Modern Physics Notes

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A. Frames of Reference

Physical systems are always observed from some point of view. That is, the displacement, velocity, and acceleration of a particle are measured *relative* to some selected origin and coordinate axes. If a different origin and/or set of axes is used, then different numerical values are obtained for $\vec{r}$, $\vec{v}$, and $\vec{a}$, even though the physical event is the same. An *event* is a physical phenomenon which occurs at a specified point in space and time.

1. Inertial Frames of Reference

a. Definition

An inertial frame is one in which Newton's "Laws" of Motion are valid. Moreover, any frame moving with constant velocity with respect to an inertial frame is also an inertial frame of reference. While $\vec{r}$ and $\vec{v}$ would have different numerical values as measured in the two frames, $\vec{F} = m\vec{a}$ in both frames.

b. Newtonian relativity

Quote: The Laws of Mechanics are the same in all inertial reference frames. What does "the same" mean? It means that the equations and formulae have identical forms, while the numerical values of the variables may differ between two inertial frames.

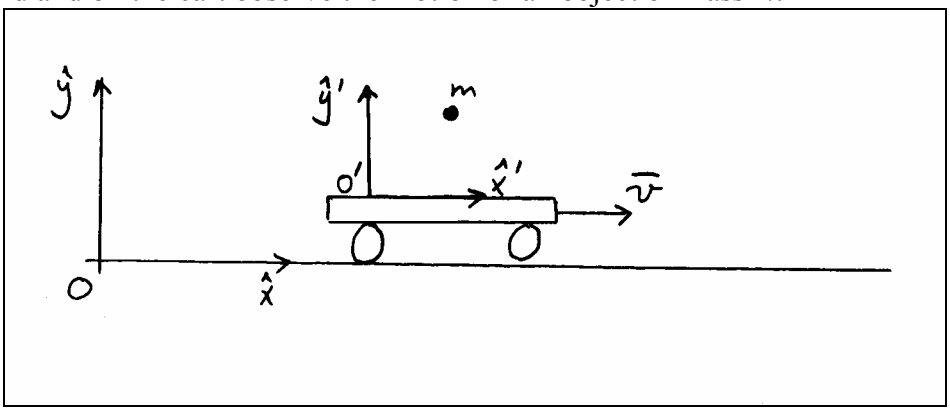
c. Fundamental frame

It follows that there is no *preferred* frame of reference—none is more fundamental than another.

2. Transformations Between Inertial Frames

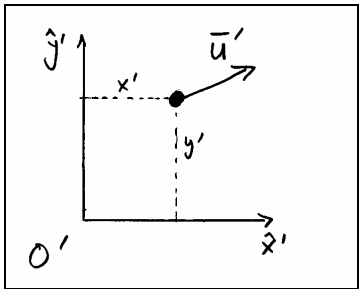
a. Two inertial frames

Consider two reference frames—one attached to a cart which rolls along the ground. Observers on the ground and on the cart observe the motion of an object of mass *m*.

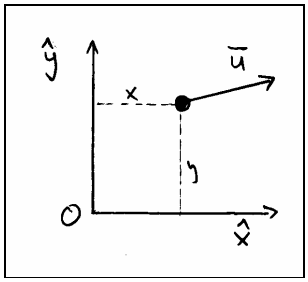


The S'-frame is moving with velocity $\vec{v}$ relative to the S-frame. As observed in the two frames:

In S' we'd measure $\Delta t'$, $\Delta x'$, and $u_x' = \dfrac{\Delta x'}{\Delta t'}$.



In S we'd measure Δt, Δx, and $u_x = \dfrac{\Delta x}{\Delta t}$.



b. Galilean transformation

Implicitly, we assume that $\Delta t = \Delta t'$. Also, we assume that the origins coincide at $t = 0$. Then

$$x = x' + v_x \Delta t'$$
$$y = y' + v_y \Delta t'$$
$$z = z' + v_z \Delta t'$$
$$\Delta t = \Delta t'$$

The corresponding velocity transformations are

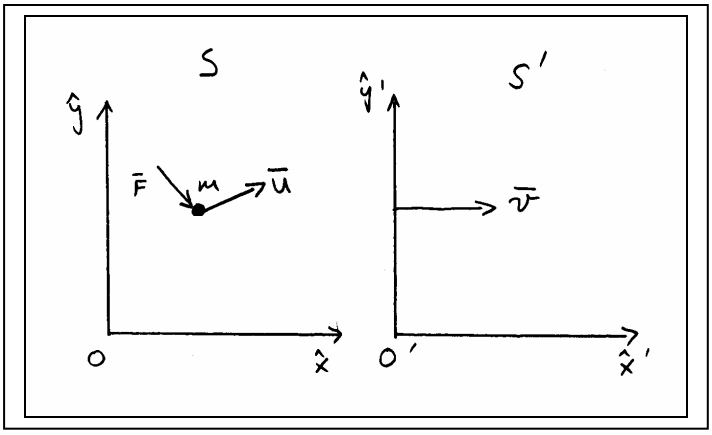
$$u_x = \frac{dx}{dt} = \frac{dx'}{dt} + v_x = u_x' + v_x$$
$$u_y = \frac{dy}{dt} = \frac{dy'}{dt} + v_y = u_y' + v_y$$
$$u_z = \frac{dz}{dt} = \frac{dz'}{dt} + v_z = u_z' + v_z$$

For acceleration

$$a_x = \frac{du_x}{dt} = a_x' + \frac{dv_x}{dt}$$
$$a_y = \frac{du_y}{dt} = a_y' + \frac{dv_y}{dt}$$
$$a_z = \frac{du_z}{dt} = a_z' + \frac{dv_z}{dt}$$

Note that for two inertial frames, the $a_x = a_x'$, $a_y = a_y'$, and $a_z = a_z'$.

Example



S-frame

$\vec{F} = m\vec{a} = m\dfrac{d\vec{u}}{dt} = \dfrac{d\vec{p}}{dt}$, if m is constant.

S'-frame

$\vec{F}' = m\vec{a}' = \dfrac{d\vec{p}'}{dt}$, where $\vec{p}' = m\vec{u}'$. But $\vec{u}' = \vec{u} - \vec{v}$, so $\vec{F}' = m\left(\dfrac{d\vec{u}}{dt} - \dfrac{d\vec{v}}{dt}\right) = m\dfrac{d\vec{u}}{dt} = \vec{F}$. That is, $\vec{a} = \vec{a}'$, as they must for 2 inertial reference frames.

Notice the technique. Write the 2nd "Law" in the S'-frame, then transform the position and velocity vectors to the S-frame.

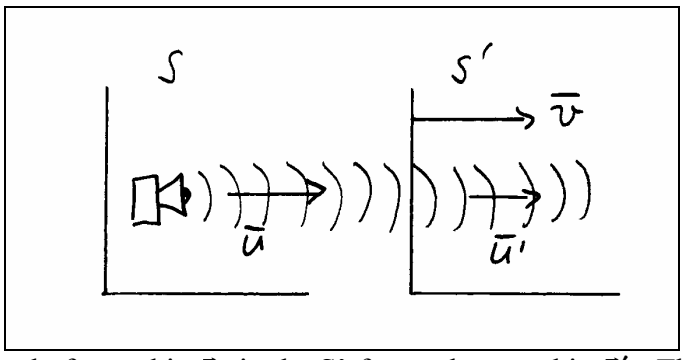
B. Special Relativity

1. Michelson-Morley

a. Wave speeds

Midway through the 19th century, it was established that light is an electromagnetic (E-M) wave. Maxwell showed that these waves propagate through the vacuum with a speed $c \approx 3x10^8$ m/sec.

Now, wave motion was well understood, so it was expected that light waves would behave exactly as sound waves do. Particularly the measured wave speed was expected to depend on the frame of reference.

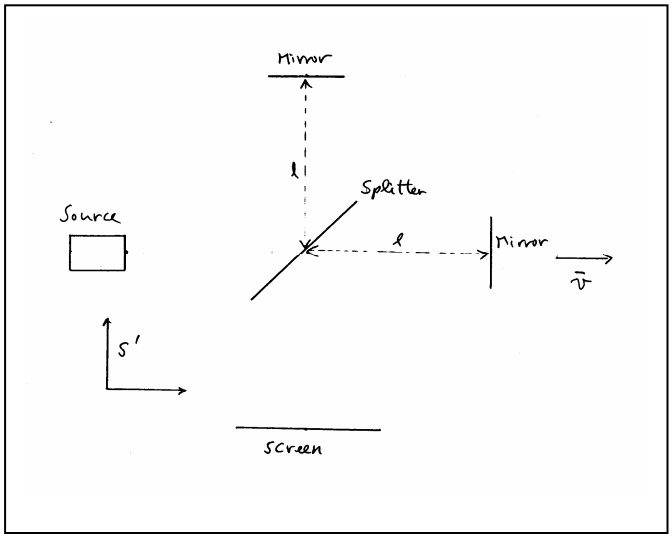


In the S-frame, the speed of sound is $\vec{u}$; in the S'-frame the speed is $\vec{u}'$. The source and the medium are at rest in the S-frame. We find (measure) that $\vec{u} = \vec{u}' + \vec{v}$, in conformity with Newtonian or Galilean relativity. We may identify a "preferred" reference frame, the frame in which the medium is at rest.

b. Michelson-Morley

Throughout the latter portion of the 19th century, experiments were performed to identify that preferred reference frame for light waves. The questions were, what is the medium in which light waves travel and in what reference frame is that medium at rest? That hypothetical medium was given the name *luminiferous ether* (*æther*). As a medium for wave propagation, the ether must be very stiff, yet offer no apparent resistance to motion of material objects through it.

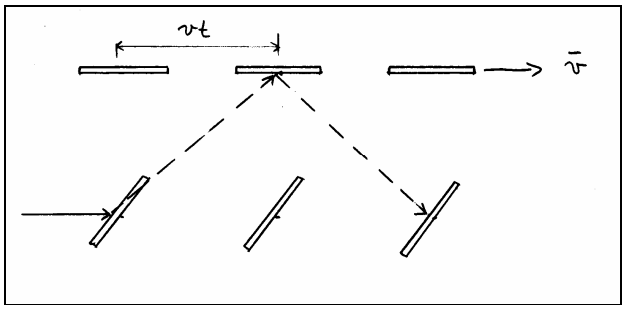
The classic experiment to detect the *ether* is the Michelson-Morley experiment. It uses interference to show a phase shift between light waves propagating the same distance but in different directions.



The whole apparatus (and the Earth) is presumed to be traveling through the ether with velocity, $\vec{v}$. A light beam from the source is split into two beams which reflect from the mirrors and are recombined at the beam splitter—forming an interference pattern which is projected on the screen. Take a look at

the two light rays as observed in the ether rest frame.

The sideward ray:



The time required for the light ray to travel from the splitter to the mirror is obtained from

$$(ct)^2 = \ell^2 + (vt)^2 \Rightarrow t = \frac{\ell}{c}\left(1 - \frac{v^2}{c^2}\right)^{-1/2}.$$

Now $c >> v$, so use the binomial theorem to simplify

$$(1-x)^{-n} = 1 + nx + \frac{n(n+1)}{2!}x^2 + \cdots$$

$$t \approx \frac{\ell}{c}\left(1 + \frac{1}{2}\frac{v^2}{c^2}\right).$$

The total time to return to the splitter is twice this: $t_1 = 2t \approx \frac{2\ell}{c}\left(1 + \frac{1}{2}\frac{v^2}{c^2}\right)$.

For the forward light ray, the elapsed time from splitter to mirror to splitter is

$$t_2 = \frac{\ell}{c-v} + \frac{\ell}{c+v} = \frac{2\ell}{c}\left(1 - \frac{v^2}{c^2}\right) \approx \frac{2\ell}{c}\left(1 + \frac{v^2}{c^2}\right).$$

The two light rays recombine at the beam splitter with a phase difference [let $\tau = \frac{\lambda}{c}$.]:

$$\frac{\Delta t}{\tau} = \frac{c}{\lambda}(t_2 - t_1) = \frac{2\ell}{c}\frac{1}{2}\frac{v^2}{c^2}\frac{c}{\lambda} = \frac{\ell}{\lambda}\frac{v^2}{c^2}.$$

Since $\frac{\Delta t}{\tau} \neq 0$, the two light rays are out of phase even though they have traveled the same distance. By measuring Δt one could evaluate $\bar{v}$.

However, no such phase difference was/is observed! So, there is no ether, no $\vec{v}$ with respect to such an ether. This null result is obtained no matter which way the apparatus is turned. The conclusion must be that either the "Laws" of electromagnetism do not obey a Newtonian relativity principle or that there is no universal, preferred, rest frame for the propagation of light waves.

c. Expedients to explain the null result

length contraction—movement through the ether causes the lengths of objects to be shortened in the direction of motion.

ether-drag theory—ether is dragged along with the Earth, so that near the Earth's surface the ether is at rest relative to the Earth.

Ultimately, the expedients were rejected as being too *ad hoc*; it's simpler to say there is no ether. This still implies that the "Laws" of electromagnetism behave differently under a transformation from one reference frame to another than do the "Laws" of mechanics.

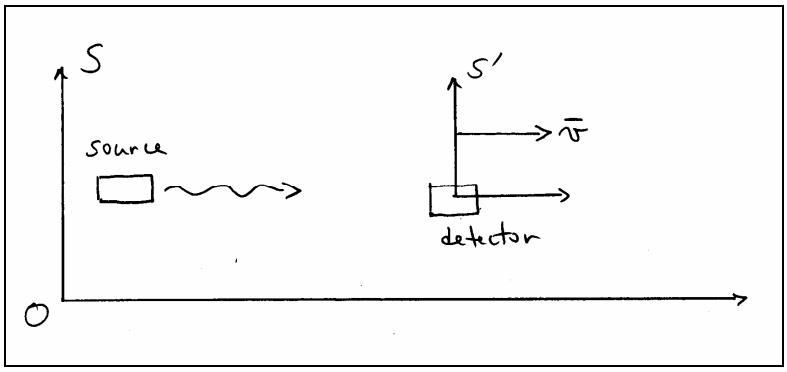
2. Postulates of Special Relativity

a. Principle of Special Relativity

It doesn't seem sensible that one "part" of Physics should be different from another "part" of Physics. Let's assume that they are not different, and work out the consequences. This is what Einstein did. He postulated that 'All the "Laws" of Physics are the same in all inertial reference frames.'

b. Second Postulate

The second postulate follows from the first. 'The speed of light in a vacuum is (measured to be) the same in all inertial reference frames.'



