum uncertainties can be derived from the mathematics of Fourier transforms

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

A Gaussian wavefunction  $\Psi(x) = Ae^{-k(x-x_0)^2}$  achieves the minimum allowable uncertainty  $\Delta x \Delta p = \hbar/2$ . Other wavefunctions have higher values of  $\Delta x \Delta p$ .

Another relation is the time-energy uncertainties principle

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

$\Delta E$  is straightforward enough: prepare a bunch of particles with identical wavefunctions, measure their energies, and see how much the results differ from the average. Roughly speaking,  $\Delta t$  is the amount of time that it takes for any property of a system to change appreciably. If the system is oscillating,  $\Delta t$  is roughly equal to the oscillation period. If some property of the system is decaying (or growing) exponentially,  $\Delta t$  is roughly the time it takes for it to reduce its value in half (or double it).

The smaller the uncertainty in a particle's energy, the longer it takes the particle's properties to change. States of definite energy are therefore "stationary states," meaning they don't change.

# Infinite Square Well

## One dimension.

A particle can move with no forces in the region  $0 < x < L$ , but cannot move anywhere outside that region. To trap the particle in this region we need the potential energy to rise steeply at the edges. In the limit where we assume it is physically impossible for the particle to escape, the potential energy everywhere outside the region would be infinitely high. In other words,  $U = \infty$  for  $x < 0$  and  $x > L$ .

In the regions  $x < 0$  and  $x > L$ , where  $U = \infty$ , the only possible solution to Schrödinger's equation is  $\psi(x) = 0$ . In  $0 < x < L$ , where  $U = 0$ ,

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

with solution

$$\psi(x) = A \sin\left(\frac{\sqrt{2mE}}{\hbar}x\right) + B \cos\left(\frac{\sqrt{2mE}}{\hbar}x\right)$$

Reminder that wavefunctions must be differentiable, and it must be normalized. However, this wavefunction are going to violate one of these conditions because they will not be differentiable at the boundaries, but still continuous. In order to achieve that, we must make the solution go to zero at both  $x = 0$  and  $x = L$ . Imposing boundary condition  $\psi(x) = 0$ , we see that  $B = 0$ , thus

$$\psi(x) = A \sin\left(\frac{\sqrt{2mE}}{\hbar}x\right)$$

Imposing the second boundary condition  $\psi(L) = 0$ , and considering that sinus function goes to zero at  $n\pi$ ,

$$\frac{\sqrt{2mE}}{\hbar} = n\pi$$

Therefore, the energy eigenvalue of our particle

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

and the energy eigenstate

$$\psi(x) = \begin{cases} 0 & x \leq 0 \\ \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) & 0 < x < L \\ 0 & x \geq L \end{cases}$$

where normalization requires  $A = \sqrt{2/L}$

**Three dimension.** Energy eigenstates particle inside infinite square well is

$$\psi_{abc}(x, y, z) = \sqrt{\frac{8}{L^3}} \sin\left(\frac{a\pi}{L}x\right) \sin\left(\frac{b\pi}{L}y\right) \sin\left(\frac{c\pi}{L}z\right)$$

while its energy eigenvalue

$$E_{abc} = \frac{\pi^2 \hbar^2}{2mL^2} (a^2 + b^2 + c^2)^2$$

## Simple Harmonic Oscillator

A classical analysis of the mass-on-spring system starts with Hooke's law,  $F = -kx$ , which becomes a differential equation

$$\frac{d^2x}{dt^2} = -\frac{k}{m}x$$

with general solution

$$x = A \sin\left(\sqrt{\frac{k}{m}}t\right) + B \cos\left(\sqrt{\frac{k}{m}}t\right)$$

The corresponding potential energy is  $U = (1/2)kx^2$ . The general solution shows that potential energy field will oscillate with angular frequency  $\omega = \sqrt{k/m}$ . Thus, simple harmonic oscillator can be defined by the potential energy function  $U(x) = (1/2)m\omega^2x^2$ . The energy eigenvalues are

$$E_n = (n + \frac{1}{2})\hbar\omega$$

for non-negative integers n. The corresponding eigenstates are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

where  $H_n(x)$  is a "Hermite polynomial," defined as

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} \left(e^{x^2}\right)$$

The eigenstates of harmonic oscillator at ground state is

$$\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

with energy eigenvalue

$$E_0 = \frac{1}{2}\hbar\omega$$

while its eigenstates at first excited state inside

$$\psi_1 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}} x \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

with energy eigenvalue

$$E_1 = \frac{3}{2}\hbar\omega$$

## Finite Square Well

A particle can move with no forces in the region  $0 < x < L$ , just like in infinite square well. However, it is not impossible for the particle to escape; the potential energy everywhere outside the region would be  $U_0$ . In other words,  $U = U_0$  for  $x < 0$  and  $x > L$ .

The Schrödinger equation and its solution inside the well are the same as they were for the infinite square well

$$\frac{d\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

with solution

$$\psi(x) = A \sin\left(\frac{\sqrt{2mE}}{\hbar}x\right) + B \cos\left(\frac{\sqrt{2mE}}{\hbar}x\right)$$

For outside the well,

$$\frac{d\psi}{dx^2} = -\frac{2m(E - U_0)}{\hbar^2}\psi$$

with real solution for  $E < U_0$

$$\psi(x) = C \exp\left(x \frac{\sqrt{2m(E - U_0)}}{\hbar}\right) + D \exp\left(-x \frac{\sqrt{2m(E - U_0)}}{\hbar}\right)$$

in the region  $x \geq L$  we have to set  $C = 0$ , while in the  $x \leq 0$  we have to set  $D = 0$ . We have now arrived at the real-valued solution for a particle in a finite square well with  $E < U_0$

$$\psi(x) = \begin{cases} C \exp\left(x \frac{\sqrt{2m(E - U_0)}}{\hbar}\right) & x \leq 0 \\ A \sin\left(\frac{\sqrt{2mE}}{\hbar}x\right) + B \cos\left(\frac{\sqrt{2mE}}{\hbar}x\right) & 0 < x < L \\ D \exp\left(-x \frac{\sqrt{2m(E - U_0)}}{\hbar}\right) & x \geq L \end{cases}$$

Unfortunately, the equation can't be solved analytically. But you can solve three of these boundary conditions to eliminate three of the arbitrary constants, leaving just one constant  $A$  in front of all the solutions. Also note that the wavefunction must be continuous, differentiable, and normalized.

Continuity at  $x = 0$  demands

$$C = B$$

and at  $x = L$

$$D \exp\left(-L \frac{\sqrt{2m(E - U_0)}}{\hbar}\right) = A \sin\left(\frac{\sqrt{2mE}}{\hbar}L\right) + B \cos\left(\frac{\sqrt{2mE}}{\hbar}L\right)$$

Differentiability requires that their first derivatives also match. Differentiating the solutions and then plugging in  $x = 0$

$$C \frac{\sqrt{2m(E - U_0)}}{\hbar} = \frac{A \sqrt{2mE}}{\hbar}$$

plugging  $x = L$

$$\begin{aligned} -D \frac{\sqrt{2m(E - U_0)}}{\hbar} \exp\left(-L \frac{\sqrt{2m(E - U_0)}}{\hbar}\right) \\ = \frac{A \sqrt{2mE}}{\hbar} \cos\left(\frac{\sqrt{2mE}}{\hbar}L\right) - \frac{B \sqrt{2mE}}{\hbar} \sin\left(\frac{\sqrt{2mE}}{\hbar}L\right) \end{aligned}$$

The last condition is normalization

$$\int_{-\infty}^0 C^2 \exp\left(2x \frac{\sqrt{2m(E-U_0)}}{\hbar}\right) dx + \int_0^L \left[ A \sin\left(\frac{\sqrt{2mE}}{\hbar}x\right) + B \cos\left(\frac{\sqrt{2mE}}{\hbar}x\right) \right]^2 dx + \int_L^\infty D^2 \exp\left(-2x \frac{\sqrt{2m(E-U_0)}}{\hbar}\right) dx = 1$$

## Free Particles

A free particle can be defined by the potential energy function  $U(x) = 0$ . The energy eigenstate of a free particle is

$$\psi(x) = Ce^{ikx}$$

with eigenvalue

$$E = \frac{k^2\hbar^2}{2m}$$

Eigenstate with time evolution is

$$\Psi(x, t) = Ce^{i(kx - \omega t)} = Ce^{i(px - Et)/\hbar}$$

Watch the signs, for example  $e^{ix}$  and  $e^{-ix}$  are different wavefunctions that correspond to the same energy; the former represents a wave moving to the right, the latter to the left. This suggest that the energy eigenstate of a free particle is a traveling wave, where

$$\omega = \frac{E}{\hbar} = \frac{k^2\hbar}{2m}$$

and travels with velocity

$$v = \omega/k$$

The free-particle eigenstates can't be normalized, so it's impossible for a particle to be in one of those states. Regardless, we could still express the wavefunction as a sum of those eigenstates. Suppose we could express a wavefunction as a sum of eigenstates, we write a wavefunction as an integral over those eigenstates. This technique is called a "Fourier transform." For any normalized wavefunction  $\psi(x)$  it is possible to find a function  $\hat{\psi}(k)$  such that both of the following equations hold:

$$\begin{aligned} \psi(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\psi}(k) e^{ikx} dk \\ \hat{\psi}(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx \end{aligned}$$

The Fourier transform of  $\psi(x)$ ,  $\hat{\psi}(k)$ , says that you are rewriting your wavefunction  $\psi(x)$  as a sum of functions of the form  $e^{ikx}$ : that is, free-particle energy eigenstates. Each such eigenfunction has a "coefficient"  $\hat{\psi}(k)$  that tells you how much of that energy eigenstate is in this superposition. Seen in this light,  $\hat{\psi}(k)$  is the formula for finding those coefficients.

Using Fourier transform, we could find the probability density function of energy. If a free particle has wavefunction  $\psi(x)$ , and  $\hat{\psi}(k)$  is its Fourier transform, then the probability of measuring the energy in a given range is given by

$$P\left(\frac{k_1^2 \hbar^2}{2m} < E < \frac{k_2^2 \hbar^2}{2m}\right) = \int_{-k_2}^{-k_1} |\hat{\psi}(k)|^2 dk + \int_{k_1}^{k_2} |\hat{\psi}(k)|^2 dk$$

We need two separate integral because  $-k_2 < k < -k_1$  represents eigenfunctions in a certain energy range, and  $k_1 < k < k_2$  represents different eigenfunctions in the same energy range

# Atom

## Quantum Numbers

The energy eigenstates of the hydrogen atom are states of definite energy, magnitude of angular momentum, and z component of angular momentum. The values of those quantities are labeled by the quantum numbers  $n$ ,  $l$ , and  $m_l$ , respectively. These three quantum numbers must be integers, and the spin quantum number  $m_s$  must be  $-1/2$  (spin-up) or  $+1/2$  (spin-down). Other restrictions are given below.