When the speed of light is measured in the two reference frames, it is found that $c \neq c' + v$, rather $c = c'$. Evidently, the Galilean Transformation is not correct, or anyway not exact. In any case, we assume the postulates are true, and work out the consequences.

C. Consequences of the Principle of Special Relativity

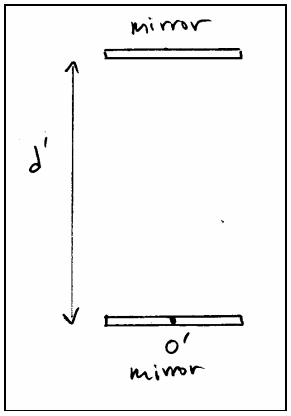
1. Time Dilation

a. Events

An *event* may be regarded as a single observation made at a specific location and time. One might say that an event is a point in space-time (x,y,z,t). Two events may be separated by intervals in either space or in time or in both.

b. Time intervals

Consider a kind of clock:

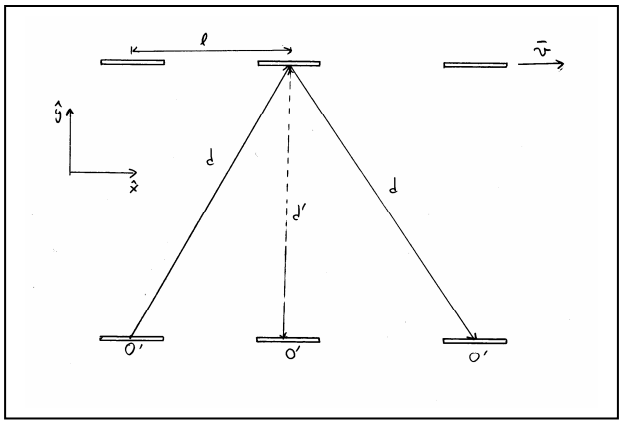


We observe two events: i) the emission of a flash at O' and ii) the reception of the flash at O'. In this case, $\Delta x' = \Delta y' = \Delta z' = 0$. The time interval between the two events is $\Delta t' = \dfrac{2d'}{c}$.

Now let's view the same two events from the point of view of another frame, S. As shown below, the S'-frame is moving to the right with speed v relative to the S-frame. In the S-frame, $\Delta x \neq 0$. The elapsed time is $\Delta t = \dfrac{2d}{c}$, where $d^2 = d'^2 + \ell^2$. Substitute for d, d', and ℓ in terms of Δt, $\Delta t'$, c, and v.

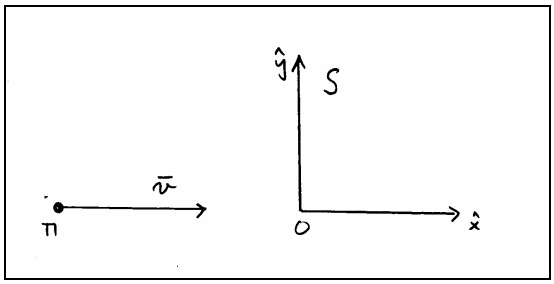
$$\frac{c^2\Delta t^2}{4} = \frac{c^2\Delta t'^2}{4} + \frac{v^2\Delta t^2}{4}$$

Solve for $\Delta t = \Delta t'\left(\dfrac{c^2}{c^2 - v^2}\right)^{1/2} = \dfrac{\Delta t'}{\sqrt{1 - \dfrac{v^2}{c^2}}}$.



example (prob. 1-11 in the text)

The lifetime of a *pion* in its own rest frame is $\Delta t' = 2.6x10^{-8}$ sec. Consider a pion moving with speed $v = 0.95c$ in a lab—what will be measured as its lifetime in the lab?



$$\Delta t = \frac{\Delta t'}{\sqrt{1-\frac{v^2}{c^2}}} = \frac{2.6x10^{-8}\ \text{sec}}{\sqrt{1-0.95^2}} = \frac{2.6x10^{-8}\ \text{sec}}{0.312} = 8.33x10^{-8}\ \text{sec}.$$

The lifetime of a fast-moving particle is measured by noting how far it travels before decaying. In this example $\ell = v\Delta t = 0.95c \cdot 8.33x10^{-8}\ \text{sec} = 23.7\ \text{m}$. In practice, we measure ℓ and compute Δt.

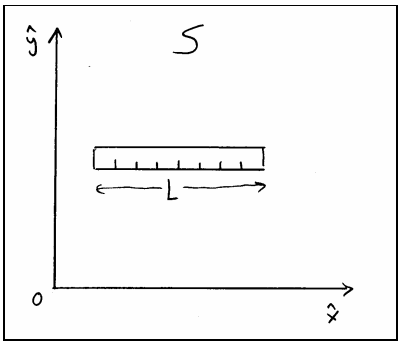
c. Proper time

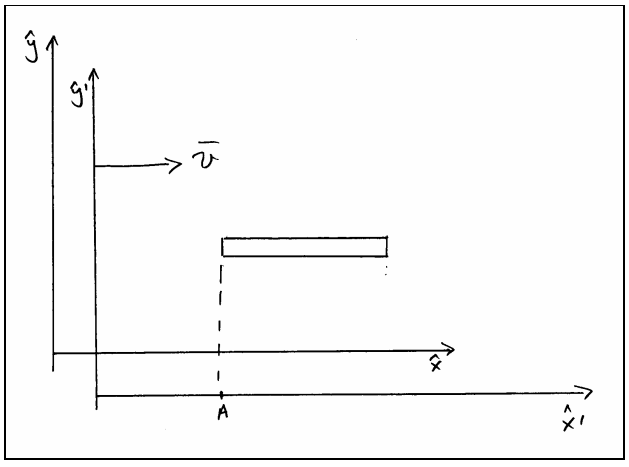
The *proper time* is the time interval measured by an observer for whom the two events occur at the same place, so that $\Delta x' = \Delta y' = \Delta z' = 0$.

2. Length Contraction

a. "Contraction"

Consider an object, such as a meter stick, of length L in its own rest frame, S.





A second frame, S', moves to the right with a speed v relative to S.
We observe two events:

i) the point A passes the left end of the stick

ii) the point A passes the right end of the stick.

As measured in the S' frame, $L' = v\Delta t'$ and $\Delta x' = 0$.

In the S frame, $\Delta x = L$ and $\Delta t = \dfrac{\Delta t'}{\sqrt{1-\dfrac{v^2}{c^2}}}$. Therefore, $L' = v\Delta t\sqrt{1-\dfrac{v^2}{c^2}} = L\sqrt{1-\dfrac{v^2}{c^2}}$.

An observer in the S' frame observes the stick to be shorter (contracted) than does the observer in the S frame. Notice particularly that the stick is at rest in the S frame.

The contraction takes place in the direction of the relative motion. Lengths perpendicular to $\bar{v}$ are not affected. So for instance in the situation discussed above the width and thickness of the meter stick are still measured the same in both reference frames.

b. Proper length

The *proper length* of an object is that length measured in the rest frame of the object.

3. Simultaneity

a. Space-time

Each event has associated with it four numbers: *x*, *y*, *z* coordinates and a "value of time" which we read off a clock located at that spatial location. There is no central universal clock, rather there is a clock at every point in space.

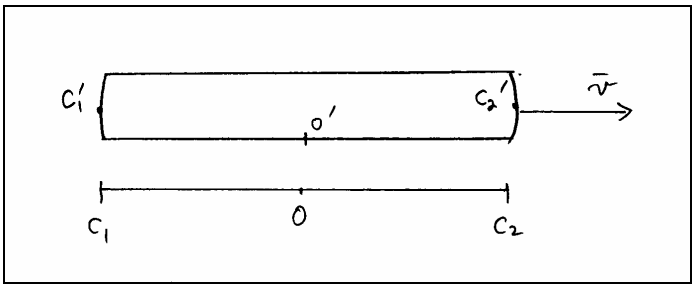
b. Synchronization

We would like all clocks in a reference frame to display exactly the same reading simultaneously, but can this be arranged? Only by the exchange of signals, which is another way of saying only in terms of intervals. However, as we have seen, intervals are not the same for observers in different inertial reference frames. Therefore, the concept of two events being simultaneous has no absolute meaning.

c. Non-simultaneity

Two events viewed as simultaneous in one frame will not be seen as occurring simultaneously in another frame.

example: a train moving with constant velocity on a straight, smooth track. One observer rides on the train, the other observer stands beside the track.



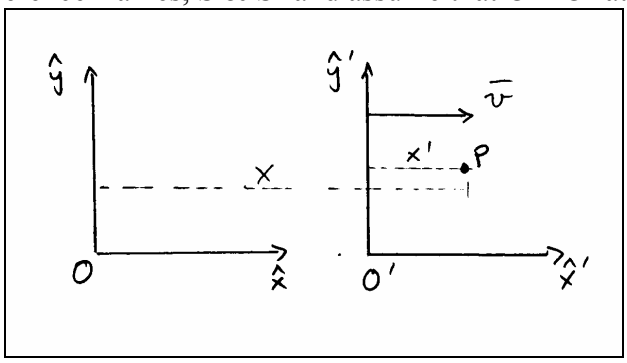
Flashes of light are emitted at the points C_1 and C_2 when the origins (O & O') of the two frames coincide. To the trackside observer at O, the flashes are simultaneous. To the observer on the train, however, the flash emitted at C'_2 is received before the flash emitted at C'_1. Yet both observers measure the same speed of light, *c*.

4. Lorentz Transformation

Now we wish to derive the transformation equations for the displacement and velocity of an object—the relativistic version of the Galilean transformation equations. In what follows, we'll be setting $\gamma = \dfrac{1}{\sqrt{1-\dfrac{v^2}{c^2}}}$.

a. Two frames

Consider two inertial reference frames, S & S' and assume that O = O' at t' = 0.



What is the x-distance from O to the point P, as measured in the S' frame? In effect, then, we'll have $\Delta t = t$ and $\Delta t' = t'$.

$$\ell' = x' + vt'$$

In the S frame, $\ell = x$, so $\ell' = \dfrac{x}{\gamma}$ also. Set 'em equal.

$$\frac{x}{\gamma} = x' + vt'$$

$$x = \gamma(x' + vt')$$

On the other hand, as measured in the S frame, $x = vt + \dfrac{x'}{\gamma}$. Set them equal.

$$\gamma(x' + vt') = vt + \frac{x'}{\gamma}$$

Solve for t.

$$vt = \gamma(x' + vt') - \frac{x'}{\gamma}$$

$$t = \gamma\left(t' + \frac{v}{c^2}x'\right)$$

b. Transformation equations

We have, then, for relative motion along the x-axis:

$$x = \gamma(x' + vt'); \quad y = y'; \quad z = z'; \quad t = \gamma\left(t' + \frac{v}{c^2}x'\right)$$

Notes: i) the inverse transformation is obtained by replacing v with $-v$.
ii) for $v << c$, these reduce to the Galilean transformation.

c. 4-vectors

Suppose that when O = O', a flash of light is emitted from the origin O. In the S frame, the distance the light wave front travels in time t is $r^2 = x^2 + y^2 + z^2 = c^2t^2$. Measured in the S' frame, it's $r'^2 = x'^2 + y'^2 + z'^2 = c^2t'^2$. Subtract the second expression from the first and collect the S frame on one side of the equal sign, the S' frame on the other side.

$$r^2 - r'^2 = c^2t^2 - c^2t'^2$$
$$r^2 - c^2t^2 = r'^2 - c^2t'^2$$

There is this quantity, a generalized displacement (call it s) which is the same in the two inertial reference frames.

$$s^2 = s'^2$$

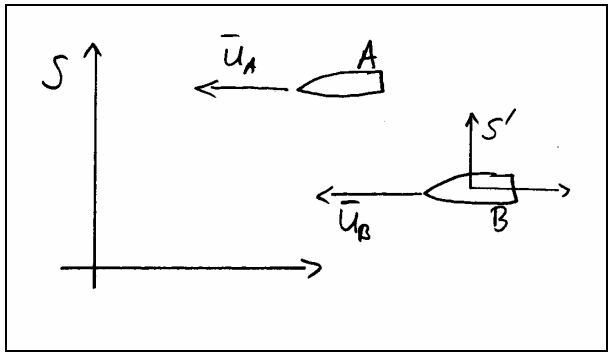
We see that the quantity (ict) "acts like" a component of displacement along a fourth axis. The *interval* between any two events in space-time is $\Delta s^2 = \Delta x^2 + \Delta y^2 + \Delta z^2 - c^2\Delta t^2$. The interval is invariant under the Lorentz Transformation. That is, as measured in any two inertial frames, $\Delta s^2 = \Delta s'^2$. This is an extension of the invariance of lengths under a rotation of the coordinate axes.

d. Transformation of velocities

Since displacements and time intervals are transformed, obviously relative velocities won't add simply, either.

In the S' frame an object moves with constant velocity along the x axis; $u'_x = \dfrac{dx'}{dt'}$. Transform to the S frame; $u'_x = \dfrac{\gamma(dx - vdt)}{\gamma\left(dt - \dfrac{v}{c^2}dx\right)} = \dfrac{\dfrac{dx}{dt} - v}{1 - \dfrac{v}{c^2}\dfrac{dx}{dt}} = \dfrac{u_x - v}{1 - \dfrac{v}{c^2}u_x}$ and similarly for the y and z components. While dy & dz are not contracted, dt is still dilated.

example:



$u_A = -0.5c$ and $u_B = -0.8c$, both as measured in the S frame. The S' frame rides along with spaceship B. Therefore, $\vec{v} = \vec{u}_B$.

$$u'_A = \frac{u_A - v}{1 - \frac{v}{c^2}u_A} = \frac{-0.5c - (-0.8c)}{1 - \frac{0.8c}{c^2}0.5c} = \frac{c}{2}$$

Be careful with the directions of the velocities.

Note that when $u << c$ and $v << c$, then $\frac{vu}{c^2} \to 0$ and $u' = u - v$. On the other hand, if $u = c$, then $u' = \frac{c - v}{1 - \frac{cv}{c^2}} = \frac{c\left(1 - \frac{v}{c}\right)}{1 - \frac{v}{c}} = c$.

D. Energy and Momentum

We require that all the "Laws" of Physics be the same in all inertial reference frames. We require further that when $v << c$, we recover the familiar Newtonian forms of the "Laws." This latter requirement is called a *Correspondence Principle*. What are those "Laws"?

1. Conservation of Momentum

We define a *relativistic momentum* so that the two conditions above are satisfied.

$$\vec{p} = \gamma m\vec{u}$$

This m is the *rest mass*—the mass measured by an observer at rest with respect to the object. This quantity should be the same in all inertial reference frames. With this definition, $\vec{p}_{initial} = \vec{p}_{final}$ in all inertial reference frames.

2. Relativistic Energy

a. Work-energy theorem (one dimensional)

The work done by a force on an object changes its kinetic energy, thus

$$\Delta K = W_{12} = \int_{x_1}^{x_2} F dx .$$

$$\Delta K = \int_{x_1}^{x_2} \frac{dp}{dt} dx$$

$$\Delta K = \int_{t_1}^{t_2} \frac{dp}{dt}\frac{dx}{dt} dt$$

$$\Delta K = \int u dp$$

Integrate by parts.

$$\Delta K = up\Big|_{u_1}^{u_2} - \int_{u_1}^{u_2} p du$$

$$\Delta K = up\Big|_{u_1}^{u_2} - \int_{u_1}^{u_2} \frac{mu}{\sqrt{1-\frac{u^2}{c^2}}} du$$

Recall that $udu = \frac{du^2}{2}$.

$$\Delta K = up\Big|_{u_1}^{u_2} - \frac{m}{2}\int \frac{du^2}{\sqrt{1-\frac{u^2}{c^2}}}$$

Look up the form $\int \frac{dx}{\sqrt{a+bx}}$ in a math tables book.

$$\Delta K = up\Big|_{u_1}^{u_2} - \frac{m}{2}\left[\frac{2\sqrt{1-\frac{u^2}{c^2}}}{-\frac{1}{c^2}}\right]_{u_1}^{u_2}$$

$$\Delta K = \left[\frac{mu^2}{\sqrt{1-\frac{u^2}{c^2}}} + mc^2\sqrt{1-\frac{u^2}{c^2}}\right]_{u_1}^{u_2}$$

$$\Delta K = \left[\frac{mu^2 + mc^2 - mu^2}{\sqrt{1-\frac{u^2}{c^2}}}\right]_{u_1}^{u_2} = \Delta\left[\frac{mc^2}{\sqrt{1-\frac{u^2}{c^2}}}\right]$$

Now, if we started from rest, then $u_1 = 0$ and $u_2 = u$ and $\Delta K = \dfrac{mc^2}{\sqrt{1-\frac{u^2}{c^2}}} - mc^2$. Therefore, we define the *relativistic kinetic energy* to be

$$K = \frac{mc^2}{\sqrt{1-\frac{u^2}{c^2}}} - mc^2 .$$

The quantity mc^2 is called the *rest energy*, because it's independent of u. The *total relativistic energy* is $E = K + mc^2 + V$, where V is the potential energy, if any. If $V = 0$, then

$$E = K + mc^2 = \gamma mc^2 .$$

b. Energy-momentum relation

Take a look at the quantity ($V = 0$)

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

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

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

For photons, $m = 0$ and $E = pc$.

c. Units of mass-energy

It is convenient to express energy in units of electron-volts (eV). An *electron-volt* is the energy gained by an electron upon being accelerated through a one Volt potential difference. Thus 1 eV = 1.60×10^{-19} Joules. The rest energy of an electron is

$$mc^2 = 9.11x10^{-31}\,kg\left(3x10^8\,m/\sec\right)^2 = 8.20x10^{-14}\,J = 0.511x10^6\,eV = 0.511MeV\ .$$

Often, mass is expressed in terms of MeV/c^2 so that the electron mass is $0.511MeV/c^2$. Sometimes, the c^2 is dropped, but it's understood to still be there. Similarly, momentum is expressed in terms of MeV/c, since pc = units of MeV.

3. Relativistic Mechanics

a. Force

We want the "Laws" of Mechanics to be invariant under the Lorentz Transformation. Also, we want to recover the classical result when $u << c$. So, we define the *relativistic force* component to be $F_x = \dfrac{dp_x}{dt}$, where $p_x = \dfrac{mu_x}{\sqrt{1-\dfrac{u^2}{c^2}}}$.

Let's say the motion and force are entirely along the x-direction.

$$F = \frac{d}{dt}\left[\frac{mu}{\sqrt{1-\frac{u^2}{c^2}}}\right] = \frac{m}{\sqrt{1-\frac{u^2}{c^2}}}\frac{du}{dt} + mu\frac{d}{dt}\left[\frac{1}{\sqrt{1-\frac{u^2}{c^2}}}\right]$$

$$F = \frac{m}{\sqrt{1-\frac{u^2}{c^2}}}\frac{du}{dt} + mu\left(-\frac{1}{2}\right)\left(1-\frac{u^2}{c^2}\right)^{-3/2}\left(-\frac{2u}{c^2}\right)\frac{du}{dt}$$

$$F = m\frac{du}{dt}\left[\left(1-\frac{u^2}{c^2}\right)^{-1/2} + \frac{u^2}{c^2}\left(1-\frac{u^2}{c^2}\right)^{-3/2}\right]$$

$$F = m\left(\frac{1}{1-\frac{u^2}{c^2}}\right)^{3/2}\frac{du}{dt}$$

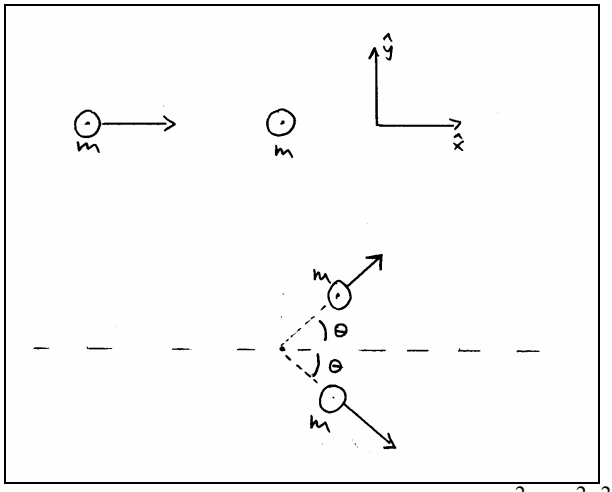
Solve for the acceleration.

$$\frac{du}{dt} = \frac{F}{m}\left(1-\frac{u^2}{c^2}\right)^{3/2}$$

The result is, that as $u \to c$, $\frac{du}{dt} \to 0$, no matter how large the applied force. At the other extreme, when $u << c$, $\frac{du}{dt} = \frac{F}{m}$.

b. Collisions—conservation of momentum

Consider the collision of two billiard balls. They have equal masses, m. Let's say that one ball is initially at rest while the second ball has momentum p_o and energy E_o before the collision. After the collision, both balls have the same energy, E, and mass, m. It's an elastic collision. Momentum and energy are conserved.



In the x direction, $p_o = 2p\cos\theta$. Substitute for p_o and p using $E^2 = p^2c^2 + m^2c^4$.

$$\frac{1}{c}\sqrt{E_o^2 - m^2c^4} = \frac{2}{c}\sqrt{E^2 - m^2c^4}\cos\theta$$

Conservation of energy allows us to eliminate E, since it was given that $E_o + mc^2 = 2E$. Keep in mind that E_o is the relativistic total energy of the second ball, while mc^2 is the rest energy of the first (target) ball. At the same time, we solve for $\cos\theta$, the cosine of the scattering angle.

$$\cos\theta = \frac{\sqrt{E_o^2 - m^2c^4}}{\sqrt{\left(E_o + mc^2\right)^2 - 4m^2c^4}} = \sqrt{\frac{\left(E_o + mc^2\right)\left(E_o - mc^2\right)}{\left(E_o + 3mc^2\right)\left(E_o - mc^2\right)}}$$

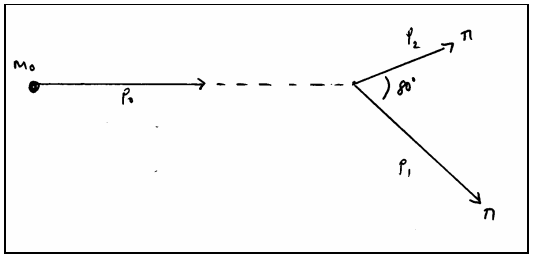
$$\cos\theta = \sqrt{\frac{E_o + mc^2}{E_o + 3mc^2}}$$

In the classical limit, $E_o \approx mc^2$ and therefore

$\cos\theta \approx \sqrt{\frac{2mc^2}{4mc^2}} = \sqrt{\frac{1}{2}} \Rightarrow \theta = 45^o$. But, as $E_o >> mc^2$, $\cos\theta \to 1 \Rightarrow \theta \to 0^o$!

c. Decay of a high-energy particle

An unidentified high-energy particle is observed to decay into two pions (π mesons), as shown.



Knowing the momenta and masses of the decay products, we determine the mass of the incident particle, hoping to identify it.

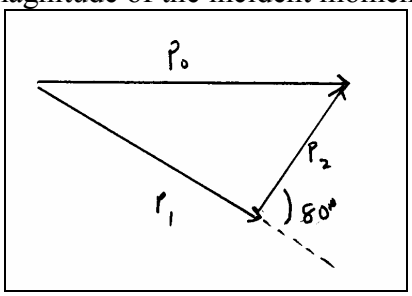
$$p_1 = 910\frac{MeV}{c},\ p_2 = 323\frac{MeV}{c},\ m_1c^2 = m_2c^2 = mc^2 = 139.6Mev.$$

The energy and momenta are conserved. The total energy is

$$E_o = E_1 + E_2 = \sqrt{p_1^2c^2 + m^2c^4} + \sqrt{p_2^2c^2 + m^2c^4}$$

$$E_o = 921MeV + 352MeV = 1273MeV$$

The quickest way to obtain the magnitude of the incident momentum is to use the law of cosines:



$$p_o^2c^2 = p_1^2c^2 + p_2^2c^2 - 2p_1p_2c^2\cos\theta = 1034229MeV^2$$

$$p_oc = 1017MeV$$

Now that we have the total energy and the kinetic energy, the mass is obtained from

$$E_o^2 = p_o^2c^2 + m_o^2c^4$$

$$m_oc^2 = \sqrt{E_o^2 - p_o^2c^2} = 765MeV$$

Evidently, the incident particle was a ρ meson. What was its speed before it decayed? Well, the total energy is also $E_o^2 = \dfrac{m_o^2c^4}{1-\dfrac{u^2}{c^2}}$, so solve that for *u*.

$$\frac{u}{c} = 1 - \sqrt{\frac{m_o^2c^4}{E_o^2}} = 0.8$$

d. Mass-energy equivalence

When we speak of the total energy being conserved that includes the total rest energy. For instance, consider the decay of a neutron that is initially at rest.

$$n \rightarrow p + e + \bar{\nu}$$

The neutron decays into a proton, an electron and an anti-neutrino. The three product particles are observed to have total kinetic energy of $K = 0.781\ MeV$. The initial energy is just the rest energy of the neutron, $E_i = 939.57\ MeV$. The total final energy is

$$E_f = m_pc^2 + m_ec^2 + K = 938.28MeV + 0.511MeV + 0.781MeV = 939.57MeV$$

Notes: i) The rest energy of the anti-neutrino is too small to bother with.

ii) Keep in mind the rounding of numbers and significant digits when substituting numerical values into the formulae.

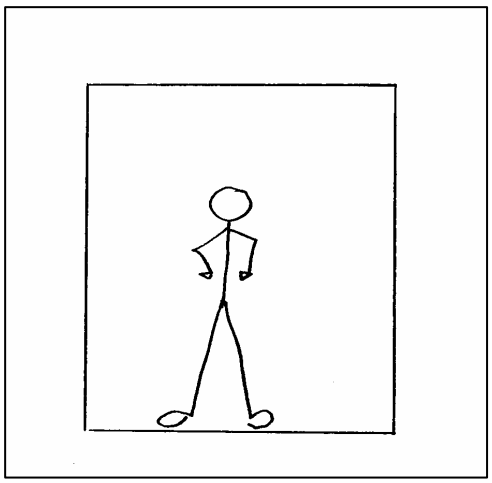
iii) Notice that $m_n \neq m_p + m_e$. A portion of the neutron's rest energy has been converted into kinetic energy.

E. A Hint of General Relativity

1. Equivalence

In Special Relativity it is asserted that all inertial reference frames are equivalent—the "laws" of physics are the same in all inertial reference frames. No experiment done in one frame can detect its uniform motion relative to another frame. Can the same be said for reference frames that have a relative acceleration?