Letter	Name	Range	Physical interpretation
$n$	Principal quantum number	$1 \leq n < \infty$	$E_n = -(1/n^2)Ry$ , with $(1 \text{ Ry} \approx 13.6 \text{ eV})$
$l$	Angular momentum quantum number	$0 \leq l \leq n - 1$	$ \vec{L}  = \sqrt{l(l+1)}\hbar$
$m_l$	Magnetic quantum number	$-l \leq m_l \leq l$	$L_z = m_l\hbar$
$m_s$	Spin quantum number	$m_s = \pm 1/2$	$S_z = m_s\hbar$

**Principal Quantum Number  $n$ .** The term “principal quantum number” refers to the fact that  $n$  determines energy: each eigenstate  $\psi_{nlm_l}$  has energy  $E_n = -(1/n^2)$  Ry, where  $1 \text{ Ry} \approx 13.6 \text{ eV}$  is a unit of energy called a “rydberg.” So the ground state of hydrogen has energy  $-1 \text{ Ry} \approx -13.6 \text{ eV}$ , the first excited state has energy  $-(1/4) \text{ Ry} \approx -3.4 \text{ eV}$ , and so on.

**Angular Momentum Quantum Number  $l$ .**  $l$  controls the magnitude of the total angular momentum of the electron about the nucleus is  $L = \sqrt{l(l+1)}\hbar$ .

**Magnetic Quantum Number  $m_l$ .** While  $l$  determines the magnitude of the angular momentum vector,  $m_l$  determine the z component of the angular momentum  $L_z = m_l\hbar$ . The name comes from the fact that the simplest way to measure a particular component of the angular momentum of a charged particle is to measure the magnetic field it creates.

**Spin  $m_s$ .** In 1924 Pauli suggested that each electron in an atom has a fourth quantum number that can only take on two possible values. He gave no physical explanation for this new electron property, which he called a “two-valuedness not describable classically.” Consider a ball spinning about its own axis, except it is not a ball and it is not spinning.

For every electron, the magnitude of spin is  $\sqrt{s(s+1)}\hbar = \sqrt{3/4}\hbar$ , with values of  $-1/2$  or  $+1/2$ . The z component of the spin is therefore  $L_z = m_s\hbar = \pm(1/2)\hbar$ .

Any particle with half-integer spin is a fermion, for example electrons, protons, and neutrons. Any particle with integer spin is a boson, for example photons. Every particle can be classified as either a

“fermion,” meaning it obeys the Pauli exclusion principle, or a “boson,” meaning it does not.

The energy eigenvalues of a hydrogen atom depend only on  $n$  (to a very good approximation). The following formulas use  $m_e$  and  $e$  for the electron mass and charge, respectively

$$E_n = -\frac{m_e e^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} = -\frac{1}{2n^2} m_e c^2 \alpha^2 = -\frac{1}{n^2} \text{Ry}$$

$$= -\frac{1}{n^2} 13.6 \text{eV} = \frac{1}{n^2} 2.18 \times 10^{-18} \text{J}$$

where  $\alpha$  is fine structure constant

$$\alpha \equiv \frac{1}{4\pi\epsilon_0} \frac{e^2}{\hbar c} \approx \frac{1}{137}$$

For a hydrogen-like atom with  $Z$  protons and one electron, the energies are

$$E_n - \frac{Z^2}{n^2} \text{Ry}$$

## Spectroscopic Notation

For many purposes the energy and total angular momentum of a state are more important than its orientation, so an atomic state is often designated by its values of  $n$  and  $l$ . Each value of  $n$  is called a “shell,” while each combination of  $n$  and  $l$  is called a “subshell.” For example, the  $n = 2$  shell consists of the subshells  $2s$  and  $2p$ . For example, the ground state of nitrogen  $Z = 7$  is written  $1s^2 2s^2 2p^3$  to indicate that it has two electrons in the state  $n = 1, l = 0$ , two electrons in the state  $n = 2, l = 0$ , and three electrons in the state  $n = 2, l = 1$ . The first four  $l$ -values are  $s, p, d$ , and  $f$ ; from there they proceed alphabetically, except they skip  $j$  because it looks too much like  $i$ .

## Energies of Different Quantum State

**Pauli exclusion principle.** Pauli exclusion principle forbid two or more of the same type of fermion in the same quantum state as each other. That means that, in the ground state of a multielectron atom, the  $Z$  electrons (fermion) fill up the  $Z$  lowest-energy states.

**$n + l$  rule.** Given two states  $\psi_{nl}$ , the subshell with the lower sum  $n + l$  will fill up first. In the case of a tie, the lower- $n$  state fills first.

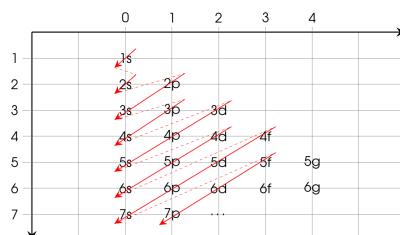


Figure: Perhaps the more familiar name for  $n + l$  rule is Aufbau rule

**Hund's Rule.** Because each electron can have spin up or spin down, two electrons can be in each combination of  $n$ ,  $l$ , and  $m_l$ . That in turn means each subshell consists of  $2(2l+1)$  degenerate states, with  $2n^2$  degenerate state for each shell. Within a particular subshell, the electrons tend to end up in the states that minimize the energy level. Two nearby electrons whose spins are identical will be, on average, farther apart from each other than if they have opposite spins. The result is that electrons with identical spins shield each other from the nucleus less than electrons with different spins, so same-spin is a lower energy state than opposite-spin.