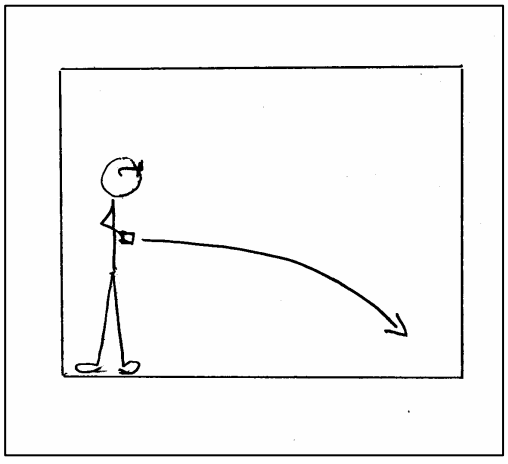
a. Elevator



Recall the past discussion of a person standing in an elevator. If the elevator moves perfectly smoothly and there are no floor indicator lights, then the person inside will have no perception of the elevator's motion, except for feeling perhaps the elevator floor pressing upward on his or her feet. [Keep in mind: the person gets no information from any source outside the reference frame of the elevator.] Contrast this situation with that of another person standing in a similar elevator, but this elevator is simply resting level on the Earth's surface. The person in this elevator also feels the floor pressing upward on his or her feet, also has no perception of the elevator's motion. We, as omniscient external observers, know that this second elevator is resting on the surface of a planet, and that what the person inside is experiencing is the gravitational force exerted by that planet. The point is that there is no experiment that either of the persons inside the elevators could perform that would distinguish between the two situations. Pendula would swing back and forth just the same; projectiles would follow the same kinds of arcs, etc.

b. Light and gravity

Imagine ourselves as observers far from any source of gravitational force. Nearby, we observe a closed "elevator" which is accelerating, relative to us, at a constant rate, $\vec{a}_o$. A person standing inside the "elevator" sends a series of light pulses toward one wall—he or she and we see the light pulses dropping toward the floor as they approach the wall. The light follows a curved path inside the elevator.



The Postulate of General Relativity asserts that the "laws" of physics have the same form for observers in any frame of reference, regardless of its acceleration relative to another frame. We have seen that an accelerated frame is equivalent to one in a gravitational field. It follows that the force of gravity must affect a beam of light just as it affects the motion of a massive projectile. Indeed, experiment has shown that it does. But, light has no mass.

2. Curvature

Classically, we would say that a mass, such as a planet, exerts a gravitational force on another mass, such as a moon or a person. However, a person in an "elevator" cannot determine whether his or her "elevator" is in the gravitational field of a planet or is being accelerated at a constant rate by, say rocket motors. If the "elevator" is in a gravitational field, we can nonetheless mathematically transform the "laws" of physics into versions of the same mathematical form that do not include gravity yet which make equally accurate predictions of the motions of particles and of light beams.

What Einstein did was to formulate such a version of the "laws" of motion. Objects and light beams move always in straight lines, but in a curved space-time. Empty space-time is flat, but the presence of mass at any location curves space-time to a degree proportional to the amount of mass that is present.

Predictions of General Relativity:

Precession of orbits—Mercury

Gravitational redshift—time runs slower in intense gravitational field

Gravitational lensing—light paths curved

Gravitational waves—ripples in space time(?); slowing binary neutron stars

II. Quantum Theory

A. Black Body Radiation

1. Equilibrium Between Matter and Radiation

a. Thermal equilibrium

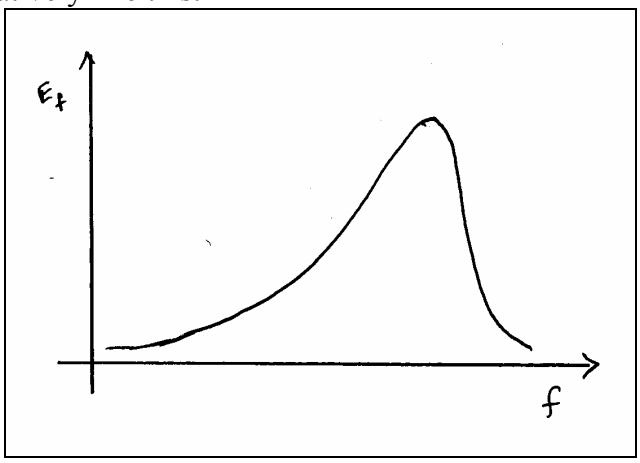
Imagine a closed oven, maintained at a constant temperature, T_o. Inside, E-M waves bounce from wall to wall, being absorbed and re-emitted over and over. Ultimately, the radiation is rendered homogeneous, isotropic and unpolarized. A thermometer placed in the center of the oven will stabilize at a temperature $T = T_o$. The radiation is said to be in *thermal equilibrium* with the walls of the oven.

b. Emissivity

From thermodynamics (Kirchhoff) the power radiated by a body in thermal equilibrium with radiation is expressed

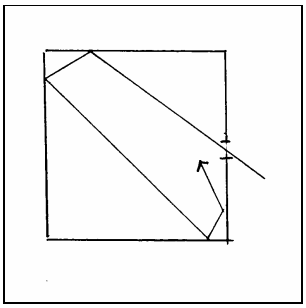
$$J(f,T) = \frac{E_f}{A_f},$$

where J is the power radiated per unit area per unit frequency, E_f is the *emissivity* or intensity per unit frequency of the radiation emitted by the body and , A_f is the fractional absorption of the body for radiation of frequency f. Notice that the substance of which the body is made is not important. For a *black body*, $A_f = 1.0$ for all f. The observed spectrum of radiation emitted by a black body looks qualitatively like this:



c. Model for a black body

One physical model for an ideal black body is a small opening in the wall of a heated cavity. Because the opening is small, a light ray entering through the opening is very unlikely to bounce back out again. Conversely, any light ray that exits through the opening will have reached equilibrium with the interior walls, having bounced off the walls many times. The black body is not the oven as a whole, but the opening in the oven wall.



2. Stefan-Boltzmann "Law"

a. Emissivity

The total emissivity is obtained by integrating $E_f df$.

$$E = \int_0^\infty E_f \, df$$

This quantity was found experimentally by J. Stefan to be proportional to T^4.

$$E = \sigma T^4$$

Subsequently, Boltzmann derived this result from Maxwell's equations. The proportionality constant is called the Stefan-Boltzmann constant, $\sigma = 5.67x10^{-8} \frac{W}{m^2 K^4}$ or $Wm^{-2}K^{-4}$. For non-black bodies, $E = a\sigma T^4$, where $a < 1$.

b. Wien's displacement "law"

Experimentally, $\lambda_{\max} \cdot T = 2.898x10^{-3} m \cdot K$, or $\frac{c}{f_{\max}} \cdot T = 2.898x10^{-3} m \cdot K$.

3. Rayleigh-Jeans "Law"

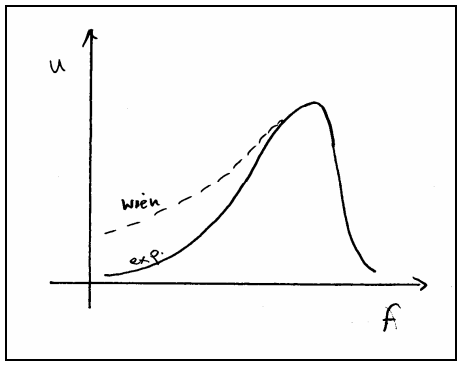
a. Wien's exponential "law"

$$u(f,T) = \frac{4}{c} J(f,T),$$

where u is the energy per unit volume per unit frequency. As derived from thermodynamics and Maxwell's equations,

$$u(f,T) = Af^3 e^{-\beta \cdot f / T}$$

where A and β are constants. When tested by experiment, this expression fails at long wavelengths. But, Wien's exponential "law" fits well near the peak, at $f_{\max}$.

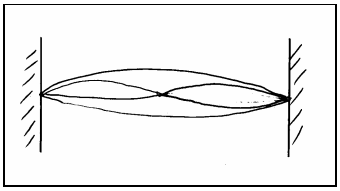


b. Rayleigh's approach

Rayliegh proposed that the energy density be expressed as the product of the number of standing wave modes in the cavity and the average energy of each mode. Let $N(f)df$ be the number of modes between f and $f+df$.

$$udf = N(f)\overline{E}df$$

We need to obtain expressions for $N(f)$ and for $\overline{E}$. Picture standing waves in a cavity. In one dimension:



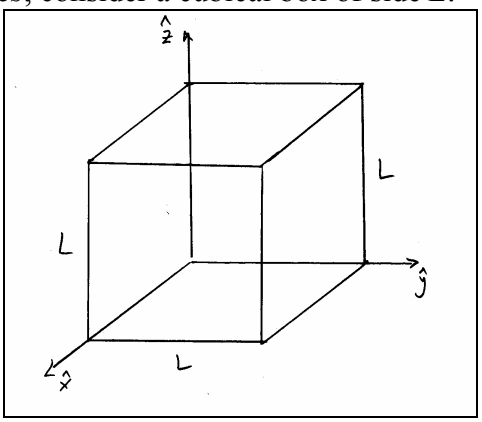
We imagine the whole volume of the cavity occupied with standing E-M waves, of many different frequencies. The radiation is in equilibrium with the walls of the cavity, at temperature T. Classically, the probability that there will be a mode of energy, E, in the cavity is given by the Boltzmann distribution.

$$P(E) = e^{-E/k_B T}$$

The average energy per mode is therefore

$$\overline{E} = \frac{\int_0^\infty E e^{-E/k_B T}\, dE}{\int_0^\infty e^{-E/k_B T}\, dE} = \frac{(k_B T)^2}{k_B T} = k_B T$$

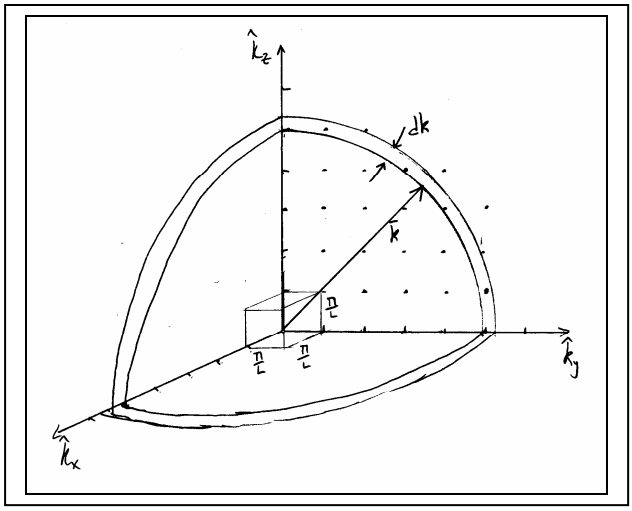
As for $N(f)$, the *density of states*, consider a cubical box of side L.



Inside the box, the x-component of the E-field satisfies the wave equation $\nabla^2 E_x + k^2 E_x = 0$. If we assume that $E_x = u(x)v(y)w(z)$, then we get three separated equations. The one for $u(x)$ is

$$\frac{d^2 u}{dx^2} + k_x^2 u = 0,$$

which has the solution $u(x) = u_o \sin k_x x$. Similarly, $v(y) = v_o \sin k_y y$ and $w(z) = w_o \sin k_z z$. The quantity k^2 is like the square of a radius in k-space: $k^2 = k_x^2 + k_y^2 + k_z^2$. Since we must have standing waves in the box, with the electric field vanishing at the walls, $k_x = \frac{n_x \pi}{L}$, $k_y = \frac{n_y \pi}{L}$ and $k_z = \frac{n_z \pi}{L}$, where the n_x, n_y and n_z are positive integers. In other words, only discrete points in k-space designate the allowed energy modes in the cubical cavity. So, we count the number of k-points lying in a spherical shell of radius k and thickness dk.



We see that each point occupies a volume $\left(\frac{\pi}{L}\right)^3$ so the number of points in the shell is

$$N(k)dk = \frac{\frac{1}{8}4\pi k^2 dk}{\left(\frac{\pi}{L}\right)^3} = \frac{Vk^2 dk}{2\pi^2},$$

where $V = L^3$. Finally, there are two perpendicular polarizations for each mode, so the number of modes per unit volume (the *density of states*) is

$$\frac{N(k)}{V}dk = \frac{k^2 dk}{\pi^2}.$$

In terms of frequency, $\frac{N(f)}{V}df = \frac{8\pi f^2 df}{c^3}$, since $f = \frac{kc}{2\pi}$.

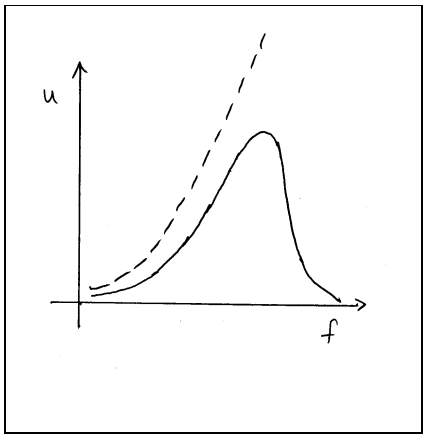
At last the energy density is

$$u(f,T)df = N(f)\bar{E}df = \frac{8\pi f^2}{c^3}k_B T df.$$

Alternatively, the energy density in terms of wavelength is

$$u(\lambda,T)d\lambda = \frac{8\pi}{\lambda^4}k_B T d\lambda$$

Compared with the observed black body spectrum, the Rayleigh-Jeans "law" is seen to diverge as $\lambda \to 0$.



What do we have so far? We have regarded the range of allowed energies for a standing wave in the cavity to be a continuous variable. The result obtained is proportional to one over the fourth power of the wavelength. This diverges for small wavelengths (the ultraviolet catastrophe).

4. Planck's "Law"

a. Quantized energy modes

Rather than visualize standing E-M waves inside a cavity, consider the atoms that form the walls of the cavity. These atoms vibrate and absorb or emit E-M waves. Let's assume that the energies of these oscillators can change only in discrete steps, rather than continuously.

Postulate: $E_n = nhf$ where n is a positive integer. No other energy values are allowed.

The average energy per vibration mode is a discrete sum $\overline{E} = \dfrac{\sum_{n=0}^{\infty} E_n e^{-E_n/k_BT}}{\sum_{n=0}^{\infty} e^{-E_n/k_BT}}$.

Firstly, the denominator. . . $\sum_{n=0}^{\infty} e^{-\frac{nhf}{k_BT}} = \dfrac{1}{1-e^{-\frac{hf}{k_BT}}}$. This follows from the series of the form

$\sum_{n=0}^{\infty} r^n = \dfrac{1}{1-r}$ with $r = e^{-\frac{hf}{k_BT}}$.

Secondly, substituting this into $\overline{E}$ . . .

$$\overline{E} = \left(1-e^{-hf/k_BT}\right)\sum_{n=0}^{\infty} nhfe^{-nhf/k_BT} = hf\left(1-e^{-hf/k_BT}\right)\sum_{n=0}^{\infty} ne^{-nhf/k_BT}.$$

Notice that $\dfrac{d}{d\left(\frac{hf}{k_BT}\right)}\sum_n e^{-nhf/k_BT} = -\sum_n ne^{-nhf/k_BT} = \dfrac{d}{d\left(\frac{hf}{k_BT}\right)}\dfrac{1}{1-e^{-hf/k_BT}}$. Therefore, we have

$$\overline{E} = -hf\left(1-e^{-hf/k_BT}\right)\frac{d}{d\left(\frac{hf}{k_Bt}\right)}\left(\frac{1}{1-e^{-hf/k_BT}}\right) = -hf\left(1-e^{-hf/k_BT}\right)\frac{-e^{-hf/k_BT}}{\left(1-e^{-hf/k_BT}\right)^2}$$

$$\overline{E} = \frac{hfe^{-hf/k_BT}}{\left(1-e^{-hf/k_BT}\right)} = \frac{hf}{e^{hf/k_BT}-1}$$

This result is multiplied by the number of modes having frequency f, $N(f) = \dfrac{8\pi f^2}{c^3}$, to obtain. . .

b. Planck's distribution formula

$$u(f,T) = \frac{8\pi f^2}{c^3} \cdot \frac{hf}{e^{hf/k_BT} - 1} = \frac{8\pi h f^3}{c^3\left(e^{hf/k_BT} - 1\right)}.$$

What do we have?

i) Assume that oscillators or standing waves are limited to discrete values of energy, $E_n = nfh$.

ii) For high f, the $\frac{1}{e^{hf/k_BT} - 1} \to 0$, therefore the probability that a high frequency or short wavelength mode is *occupied* or present is very low.

iii) An oscillator that emits energy can change its energy only in steps of $\Delta E = nhf$, where f is the vibration frequency of the oscillator.

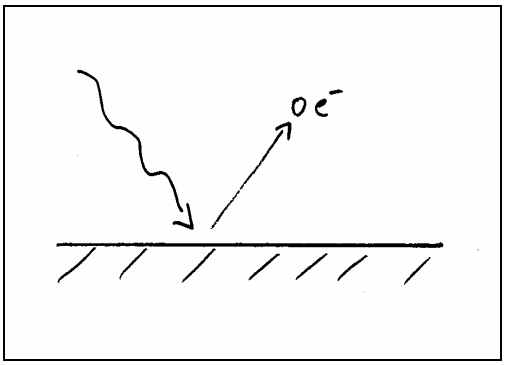
Fitting Planck's formula to the observed black body radiation yields a value for Planck's constant, $h = 6.626 \times 10^{-34}$ J sec.

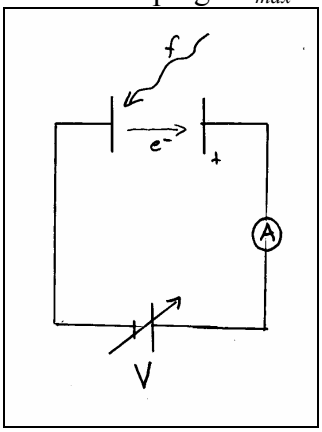
B. Photons

1. Photo-electric Effect

a. Kinetic energy

When a metal surface is exposed to intense monochromatic E-M radiation, electrons are expelled from the metal. A certain amount of energy, called the *work function*, is required to liberate an electron from the metal. Once liberated, the *photoelectrons* have a distribution of kinetic energies. We can evaluate the maximum, K_{max}, of the kinetic energy distribution by applying a voltage, V_s, large enough to stop the fastest-moving electron from escaping. $K_{max} = eV_s$.



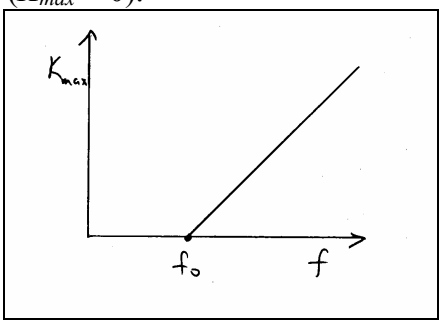


Finding: K_{max} is independent of the incident intensity, while the *photocurrent* is proportional to the incident intensity.

Interpretation: Increasing the intensity of the incident radiation does not increase the left over kinetic energy of the photoelectrons, only the number of electrons ejected from the metal.

b. Work function

Finding: K_{max} is proportional to the frequency, f, of the incident radiation with an f_o below which no photoelectrons are produced ($K_{max} = 0$).



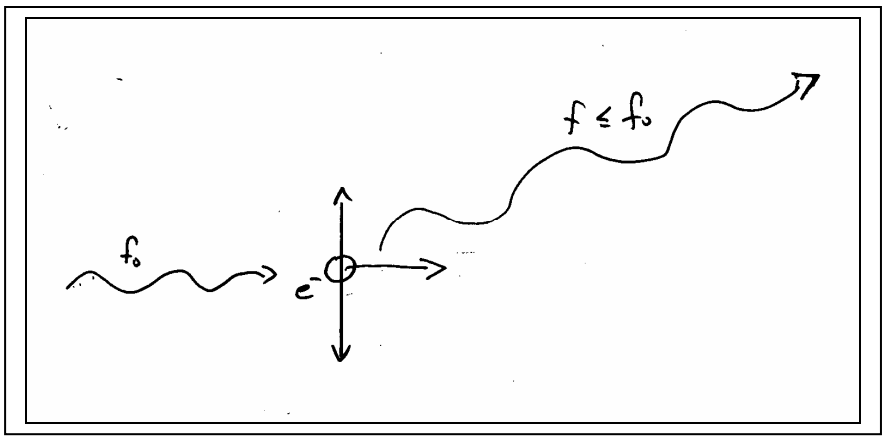
Interpretation: $K_{\max} = eV_s = hf - \phi$, where ϕ is the work function of the metal, f is the frequency of the incident radiation and h is Planck's constant. That is, the light is absorbed in discrete portions, $\Delta E = hf$, only. If $hf < \phi$, then no photoelectrons are produced; if $hf > \phi$, increasing the intensity only liberates more electrons, each one absorbing one hf and no more. If the incident frequency is such that $hf \leq \phi$, then $K_{max} = 0$ and no electrons escape from the metal.

We conclude that E-M radiation is not a continuous wave form, but consists of discrete, localized wave packets, called a *photon*. Either a photon is absorbed entirely, or not at all. Likewise, light is emitted in the form of one or more discrete photons.

2. Compton Effect

a. Absorption of a classical E-M wave

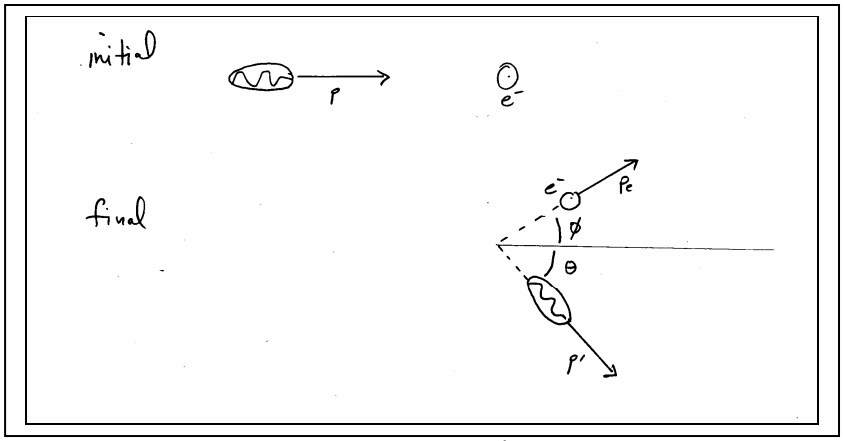
Suppose a continuous E-M wave (frequency f_o) is incident on a free electron. The classical prediction is that the electron will experience acceleration causing the electron to oscillate transversely and to move in the direction the light wave is traveling. The accelerated electron in its turn emits a new E-M wave. Since the electron is now moving, the emitted wave has a Doppler-shifted frequency. The longer the electron is exposed to the incident radiation, the faster it translates and the greater is the Doppler shift. The intensity of the incident radiation also influences the Doppler shift, since it influences the electron's acceleration.



This is <u>not</u> what is observed.

b. Collision between a photon and an electron

Consider a collision between an x-ray photon and a stationary free electron.



Qualitatively, what is observed is that the frequency, f', of the scattered photon depends only on the scattering angle, θ. Usually, the effect is expressed in terms of the shift in wavelength, thusly:

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

The quantity $\frac{h}{m_e c} = 0.0243$ Å is called the *Compton wavelength* of the electron.

c. Theoretical treatment as a collision

As a collision between two particles, both energy and momentum are conserved. It is necessary to use the relativistic forms of energy and momentum, since the photon is certainly moving at a speed close to, if not equal to *c*.

Energy

$$E + m_e c^2 = E' + E_e$$

$$hf + m_e c^2 = hf' + E_e$$

momentum components

$$p = p'\cos\theta + p_e \cos\phi$$

$$0 = p_e \sin\phi - p'\sin\theta$$

The first step is to eliminate ϕ from the momentum component equations.

$$p = p'\cos\theta + p_e\sqrt{1 - \left(\frac{p'}{p_e}\sin\theta\right)^2}$$

Square both sides and solve for $p_e^2 = p'^2 + p^2 - 2pp'\cos\theta$. For the photon, $p = \frac{E}{c} = \frac{hf}{c} = \frac{h}{\lambda}$.

On the other hand, the energy of the electron is also $E_e^2 = p_e^2 c^2 + m_e^2 c^4$. Substitute for E_e and p_e.

$$\left(hf - hf' + m_e^2 c^4\right)^2 = c^2\left[\left(\frac{hf'}{c}\right)^2 + \left(\frac{hf}{c}\right)^2 - 2\frac{h^2 ff'}{c^2}\cos\theta\right] + m_e^2 c^4$$

$$2h^2 ff' + 2hfm_e c^2 - 2hf'm_e c^2 = -2h^2 ff'\cos\theta$$

$$-2hm_e c^2(f - f') = 2h^2 ff'(1 - \cos\theta)$$

$$\frac{f - f'}{ff'} = \frac{1}{f'} - \frac{1}{f} = \frac{h}{m_e c^2}(1 - \cos\theta)$$

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

This *Compton shift formula* exactly matches the observations. We conclude, then, that a photon behaves like a particle having relativistic energy *hf* and momentum $\frac{h}{\lambda}$.

C. Matter Waves

We find that light is quantized and may be regarded in some circumstances as being particles of zero mass, momentum h/λ, and energy hf. Some persons use the quantum point of view exclusively. Might it be useful to investigate whether non-zero mass particles can be treated as having wave properties?

1. deBroglie's Postulate

a. deBroglie wavelength

For a photon, $p = h/\lambda$. In a similar vein, define for any particle a wavelength $\lambda = h/p$, where p is the momentum (magnitude) of the particle. Further, if E is the total relativistic energy of the particle, a frequency is defined as $f = E/h$.

b. Phase velocity of a wave

The phase velocity of a wave is $v_p = f\lambda = E/p$. If the relativistic expressions for E & p are used, then we get a phase velocity for a massive particle

$$v_p = \frac{mc^2}{\sqrt{1 - v^2/c^2}} \frac{\sqrt{1 - v^2/c^2}}{mv} = \frac{c^2}{v}.$$

2. Group velocity

A particle occupies a limited volume, so if we are to represent it with a waveform, the waveform amplitude must be non-zero only in a limited region of space. We accomplish this by superimposing many waves of differing wavelengths and amplitudes and phases.

a. Waves in one dimension

$$y = A\cos\left(\frac{2\pi x}{\lambda} - 2\pi f t\right) \text{ and } v_p = \lambda f .$$

We define the angular frequency, $\omega = 2\pi f$ and the wave number, $k = 2\pi/\lambda$. Using these quantities,

$$y = A\cos(kx - \omega t) \text{ and } v_p = \frac{\omega}{k}.$$

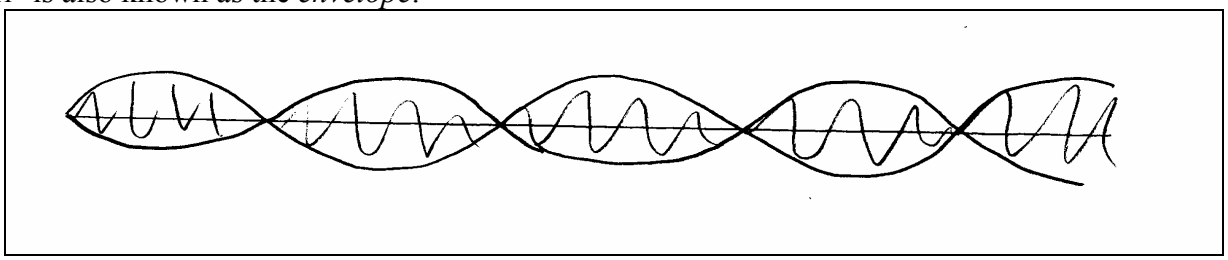
b. Beats

Superimpose two waves: $y = y_1 + y_2 = A\cos(k_1 x - \omega_1 t) + A\cos(k_2 x - \omega_2 t)$.

$$y = 2A\cos\left(\frac{1}{2}\{(k_2 - k_1)x - (\omega_2 - \omega_1)t\}\right) \cdot \cos\left(\frac{k_1 + k_2}{2}x - \frac{\omega_1 + \omega_2}{2}t\right).$$

[Note: cos(a) + cos(b) = 2cos(½ (a-b)·cos(½ (a+b).]

We have a traveling wave whose amplitude is not constant. $y = A'\cos(k'x - \omega' t)$, where $k' = \frac{k_1 + k_2}{2}$ and $\omega' = \frac{\omega_1 + \omega_2}{2}$. The time-varying amplitude is $A' = 2A\cos(\Delta k x - \Delta\omega t)$. This A' is also known as the *envelope*.