## Electron Screening Model

Consider lithium ( $Z = 3$ ), which in its ground state has two electrons in the  $1s$  subshell and one in the  $2s$  subshell. We approximate two inner electrons as uniform spherical shells of negative charge at the Bohr radius  $a_0$ . Approximation it feels a net charge of  $+e$  coming from the nucleus. We say that the inner electrons “screen” the nuclear charge.

According to this model, the outer electron in lithium should be just like a  $2s$  electron in hydrogen. So the model predicts that the “ionization energy” of lithium should be

$$E = \frac{Z_{\text{eff}}^2}{n^2} 13.6 \text{ eV} = 3.4 \text{ eV}$$

## Periodic Table

Alkali		Noble gases																																			
1s	1	Alkaline earths		18																																	
	H	Hydrogen		He																																	
2s	Li	Be		Helium																																	
3s	Na	Mg		18																																	
4s	K	Ca		2																																	
5s	Rb	Sr		He																																	
6s	Cs	Ba		He																																	
7s	Fr	Rb		He																																	
Alkaline earth metals		He																																			
Transition metals		He																																			
3d	21	Sc		He																																	
4d	39	Y		He																																	
5d	71	Lu		He																																	
Lanthanides		He																																			
6d	103	Irradiated		He																																	
7d	104	Lawrencium		He																																	
Actinides		He																																			
Rare earths		He																																			
4f	57	La		He																																	
Actinides		He																																			
5f	89	Ac		He																																	

Figure: Periodic table

Each subshell is labeled with a number for  $n$  and a letter for  $l$ .  
 $s(l=0), p(l=1), d(l=2), f(l=3)$

Most electron configurations fill in according to the  $n+l$  rule. The exceptions are marked below, showing the previous noble gas plus the electrons added beyond it.  
 (Subshells without a superscript have a single electron.)

: Metal     : Non-Metal     : Metalloid

Transition metals

## Energy Eigenstates

The energy eigenstates of the hydrogen atom are of the form

$$\psi_{nlm_l}(r, \theta, \phi) = R_{nl}(r)Y_l^{m_l}(\theta, \phi).$$

A full specification of the quantum state of a hydrogen atom also includes the spin state (up or down) of the electron.

## Radial Wavefunction

The radial wavefunction is given by the following:

$$R_{nl}(r) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}} \left(\frac{2r}{na_0}\right)^l \exp\left(-\frac{r}{na_0}\right) L_{n-l-1}^{2l+1} \left(\frac{2r}{na_0}\right)$$

where  $L$  is called an associated Laguerre polynomial and is defined as

$$L_n^k(x) = (-1)^k \left(\frac{d}{dx}\right)^k \left[ e^x \frac{d^{p+k}}{dx^{p+k}} (e^{-x} x^{p+k}) \right]$$

As you know,  $k = 0$  then the above formula calls for the “zeroth derivative,” or the function itself.  $R_{nl}(r)$  is a polynomial in  $r$  times a decaying exponential  $e^{-r/(a_0 n)}$ , where  $a_0$  is a constant called the “Bohr radius”

$$a_0 \equiv \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} \approx 5 \times 10^{-11} \text{ m}$$

Here's first few Radial Wavefunctions: for  $n = 1$

$$R_{1,0} = 2a_0^{-3/2} \exp\left(-\frac{r}{a_0}\right)$$

for  $n = 2$

$$R_{2,0} = \frac{1}{\sqrt{2}} a_0^{-3/2} \left(1 - \frac{r}{2a_0}\right) \exp\left(-\frac{r}{2a_0}\right)$$

$$R_{2,1} = \frac{1}{\sqrt{24}} a_0^{-3/2} \frac{r}{a_0} \exp\left(-\frac{r}{2a_0}\right)$$

for  $n = 3$

$$R_{3,0} = \frac{2}{\sqrt{27}} a_0^{-3/2} \left[1 - \frac{2r}{3a_0} + \frac{2}{27} \left(\frac{r}{a_0}\right)^2\right] \exp\left(-\frac{r}{3a_0}\right)$$

$$R_{3,1} = \frac{8}{27\sqrt{6}} a_0^{-3/2} \left(1 - \frac{r}{6a_0}\right) \frac{r}{a_0} \exp\left(-\frac{r}{3a_0}\right)$$

$$R_{3,2} = \frac{4}{81\sqrt{30}} a_0^{-3/2} \left(\frac{r}{a_0}\right)^2 \exp\left(-\frac{r}{3a_0}\right)$$

## Spherical Harmonics

Spherical harmonics are products of complex exponentials in  $\phi$  and polynomials in  $\cos\theta$ :

$$Y_l^{m_l}(\theta, \phi) = \pm \sqrt{\frac{2l+1}{4\pi} \frac{(l-|m_l|)!}{(l+|m_l|)!}} P_l^{m_l}(\cos\theta) \exp(im_l\phi)$$

where  $l$  and  $m_l$  are integers and  $-l \leq m_l \leq l$ . The plus minus comes from +1 for all negative  $m_l$  and all even values of  $m_l$ , and -1 for odd positive values. So the only differences between  $Y_l^{m_l}$  and  $Y_l^{-m_l}$  are that they have different signs if  $m_l$  is odd, and the exponent in  $e^{im_l\phi}$  changes sign between them. Also, P is an “associated Legendre polynomial”

$$P_l^{m_l}(x) \equiv (1-x^2)^{|m_l|/2} \left( \frac{d}{dx} \right)^{|m_l|} \left[ \frac{1}{2^l l!} \left( \frac{d}{dx} \right)^l (x^2 - 1)^l \right]$$