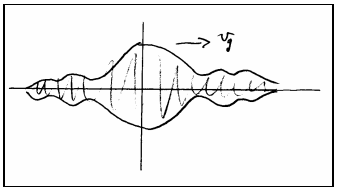
The envelope also travels at a speed called the *group velocity*, $v_g = \frac{\Delta\omega/2}{\Delta k/2} = \frac{\Delta\omega}{\Delta k}$.

Evidently, from the form of A', $\Delta k \cdot \Delta x = 2\pi$ and $\Delta\omega \cdot \Delta t = 2\pi$. With sound waves, the regular rises and falls of the amplitude are known as *beats*.

c. Wave packets

The beating waveform still extends to ± ∞ in *x*. That combination is constructed only of two waves having the same amplitude but slightly different frequencies or wave numbers. We can construct a *wave packet* that is non-zero only in a small region by superimposing many waves having different amplitudes, and having a range of wave numbers centered on a k_o. The mathematics of the superposition will be explored in paragraph 4. For the time being, we are concerned with the group velocity of the wave packet:

$v_g = \left.\frac{d\omega}{dk}\right|_{k_o} = v_p\big|_{k_o} + k\left.\frac{dv_p}{dk}\right|_{k_o}$, since $\omega = kv_p$.



d. Dispersion

If $v_p = v_p(\lambda)$, then the medium through which the waves are propagating is said to be *dispersive*. The individual harmonic waves travel at different speeds, so the wave packet or wave group spreads out with time.

e. Application to a massive particle

We consider a massive particle (in this context, massive means having a non-zero mass), such as the electron. Its mass is *m* and it is moving uniformly with speed *v*. We postulate that the motion of the particle can be modeled by a traveling wave packet with frequency $f_o = E/h$ and wavelength $\lambda_o = h/p$ where *E* is the total relativistic energy and *p* the total relativistic momentum of the particle. The wave packet would be constructed by a superposition of harmonic waves having wavelengths centered on λ_0.

The phase velocity is $v_p = f\lambda = E/p$. Putting E in terms of *p* and *p* in terms of the wave number *k* yields $[E = \frac{p^2}{2m} \text{ and } p = \frac{h}{2\pi k}]$

$$v_p = c\sqrt{1+\left(\frac{mc}{\hbar k}\right)^2}\ , \text{ where } \hbar = h/2\pi\ .$$

From this expression, we obtain the group velocity

$$v_g = \left.\frac{d\omega}{dk}\right|_{k_o} = v_p\big|_{k_o} + k\left.\frac{dv_p}{dk}\right|_{k_o}$$

$$v_g = c\sqrt{1+\left(\frac{mc}{\hbar k_o}\right)^2} + k_o\,\frac{c}{2}\,\frac{(-2)\left(\frac{mc}{\hbar}\right)^2\frac{1}{k_o^3}}{\sqrt{1+\left(\frac{mc}{\hbar k_o}\right)^2}}$$

$$v_g = \frac{c}{\sqrt{1+\left(\frac{mc}{\hbar k_o}\right)^2}} = \frac{c^2}{v_p\big|_{k_o}}\ .$$

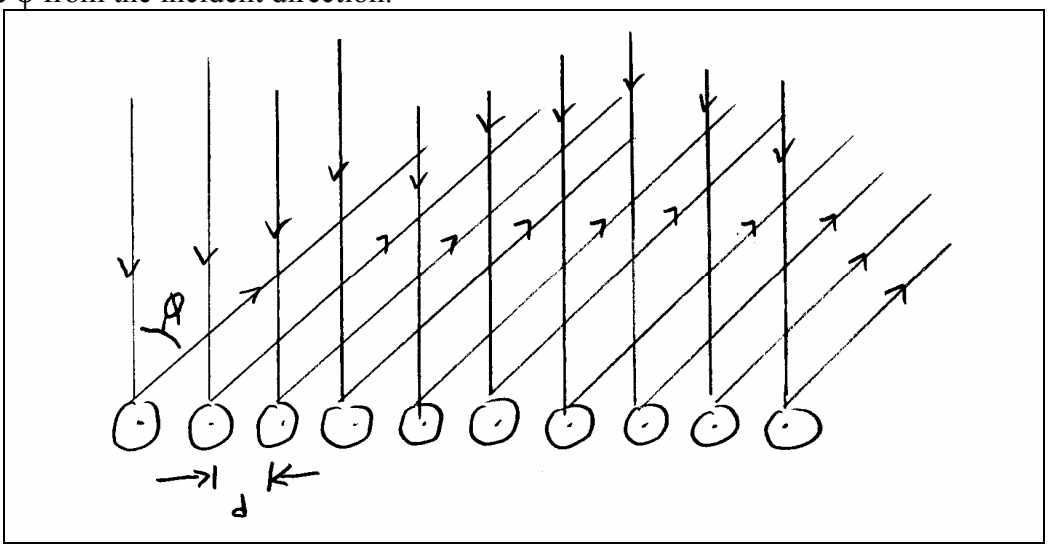
Previously, we saw that the phase velocity also equals c^2/v. Therefore, the group velocity of the wave packet coincides with the velocity of the massive particle: $v_g = v$.

3. Davisson-Germer experiment

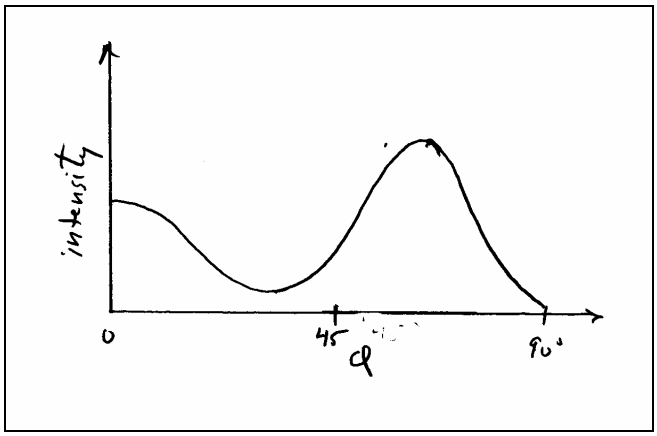
How might wave-like behavior of massive particles be observed? One of the prominent characteristics of waves is the fact that they interfere with each other to form interference patterns. When a monochromatic light beam is incident on a diffraction grating, a characteristic interference pattern is observed, entirely understood in terms of the constructive and destructive interference among the scattered light waves.

a. Electron diffraction

Consider a mono-energetic beam of electrons incident on a crystal lattice. The electrons will be scattered from regularly spaced centers. We count the number of electrons that are scattered at an angle φ from the incident direction.



We do not observe either a uniform distribution with scattering angle, nor a sharp peak at $\varphi = 0$ and no particles elsewhere. Rather, we observe a distribution of scattered electrons something like this:



b. Interpretation

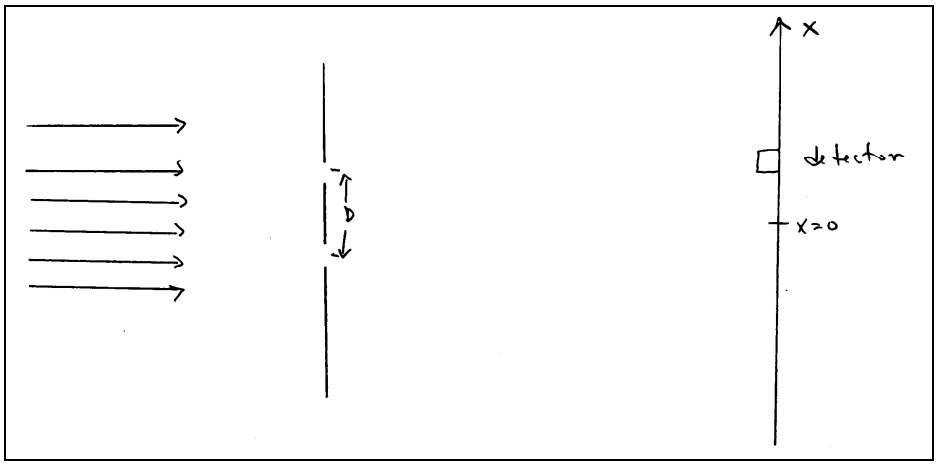
If this result is interpreted as wave-like interference, then the peak at $\varphi = \varphi_{max}$ occurs when $d \cdot \sin\varphi = \lambda$, where d is the spacing between neighboring atoms in the crystal. [We are imagining that the rows of atoms forming the surface of the crystal correspond to the closely spaced lines of a grating.] We might solve for the wavelength: $\lambda = d \cdot sin(\varphi_{max})$.

Specifically, for 54 eV electrons impinging on a Ni crystal, $\varphi_{max} = 50^o$ and $d = 2.15$Å whence we obtain $\lambda = 1.65$Å. The question is, does this wavelength correspond to the deBroglie wavelength of such an electron?

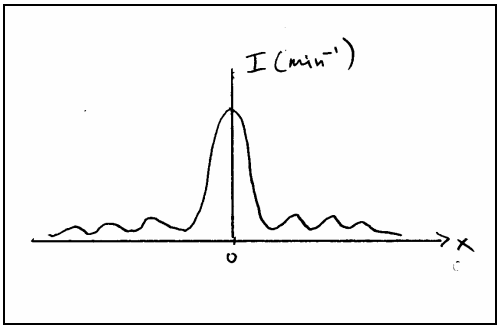
Firstly, it will be easier if the relativistic formulae are unnecessary. So check how fast the electrons are moving. The kinetic energy is $K = \gamma mc^2 - mc^2$. We have $K = 54$ eV and $mc^2 = .511$ MeV. Thus $\gamma - 1 = 0.0001$. We can use the classical expression $K = p^2/2m$. Therefore, $p = \sqrt{2mK}$. The deBroglie wavelength is $\lambda = \dfrac{h}{p} = \dfrac{4.136x10^{-15} eV \cdot s}{\sqrt{2 \cdot 0.511 \dfrac{MeV}{c^2} \cdot 54eV}} = 1.67$Å. That is close enough in view of the rounding used in the calculation. It appears that the deBroglie postulate has some physical reality.

4. Uncertainty and probability

Consider a simplified electron diffraction experiment: a mono-energetic beam of electrons impinging on two narrow slits. The electrons all have the same kinetic energy and the same velocity. Beyond the slits is a detector, which can be moved along the x-axis.



The observed result:

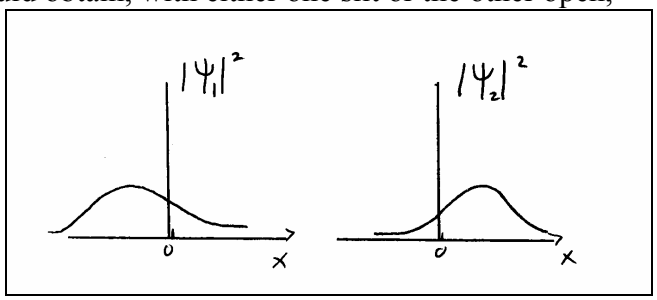


Note that at a specific location, *x*, the detector counts electrons one at a time. After counting for a "long" time at several *x*-values, the interference pattern is obtained.

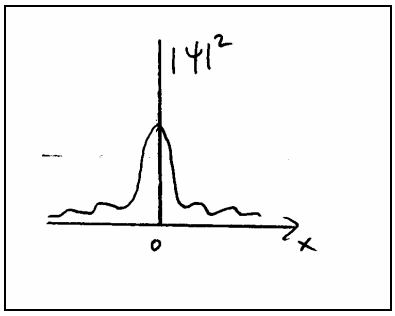
a. Probability

We have a stream of many electrons incident on the double slits, passing through them, and being counted by the detector. The detector counts the number of electrons arriving at *x* per unit time, so the intensity being measured is *I(x)* in particles per minute. The number of particles we expect to count in the interval x *'* to *x'*+Δ*x* is proportional to the probability that an electron will be counted at *x* lying between *x'* and *x'*+Δ*x*. Define a *wave function*, such that $|\Psi|^2$ equals that probability. This parallels the definition of *intensity* for light waves.

For a single slit we would obtain, with either one slit or the other open,



For two slits spaced a distance *D* apart, open however just one at a time in succession, we would observe a superposition of the single-slit distributions. If both the slits are open while electrons are being counted, we obtain, not the superposition of two single-slit distributions, but the following interference pattern:



Evidently, $|\Psi|^2 = |\Psi_1 + \Psi_2|^2 \neq |\Psi_1|^2 + |\Psi_2|^2$, rather,

$$|\Psi|^2 = \Psi_1^*\Psi_1 + \Psi_1^*\Psi_2 + \Psi_1\Psi_2^* + \Psi_2^*\Psi_2 = |\Psi_1|^2 + |\Psi_2|^2 + \left(\Psi_1^*\Psi_2 + \Psi_1\Psi_2^*\right).$$

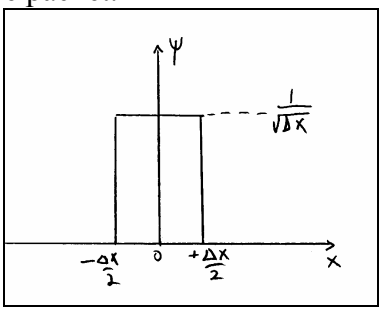
Those additional terms in the parentheses are called *interference terms*. Ψ^* is the complex conjugate of Ψ so that $|\Psi|^2 = \Psi^*\Psi$.

b. Uncertainty.

The wave function is interpreted as being related to the probability that a measurement will find a particle at a specified location, *x'*. It is constructed by a superposition of plane waves $\Psi = \int_0^\infty a_k \cdot \cos(kx - \omega t)dk$, where *k* is the wave number and a_k is a Fourier coefficient. As is often the case, we find it convenient to use the complex version:

$$\Psi = \int_0^\infty a_k \cdot e^{i(kx-\omega t)}dk .$$

This wave packet is to be zero everywhere except within a region of width Δx. To illustrate, consider a simple rectangular wave packet.



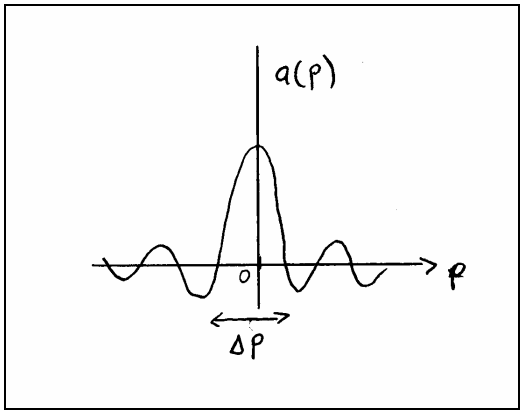
The wave function is non-zero for a region on the *x*-axis of width Δx centered on $x = 0$. The total probability that the particle will be observed somewhere on the *x*-axis must be 1.0, so the wave function is $\Psi(x) = 1/\sqrt{\Delta x}$.

The Fourier transform of Ψ will yield a momentum wave packet, *a(k)*. That is, $|a(k)|^2$ will tell us the probability that a particle will be observed to have momentum $p = \hbar k$.

$$a(k) = \frac{1}{\sqrt{2\pi}} \int_{-\Delta x/2}^{\Delta x/2} \frac{e^{ikx}}{\sqrt{\Delta x}} dx = \sqrt{\frac{2}{\pi \Delta x}} \frac{\sin\left(\frac{\Delta x k}{2}\right)}{k}.$$

In terms of the momentum, $p = \hbar k$,

$$a(p) = \sqrt{\frac{2}{\pi \Delta x}} \frac{\sin\left(\frac{p\Delta x}{2\hbar}\right)}{\frac{p}{\hbar}} = \sqrt{\frac{\Delta x}{2\pi\hbar}} \frac{\sin\left(\frac{p\Delta x}{2\hbar}\right)}{\frac{p\Delta x}{2\hbar}}.$$



The height of the central peak is much greater than the side-peaks, and the width of the central peak is roughly $\Delta p \approx \frac{\hbar}{\Delta x}$. Now, look at the product $\Delta x \cdot \Delta p \approx \Delta x \frac{\hbar}{\Delta x} = \hbar$. This is an *uncertainty relation*, saying that it is impossible to measure *simultaneously* both the position (x) and momentum (p) of a particle to arbitrary precision.

In fact, a rectangular wave packet is not physical, since it is a discontinuous function. Much theoretical work has gone into determining what sort of mathematical construction will give smooth wave packets with minimum initial uncertainty, Δx. For a physically realistic wave packet, it was found that $\Delta x \Delta p \geq \frac{\hbar}{2}$.

This relation holds for any pair of conjugate variables, e.g., $\Delta t \Delta E \geq \frac{\hbar}{2}$.

[$\Delta x \Delta p = v \Delta t \frac{\Delta E}{v} = \Delta t \Delta E$] [The time rate of change of a particle's kinetic energy: $\Delta E = v \Delta p$.]

D. Atoms

The history of the concept of material objects being composed of small particles goes back to the ancient Greeks, and is beyond the scope of this course. The "modern" picture of an atom was assembled in a series of experiments during the 19th and early 20th centuries.

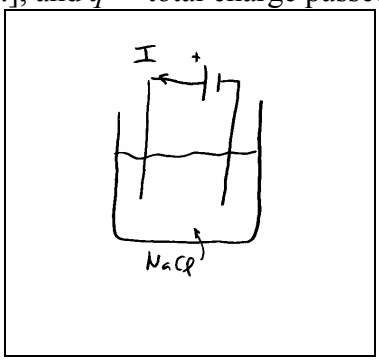
1. Charges/particles; *e/m*

a. Faraday's "Law" of Electrolysis

When an electrical current is passed through molten NaCl, chlorine and sodium are deposited on the anode and cathode, respectively. Quantitatively,

$$m = M \cdot \frac{q}{96500 Coul \cdot \nu},$$

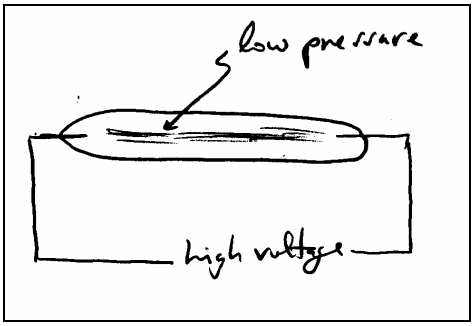
where m = mass deposited on the anode or cathode, M = molecular weight, ν = valance of the atoms [1 for Na & Cl, 2 for O, etc.], and q = total charge passed through the NaCl.



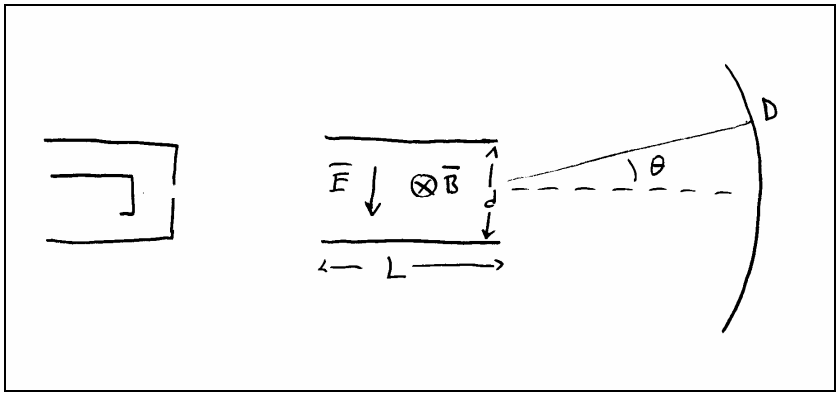
Faraday's "Law" of Electrolysis demonstrates that i) molecules [NaCl] consist of elemental atoms and ii) subatomic particles have electric charge.

b. Cathode Rays

J. J. Thomson showed that *cathode rays* are streams of electrons. As we know now, when a high voltage is applied to the ends of a partially evacuated glass tube, a glowing path of ionized air is formed inside the tube between the electrodes. The ionization is caused by collisions between air molecules and fast-moving electrons. Those electrons escape from one electrode and are accelerated toward the opposite electrode by the applied voltage. The ionized air molecules emit the light seen along the glowing path. At the time, the glowing path was mysterious. Thomson's experiments established that cathode rays were caused by charged particles, subatomic in mass and apparently present in all matter.



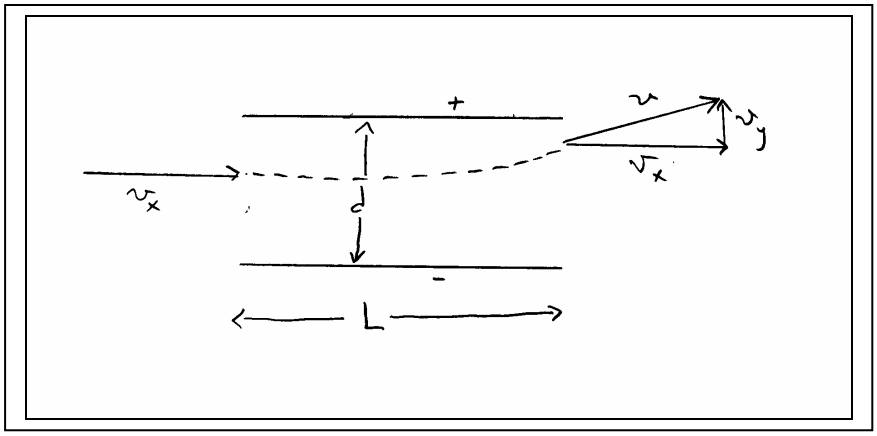
Pass a stream of electrons through a electric field and a magnetic field oriented at right angles to each other, as shown here:



With no *B*-field, the electron stream hits the screen at the point D. The deflection angle is $\tan\theta = \frac{v_y}{v_x}$, where $v_y = a_y \cdot t = \frac{eE}{m} \cdot t$. But $t = \frac{L}{v_x}$, so $v_y = \frac{eEL}{mv_x} = \frac{eVL}{mdv_x}$. Therefore,

$$\tan\theta = \frac{eVL}{mdv_x^2} = \left(\frac{e}{m}\right)\frac{VL}{dv_x^2}.$$

So, knowing v_x and measuring θ, we could obtain *e/m*, the charge to mass ratio of the electron. To know v_x, we turn up the *B*-field until there is no deflection—the magnetic force on the moving electrons balances the electrostatic force. $eE = ev_xB$ whence $\frac{e}{m} \cong \frac{\theta \cdot d \cdot V^2}{VL(Bd)^2} = \frac{\theta \cdot V}{LdB^2}$.



The electron as a universal constituent of matter is supported by the fact that the same *e/m* is obtained when i) different gases are in the tube, ii) different metals are used for the electrodes, and iii) the electrons are released via the photoelectric effect rather than by heating the cathode.

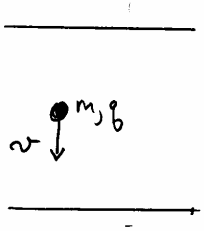
e/m for the electron is many orders of magnitude smaller than *e/m* for the Hydrogen nucleus, so the electron mass is many orders of magnitude smaller than that of an atom.

c. Millikan's experiment

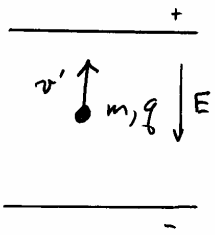
The charge to mass ratio of a particle has two properties mixed together. We'd like to get them separately. For instance, what is the smallest possible charge a particle might have? We suspend a small object, such as a droplet of oil or a tiny plastic bead, between two plates. We may apply

a voltage between the plates and observe the vertical motion of the droplet or bead, and do the same with zero applied voltage.
Forces on the droplet:
D is the air resistance, C is the drag coefficient, and W is the weight of the droplet.

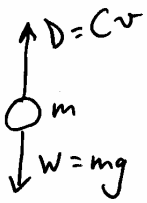
Without E-Field



With E-Field



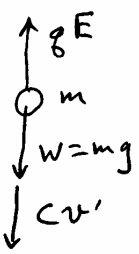
At terminal velocity



$$Cv - mg = 0$$

$$C = \frac{mg}{v}$$

Set E-Field such that *v*' = constant



$$qE - mg - Cv' = 0$$

Substitute for *C* in the right hand equation, $qE - mg - mg\frac{v'}{v} = 0$, solve for *q/m*.

$$\frac{q}{m} = \frac{g}{E}\left(1 - \frac{v'}{v}\right)$$

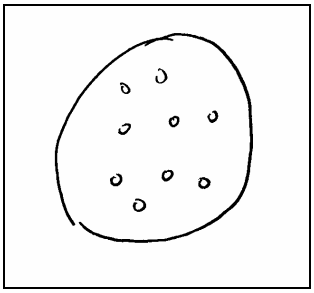
Now, *m* is the mass of the droplet and *q* is the excess electric charge on the droplet. The volume of the droplet can be obtained from Stoke's "Law" for a sphere falling through a fluid medium. From the volume and density of the droplet, we obtain its mass, *m*. We repeat the experiment for many, many droplets and find that always $q = -ne$, where *n* is an integer and $e = 1.602 \times 10^{-19}$ Coulombs.

2. Atomic architecture

If atoms are made of smaller building blocks, such as electrons, how are those blocks arranged? We know, so far, that there are both positive and negative charges within an atom. The problem is to arrange them in such a way that they stick together—the atom is stable.

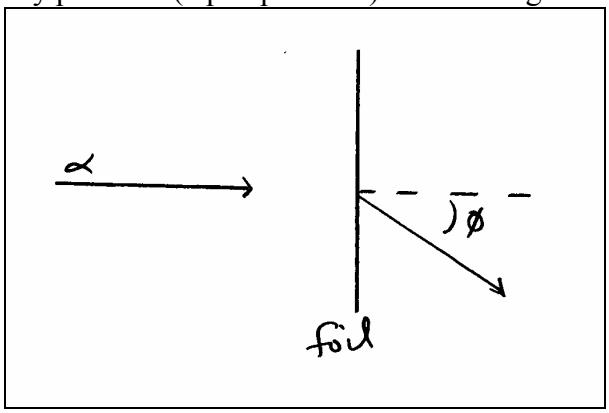
a. Thomson

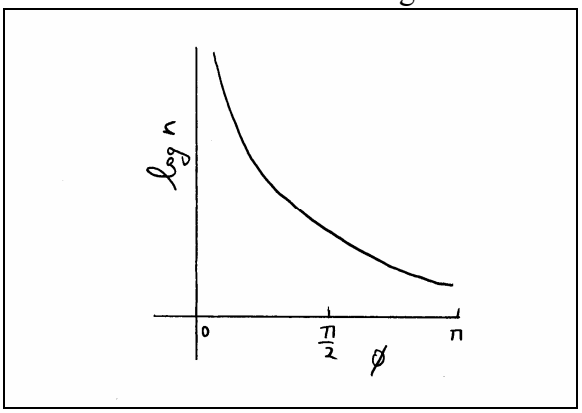
Atoms consist of a uniform, positively charged sphere throughout which are embedded tiny negative particles—the electrons. This model gives a stable arrangement of +/- charges. However, it fails to account for the observed emission & absorption spectra.



b. Rutherford

To determine the size of something too small to see, we can bombard that something with tiny projectiles and observe how those projectiles are scattered. Rutherford (et al.) sent a beam of heavy particles (alpha particles) into a thin gold foil. The result was the following:





Most α-particles are undeviated, which means that the target gold atoms are not big mushy balls. As the scattering angle, ϕ, increases, fewer α-particles are scattered through that angle, but not zero, and some even bounce backward, $\phi > \pi/2$. We conclude that the target atoms are several times more massive than the α-particle and compact. Just how compact we can estimate by using conservation of energy in a collision. In a direct, head-on collision the α-particle reaches closest approach to the target atom when

$$\frac{1}{2} m_\alpha v_\alpha^2 = k \frac{Ze \cdot 2e}{r}.$$

Solve for that $r = \dfrac{kZe \cdot 2e}{\frac{1}{2} m_\alpha v_\alpha^2} = f(Z)$. We find that $r \approx 10^{-14}$ meters and that Z is roughly ½ the atomic weight of the target atom. In other words, we find that the positive charge is confined to a very tiny volume. However, the experiment does not tell us how the electrons in the target atom are arranged within the atom's structure. Rutherford proposed that either the electrons were indeed mixed in the positive nucleus, or they orbited the positive nucleus. Just how the positive nucleus could stay together was still a puzzle. Also still a puzzle was the emission & absorption spectra of atoms.

c. The problem of atomic spectra

Certainly, an electron could orbit a positively charged nucleus just as planets orbit the Sun. After all, the form of Coulomb's "Law" is exactly the same as the "Law" of Universal Gravitation. But, according to classical Electro-Magnetism, an accelerated charge emits radiation. That's how radio signals are generated, for instance. An electron in an orbit is certainly accelerated; it should continuously emit radiation. Further, the emitted radiation should increase in wavelength as the electron continuously loses energy and spirals inward toward the nucleus. What is observed? i) Atoms do not emit continuous spectra nor ii) do atoms collapse—they are stable objects.