Not to be confused by Legendre polynomials (defined by Rodrigues formula)

$$P_l(x) \equiv \frac{1}{2^l l!} \left( \frac{d}{dx} \right)^l (x^2 - 1)^l$$

$Y_l^{m_l}$  is a polynomial in  $\sin \theta$  and  $\cos \theta$  multiplied by  $e^{im_l\phi}$ . Here's first few Spherical Harmonics: for  $l = 0$

$$Y_0^0 = \sqrt{\frac{1}{4\pi}}$$

for  $l = 1$

$$\begin{aligned} Y_1^0 &= \sqrt{\frac{3}{4\pi}} \cos \theta \\ Y_0^{\pm 1} &= \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi} \end{aligned}$$

for  $l = 2$

$$\begin{aligned} Y_2^0 &= \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1) \\ Y_2^1 &= \mp \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{\pm 2i\phi} \\ Y_2^2 &= \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\phi} \end{aligned}$$

## Probability Distributions

For any particle with wavefunction  $\Psi$  in 3D, the probability per unit volume of finding the particle in a given region is  $|\Psi|^2$ . For an electron in a hydrogen atom energy eigenstate  $\psi_{nlm_l}$ , probability of finding the electron between radii  $r_1$  and  $r_2$

$$P(r_1 \leq r \leq r_2) = \int_{r_1}^{r_2} r^2 R^2 dr$$

while the probability of finding the electron in a specified range of angles is

$$\int_{\theta_1}^{\theta_2} \int_{\phi_1}^{\phi_2} \sin \theta |Y_l^{m_l}|^2 d\psi d\theta$$

These integrals are normalized so that

$$\int_0^\infty r^2 R^2 dr = \int_0^\pi \int_0^{2\pi} \sin \theta |Y_l^{m_l}|^2 d\psi d\theta = 1$$

## Zeeman Effect

The Zeeman effect refers to the changes in atomic spectra caused by an external magnetic field. In classical electrodynamics, magnets tend to align with magnetic fields, or magnet pointing along an external magnetic field has less energy than one pointing opposite to the external field. Because an electron is negatively charged, its magnetic moment points opposite to its angular momentum. So a positive  $m_l$  means its magnetic moment is pointing opposite external field, if we define positive z axis as the direction of external field. A negative  $m_l$  means the electron's magnetic field is pointing with the external field, which is the preferred (low-energy) orientation.

Therefore, in an external magnetic field pointing in the positive z direction, higher  $m_l$  leads to higher energy. For weak magnetic fields (neglecting spin), the Zeeman contribution to the energy of a state is

$$\Delta E = m_l \mu_B B$$

where  $\mu_B$  is Bohr magneton

$$\mu_B = \frac{e\hbar}{2m_e}$$

If an atom transitions between states in which all its electron spins cancel, then you can ignore spin. In that case the splitting caused by a magnetic field is called the “normal Zeeman effect.” in the presence of an external magnetic field, the normal Zeeman effect splits the  $n = 2$  to  $n = 1$  transition into three separate transitions based on  $\Delta m_l$ . The selection rule limits which electron transitions generally occur

$$\Delta l = \pm 1$$

$$\Delta m_l = -1, 0, 1$$

## Appendix

### Electron screening model prediction.

The ground state of nitrogen ( $Z = 7$ ) is  $1s^2 2s^2 2p^3$ . Using the model, predicts the ionization energy of a nitrogen atom.

The nucleus has 7 protons. The 4 inner electrons provide full shielding, and the other two electrons in the  $2p$  state provide half-shielding:

$$Z_{\text{eff}} = 7 - 4 - 2(1/2) = 2$$

the energy ionization is therefore

$$E = \frac{2^2}{2^2} 13.6 \text{ eV} = 13.6 \text{ eV}$$

# Statistical Mechanics

## Introduction

Here's few short definition used in Statistical Mechanic

Term	Definition
Binomial coefficient	Used to determine number of ways to choose a group of m items from a list of n distinct items: $\binom{n}{m} = \frac{n!}{m!(n-m)!}$
Boltzmann's constant $k_B$	$k_B = 1.38 \times 10^{-23} \text{ J/K} = 8.62 \times 10^{-5} \text{ eV/K}$
Density of states $g(E)$	The number of states per unit energy
Entropy $S$	$S = k_B \ln \Omega$
Heat $Q$	Energy transferred spontaneously from a hot system to a cold system. When heat $Q$ flows into a system, $\Delta S \geq Q/T$
Heat capacity $C$	Formula for heat capacity is: $C = \frac{dE}{dT}$ taking $dE$ to be the heat input, not work. Heat capacity is written $C_P$ if heat is added at constant pressure, and $C_V$ if it's added at constant volume. In general, $C_P > C_V$
Ideal gas	A gas of non-interacting, free molecules
Multiplicity $\Omega$	The number of microstates associated with a macrostate
Temperature $T$	Defined using second law of Thermodynamics $T = \frac{1}{dS/dE}$ assuming $dE$ is only heat and there are no other changes
Work $W$	Any energy transfer other than heat (e.g. via macroscopic forces)

## Boltzmann Distribution

For a system in equilibrium with a large reservoir at temperature  $T$ , the probability of its being in a given microstate with energy  $E$  is

$$P = \frac{1}{Z} e^{-E/(k_B T)}$$

The “partition function”  $Z$  is defined to normalize the probabilities:

$$Z = \sum_{\text{all microstates}} e^{-E/k_B T} = \sum_{\text{all microstates}} \Omega(E) e^{-E/k_B T}$$

## Equipartition Theorem

If the energy of a system in equilibrium with a large reservoir at temperature  $T$  depends quadratically on a continuous degree of freedom (e.g.  $x, y, v_x, \omega_x, \dots$ ), the average thermal energy associated with that degree of freedom is  $(1/2)k_B T$ . If the degree of freedom is quantized, the equipartition theorem still holds in the limit where the spacing between energy levels is small compared to the system’s energy. Even when the conditions for the equipartition theorem don’t apply, it is usually still true that the thermal energy of a single particle, atom, or molecule is of order  $k_B T$ , provided the density of states is relatively uniform and the spacing between available energy levels is much smaller than  $k_B T$ . Few examples where equipartition theorem holds

1. A free, classical particle in three-space has a translational kinetic energy that depends quadratically on three degrees of freedom ( $v_x, v_y$ , and  $v_z$ ), so its average thermal energy is  $(3/2)k_B T$ .
2. A monatomic atom (He) has no rotational degrees of freedom. A diatomic molecule (H<sub>2</sub>) has two, so  $K_{rot} = k_B T$ . A polyatomic molecule (CO<sub>2</sub>) has three, so  $K_{rot} = (3/2)k_B T$ . (Molecular vibrations are typically frozen out at room temperature.)
3. A one-dimensional simple harmonic oscillator has two quadratic degrees of freedom,  $E = (1/2)mv^2 + (1/2)kx^2$ , so its average thermal energy is  $k_B T$ .

## Quantum Statistics

For a system of identical particles in equilibrium with a large reservoir at temperature  $T$ , the average occupation number  $\bar{n}$  of a microstate is given by Fermi-Dirac distribution (for fermions) and Bose-Einstein distribution (for bosons). Fermi-Dirac distribution predicts

$$\bar{n} = \frac{1}{e^{(E-\mu)/(k_B T)} + 1}$$

while Bose-Einstein distribution predicts

$$\bar{n} = \frac{1}{e^{(E-\mu)/(k_B T)} - 1}$$

The “chemical potential”  $\mu$  is defined to normalize the total occupation number ( $\sum \bar{n} = N$ ). The value  $\mu$  for massless particles such as photons

is  $\mu = 0$ ; for fermions  $\bar{n}$  is greater than 1/2 for energies below  $\mu$ , and less than 1/2 for higher energies; for bosons,  $\mu$  is always below the ground state energy.

## Blackbody Spectrum

An object that absorbs all electromagnetic radiation is called a “blackbody.” Many objects, ranging from stars to a human body, emit radiation that is approximately the same as what we find inside a cavity in equilibrium. The spectrum of radiation inside a cavity is also the spectrum emitted by a blackbody, because in equilibrium, the blackbody must be emitting the same spectrum that it’s absorbing.

To find the energy density  $\rho$  in a given range of frequency, we then integrate spectrum function  $S(\nu)$  (energy density per unit frequency) with respect to frequency.

$$\rho = \int_0^\infty S(\nu) d\nu$$

where

$$S(\nu) = \frac{8\pi}{c^3} v^2 E_w(\nu)$$

The function  $E_w(\nu)$  represents the energy of each wave of frequency  $\nu$ . We will now derive  $E_w(\nu)$  classically, from which the ultraviolet catastrophe emerges. Now suppose a wave in our cavity has energy levels: 0,  $2k_B T$ ,  $4k_B T$ ,  $6k_B T$ , and  $8k_B T$ . Using Boltzmann distribution, we find the expectation value:

$$\begin{aligned} \langle E_w \rangle &= \sum_E EP(E) = \frac{1}{Z} \sum_{n=0,2,4,\dots} E e^{-E/(k_B T)} \\ &= \frac{(0)(C) + (Ce^{-2})(2k_B T) + (Ce^{-4})(4k_B T) + (Ce^{-6})(6k_B T) + (Ce^{-8})(8k_B T)}{C + Ce^{-2} + Ce^{-4} + Ce^{-6} + Ce^{-8}} \\ &\approx 0.31k_B T \end{aligned}$$

Notice that the way we “chunk” our energy will result in different expectation value. Average energy of a given wavelength as a function of the “chunking” of discrete allowed energy levels are as follows

$\Delta E$	Allowed energy levels	Calculated $E_w$
$5k_B T$	$0, 5k_B T, 10k_B T, \dots$	$0.034k_B T$
$2k_B T$	$0, 2k_B T, 4k_B T, \dots$	$0.31k_B T$
$k_B T$	$0, k_B T, 2k_B T, \dots$	$0.58k_B T$
$0.5k_B T$	$0, 0.5k_B T, 1k_B T, \dots$	$0.77k_B T$
$0.1k_B T$	$0, 0.1k_B T, 0.2k_B T, \dots$	$0.95k_B T$

As you the limit where  $\Delta E$  approaches 0,  $E_w$  rises toward  $k_B T$ ; on the other hand,  $E_w$  drops toward 0 as limit where  $\Delta E$  approaches  $\infty$ . Classically, the next step was obvious. Energy can be any real positive number, so the correct  $E_w$  is the limit of this process as  $\Delta E$

approaches 0. This result is called the “Rayleigh-Jeans spectrum.” The energy density then become

$$\rho = \int_0^\infty \frac{8\pi}{c^3} v^2 k_B T \, dv \quad \text{Diverges}$$

In other words, classical theory predicted that a cavity in equilibrium should have infinite energy density. Because the blow-up occurs at high frequencies, this prediction was called the “ultraviolet catastrophe.”

To fix this problem, Planck made  $\Delta E$  proportional to the frequency, introducing a constant of proportionality that we now call Planck’s constant:

$$\Delta E = h\nu$$

The Spectrum function, which can be expressed in terms of frequency or wavelength, become

$$u(v) = \frac{8\pi h}{c^3} \frac{v^3}{e^{hv/k_B T} - 1}$$

$$u(\lambda) = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{hc/k_B T} - 1}$$

and energy density of radiation inside an enclosed cavity in equilibrium

$$\rho = \int_0^\infty u(v) \, dv = \int_0^\infty u(\lambda) \, d\lambda$$

actually converge this time.

The intensity (energy per time per surface area) emitted by a black-body is  $c/4$ times the energy density of radiation in a cavity

$$I = \frac{c}{4} \rho = \sigma T^4$$

Wien’s law for peak frequency

$$hv_{peak} = 2.82k_B T$$

while wavelength

$$hc/\lambda_{peak} = 4.97k_B T$$

Stefan’s law for total intensity

$$I = \sigma T^4 \quad \text{where} \quad \sigma = 5.67 \times 10^{-8} \text{ Wm}^{-2}\text{K}^{-4}$$

## Maxwell Speed Distribution

The probability that a (non-relativistic) molecule of mass  $m$  in an ideal gas at temperature  $T$  has speed in the range  $v_1 < v < v_2$  is

$$P = 4\pi \left( \frac{m}{2\pi k_B T} \right)^{3/2} \int_{v_1}^{v_2} v^2 e^{-mv^2/(2k_B T)} \, dv \quad (1)$$

# Wave

## One Variable Function

Wave can be represented by function of time or space. As function of time

$$y = A \sin(\omega t) = A \sin(2\pi\nu t) = A \sin \frac{2\pi}{T} t$$

while as function of space

$$y = A \sin(kt) = A \sin(2\pi f x) = A \sin \frac{2\pi}{\lambda} x$$

The definition of Variable are as follows

Variable	Definition
$T$ and $\lambda$	$T$ represented period, and $\lambda$ represented wavelength
$\omega$ and $k$	$\omega$ represented angular frequency, while $k$ represented wave number; which related by: $\omega = \frac{w\pi}{T} \quad \text{and} \quad k = \frac{2\pi}{\lambda}$
$\nu$ and $f$	$\nu$ represented frequency, while $f$ represented spatial frequency; which related by: $\nu = \frac{\omega}{2\pi} = \frac{1}{T} \quad \text{and} \quad \nu = \frac{k}{2\pi} = \frac{1}{\lambda}$

Using Euler's formula, sinusoidal wave can also be represented

$$y = Ae^{i\omega t}$$

## Standing and Traveling Waves

standing wave is a wave in space with fixed nodes and antinodes and a time-varying amplitude

$$y = A \sin(\omega t) \sin(kx)$$

A traveling wave keeps the same amplitude and shape but moves through space:

$$y = A \sin(kx - \omega t) = Ae^{ikx-i\omega t}$$

The velocity of a traveling wave can equivalently be written  $v = \lambda\nu = \omega/k$ . Note the difference between  $v$  and  $\nu$ .

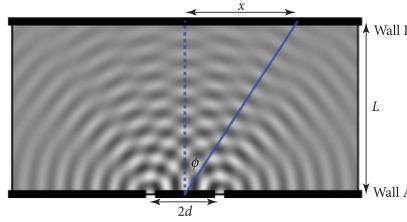


Figure: Double slit

## Simple Harmonic Oscillator

Many waves arise as solutions to the following differential equation

$$\frac{d^2y}{dx^2} = -\omega^2 y$$

The general solutions below are

$$\begin{aligned} y(t) &= A \sin(\omega t) + B \cos(\omega t) \\ &= C \sin(\omega t + \phi) \\ &= D e^{i\omega t} + F e^{-i\omega t} \end{aligned}$$

## Double Slit Interference

Consider two waves that are identical in every way meet at same space. Those two will Interfere. Suppose a wave of wavelength  $\lambda$  passes through two narrow slits separated by a distance  $2d$ . The wave is then measured on a back wall a distance  $L$  behind the wall with the slits. Places where the waves from the different paths interfere constructively to produce the maximum possible amplitude are called antinodes (bright), and places where they interfere destructively to produce no oscillation are called nodes (dark). The distance from the center of the back wall to the  $n$ th antinode is

$$x_n = \frac{n\lambda}{2} \sqrt{\frac{4(d^2 + L^2) - n^2\lambda^2}{4d^2 - n^2\lambda^2}}$$

This equation then can be approximated. For far-field approximation, we assume the back wall is much farther away than the spacing between the slits  $L \gg d$ . The antinodes occur at evenly spaced values of  $\sin \phi$

$$\sin \psi \approx \frac{n\lambda}{2d}$$

For small-angle approximation, we additionally assume  $d \gg n\lambda$ . Then  $\phi \ll 1$  and we can use  $\sin \psi \approx \tan \theta x/L$ . This approximation is never valid if  $d \gg \lambda$ , but if  $d \gg \lambda$  then it works for all the peaks up to  $d \approx n\lambda$

**Diffraction grating.** Diffraction grating is a long line of evenly spaced slits. Assuming the back wall is far enough away that the waves from all slits travel at approximately the same angle to each point, the nodes and antinodes follow the same equations as the far-field and small-angle equations for a double slit. The difference is that the fringes show greater contrast when there are more slits.

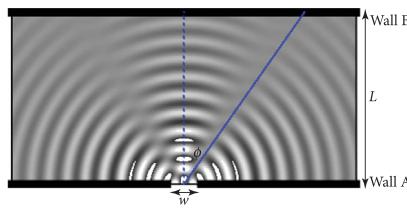


Figure: Single slit

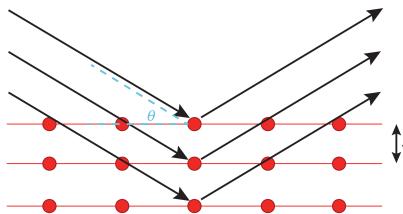


Figure: Waves reflecting off a crystal

## Single Slit

A diffraction pattern occurs when a wave passes through a single slit whose width  $w$  is comparable to the wavelength  $\lambda$ . This produces one intense central maximum with smaller maxima on the sides, separated by nodes (dark fringes). In the far-field approximation the nodes occur at the following angles for positive integers  $n$ :

$$\sin \psi = \frac{n\lambda}{w}$$

## Bragg's Law

Bragg's law refers to the scattering of an incoming wave off multiple layers of a crystal. You get a strong reflected beam when the glancing angle  $\theta$  meets the following condition for integer  $n$

$$\sin \theta = \frac{n\pi}{2s}$$

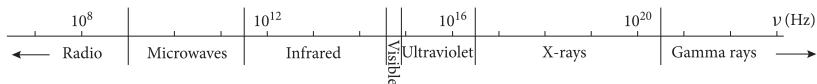
This looks similar to the far-field formula for a double slit, but here  $\theta$  is the angle of the incoming beam and  $s$  is the spacing between atomic layers. By convention, Bragg's law is expressed in terms of glancing angle  $\theta$  rather than angle of incidence ( $\pi/2 - \theta$ ).

## Electromagnetic Spectrum

There are no universally accepted conventions for the exact cutoffs between the different types,<sup>1</sup> but this gives a general idea. The columns of the table are the frequency  $\nu$ , the wavelength ( $\lambda = c/\nu$ ), the energy of a photon with that frequency ( $E = h\nu$ ), and the temperature of a blackbody whose spectrum would peak at that frequency ( $T \approx h\nu/2.82 k_B$  ).

Category	$\nu$ (Hz)	$\lambda$ (m)	$E$ (eV)	$T$ (K)
Gamma rays	$3 \times 10^{20} \rightarrow$	$\leftarrow 10^{-12}$	$1.2 \times 10^6 \rightarrow$	$5 \times 10^9 \rightarrow$
X-Rays	$3 \times 10^{16} \leftrightarrow 3 \times 10^{20}$	$10^{-12} \leftrightarrow 10^{-8}$	$1.2 \times 10^2 \leftrightarrow 1.2 \times 10^6$	$5 \times 10^5 \leftrightarrow 5 \times 10^9$
Ultraviolet	$7.7 \times 10^{14} \leftrightarrow 3 \times 10^{16}$	$10 - 8 \leftrightarrow 3.9 \times 10^{-7}$	$3 \leftrightarrow 120$	$1.3 \times 10^4 \leftrightarrow 5 \times 10^5$
Visible	$3.8 \times 10^{14} \leftrightarrow 7.7 \times 10^{14}$	$3.9 \times 10^{-7} \leftrightarrow 7.8 \times 10^{-7}$	$1.6 \leftrightarrow 3$	$6000 \leftrightarrow 13000$
Infrared	$3 \times 10^{11} \leftrightarrow 3.8 \times 10^{14}$	$7.8 \times 10^{-7} \leftrightarrow 10 - 3$	$0.0012 \leftrightarrow 1.6$	$5 \leftrightarrow 6000$
Microwave	$10^9 \leftrightarrow 3 \times 10^{11}$	$10^{-3} \leftrightarrow 3 \times 10^{-1}$	$4 \times 10^{-6} \leftrightarrow 1.2 \times 10^{-3}$	$0.02 \leftrightarrow 5$
Radio	$\leftarrow 10^9$	$0.3 \rightarrow$	$\leftarrow 4 \times 10^{-6}$	$\leftarrow 0.02$

Next, is electromagnetic radiation graph against frequency



For visible light

Color	Frequency (THz)	Wavelength (nm)
Red	$384 \leftrightarrow 482$	$622 \leftrightarrow 781$
Orange	$482 \leftrightarrow 503$	$596 \leftrightarrow 622$
Yellow	$503 \leftrightarrow 520$	$577 \leftrightarrow 596$
Green	$520 \leftrightarrow 610$	$492 \leftrightarrow 577$
Blue	$610 \leftrightarrow 659$	$455 \leftrightarrow 492$
Violet	$659 \leftrightarrow 769$	$390 \leftrightarrow 455$