During the latter part of the 19th century, many individuals measured the spectra of many substances. Their findings are summarized by the following relation:

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

where n_i and n_f are integers and R is the Rydberg constant, $R = 1.0973732 \times 10^7 \text{m}^{-1}$.

For Hydrogen:

Balmer series: $n_f = 2$ and $n_i = 3, 4, 5, 6, \ldots$

etc. see the Table 4.1 in the text.

Note the spacing of the lines in each series, and that the series fall in different regions of the E-M spectrum. These are the experimental results that Bohr set out to explain in his model of the atom.

3. The Bohr Model of the Hydrogen Atom

Bohr inferred certain properties of the atom from the observed spectra.

a. Assumptions/Postulates

i) The electron moves in stable circular orbits about the proton. The attractive force is the Coulomb force.

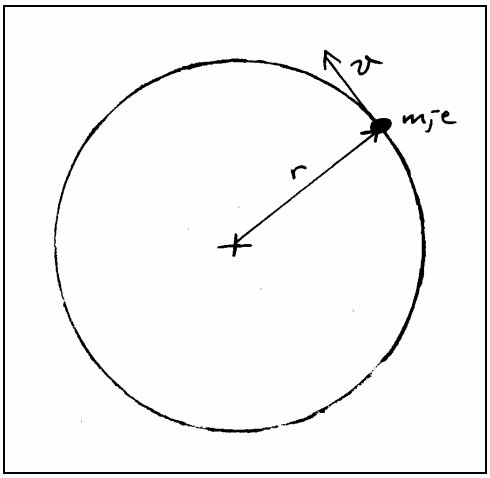
ii) Only certain orbits are stable. In a stable orbit, the electron does not radiate, so the energy is constant.

iii) Radiation is emitted when the electron makes a transition from one stable orbit to another, and $|\Delta E| = hf$.

iv) The angular momentum of the electron in its orbit is quantized, $mvr = n\hbar$. This postulate arises in part from the idea of a standing deBroglie matter wave filling the orbital circumference.

b. Energy levels of the Bohr H-atom

We use the assumptions mentioned above to see if we can reproduce the observed emission spectra for Hydrogen. We have two threads: the conservation of energy and the quantization of angular momentum.



The total energy is $E = \frac{1}{2}mv^2 - k\frac{e^2}{r}$. Now, the *v* and *r* are not independent, since for a circular orbit Newton's 2nd Law says that $k\frac{e^2}{r^r} = \frac{mv^2}{r}$, or $mv^2 = k\frac{e^2}{r}$. Substitute this for mv^2 in *E*,

$$E = \frac{1}{2}\frac{ke^2}{r} - \frac{ke^2}{r} = -\frac{ke^2}{2r}.$$

This is the total mechanical energy of an electron in a circular orbit of radius, *r*. However, we know that not all values of E are to be permitted, so at this point we invoke the quantization of angular momentum, setting $mvr = n\hbar$, which leads to $v^2 = \frac{n^2\hbar^2}{m^2r^2}$. At the same time, $v^2 = \frac{ke^2}{mr}$. So we have two expressions for v^2; set 'em equal.

$$\frac{n^2\hbar^2}{m^2r^2} = \frac{ke^2}{mr}$$

Solve for $r = r_n$

$$r_n = \frac{n^2\hbar^2}{mke^2},\ n = 1, 2, 3, 4, \ldots$$

Finally, substitute this r_n for *r* in the expression for *E*

$$E = -\frac{ke^2}{2r_n} = -\frac{ke^2}{2\frac{n^2\hbar^2}{mke^2}} = -\frac{mk^2e^4}{2\hbar^2}\cdot\left(\frac{1}{n^2}\right).$$

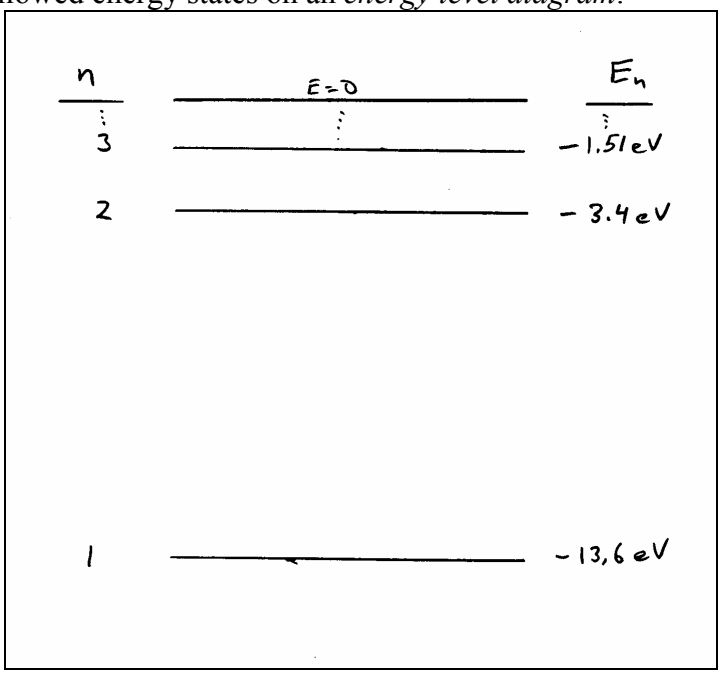
Notice the factor of $\frac{1}{n^2}$! These are the allowed *energy states* of the H-atom, according to the Bohr Model, where *m* = mass of the electron, *e* = electric charge of the electron, *k* = coulomb constant, and *n* is the *principle quantum number*. The lowest energy, and the smallest orbit, is for *n* = 1. The radius of that *n* = 1 orbit is called the *Bohr Radius*, a_o.

$$r_1 = a_o = \frac{\hbar^2}{mke^2} = 0.529\ \text{Å}.$$

The corresponding lowest, or *ground state* energy is E_1 = -13.6 eV. The first excited state is for *n* = 2, $E_2 = \frac{-13.6eV}{4} = -3.4eV$, etc.

c. H-atom spectrum in the Bohr Model

Often we chart the allowed energy states on an *energy level diagram*:



The frequency of a photon emitted (or absorbed) in a transition between levels is

$$f = \frac{\Delta E}{h} = \frac{ke^2}{2a_o h} \cdot \left| \frac{1}{n_f^2} - \frac{1}{n_i^2} \right|.$$

In terms of wavelength, λ,

$$\frac{1}{\lambda} = \frac{f}{c} = \frac{ke^2}{2a_o hc} \cdot \left| \frac{1}{n_f^2} - \frac{1}{n_i^2} \right| = R \cdot \left| \frac{1}{n_f^2} - \frac{1}{n_i^2} \right|.$$

The quantity $\frac{ke^2}{2a_o hc}$ is exactly equal to the experimentally derived Rydberg constant, *R*. So, the Bohr Model of the H-atom can reproduce the observed emission/absorption spectrum.

d. Hydrogenic atoms

We may imagine extreme conditions wherein an atom is almost completely ionized, so that a single electron orbits a nucleus with charge *Ze*. Then the Bohr Model would say:

$$r_n = n^2 \frac{a_o}{Z} \text{ and } E_n = -\frac{ke^2}{2a_o}\left(\frac{Z^2}{n^2}\right).$$

An atom having a single electron orbiting a nucleus is called a *hydrogenic atom*.

4. Correspondence Principle

Classical, or preModern, Physics is not incorrect, only approximate and inaccurate for atomic-scale systems, just as it was for fast-moving systems. Thus, we would expect to be able to extend quantum-based predictions to macroscopic systems and recover the classical result, again just as the classical equations of motion were recovered for speeds small compared to *c*. This

expectation is called a *correspondence principle*. Such a principle serves as a check on quantum-based reasoning and derivations.

E.g. In the case of a quantized oscillator (such as a mass vibrating on a spring), where $E_n = n\hbar\omega$ and $\omega = \sqrt{\frac{k}{m}}$, on the macroscopic scale, we might have $m \approx 1kg$ and $k \approx 1\frac{N}{m}$, so that $\omega \approx 1\frac{rad}{\sec}$. The spacing between energy levels would be $\Delta E \approx \hbar \approx 1x10^{-34} J$. Similarly, the spacing between adjacent energy levels of the H-atom approaches zero as the principle quantum number, *n*, increases. To put it another way, in macroscopic systems, the level spacing is too fine to be perceived by the human observer, so the energy *appears* to be a continuous variable.

III. Quantum Mechanics & Atomic Structure (abbreviated)

We now seek a full treatment of particle dynamics in terms of matter-waves. That is, we want a scheme of producing equations of motion.

A. Schrödinger Wave Equation—One Dimensional

1. Free Particle

A free particle is one subject to no external forces.

a. Einstein-deBroglie relation

$E = \hbar\omega$ and $p = \hbar k$. A plane wave with this E and p would be written: $y = e^{\frac{i}{\hbar}\left(px - \frac{p^2}{2m}t\right)}$, where p is the momentum, m is the mass, $E = \frac{p^2}{2m}$ is the kinetic energy and $k = \frac{p}{\hbar}$ is the wave number.

An alternative form is $y = A\sin\left(px - \frac{p^2}{2m}t\right) + B\cos\left(px - \frac{p^2}{2m}t\right)$. Which form is used in a given case is a matter of convenience.

b. Free wave packet

A wave packet for a free particle is constructed of many plane waves:

$$\Psi(x,t) = \int_{-\infty}^{+\infty} a(k)e^{i(kx-\omega t)}dk = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} a(p)e^{\frac{i}{\hbar}\left(px - \frac{p^2}{2m}t\right)}dp\,.$$

The transform gives the coefficients: $a(k) = \int_{-\infty}^{+\infty}\Psi(x,0)e^{i(kx-\omega t)}dx$.

c. Wave equation

This Ψ, a superposition of plane waves, satisfies the following differential equation:

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

which can be verified by substitution. This equation is known as the Schrödinger Wave Equation for a free particle.

2. Interpretation of the Wave Function, Ψ

a. Claim

The wave function contains all the information that can be known about a particle—its mass, charge, energy, momentum, etc.

b. Proposed interpretation

The probability that the particle will be observed to be at a location between x and $x+dx$ at time t is given by $P(x,t)dx = |\Psi(x,t)|^2 dx$, where $|\Psi|^2 = \Psi^* \Psi$ and $P(x,t)$ is the *probability density*. To be realistic, Ψ must be continuous and single valued and must be normalized, since $\int_{-\infty}^{+\infty} |\Psi|^2 dx = 1$. That is, the particle must be *somewhere* on the x-axis. This proposed interpretation is to be validated by experiment.

c. Solving for the motion

The problem, then, is to find $\Psi(x,t)$, given $\Psi(x,0)$, rather than $x(t)$ given $x(0)$, as in Newtonian mechanics. We shall have to make the connection between $|\Psi|^2$ and the physical motion of the particle explicit subsequently. That is, later.

3. Particle Experiencing a Conservative Force

We draw an analogy with a wave propagating in a dissipative medium.

a. Schrödinger equation

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

where $U(x)$ is the potential energy function for the external conservative force. The solution of this equation may be easy or difficult, depending on the form of the $U(x)$. Even so, we're assuming the potential energy function is constant in time.

b. Time independent Schrödinger equation

If the U is not a function of time, then the differential equation is separable, in the usual way. We assume that $\Psi(x,t) = \psi(x) \cdot \phi(t)$. Then

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

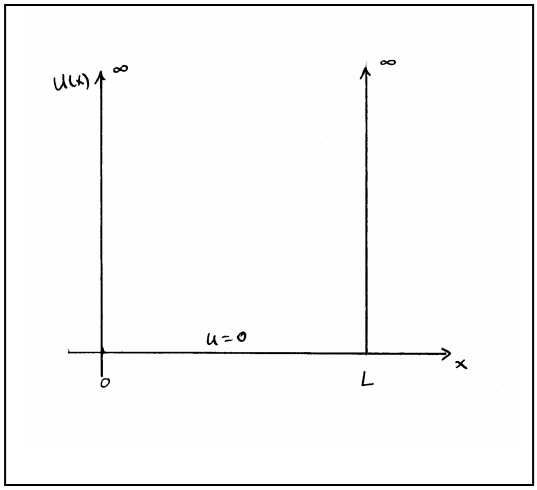
where E is the constant total energy of the particle. The space (x) equation to be solved is

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

To go farther, we need to consider specific potential energy functions.

B. One-Dimensional Potentials

1. Infinite Well or One-Dimensional Box



a. $U(x)$

$$U(x)=\begin{cases}\infty & x\le 0\\ \infty & x\ge L\\ 0 & 0<x<L\end{cases}$$

b. Conditions on ψ

$$\psi=\begin{cases}0 & x\le 0\\ 0 & x\ge L\\ \psi(x) & 0<x<L\end{cases}$$

c. Solution

We have 3 regions in which the Schrödinger equation must be solved. Two regions are taken care of already in this case, as $\psi = 0$ outside the potential well. Inside the well, $U = 0$, so the particle is free.

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

This is the equation for a plane wave, so for $0 < x < L$,

$$\psi(x)=A\sin(kx)+B\cos(kx).$$

To evaluate the coefficients, A & B, we apply the boundary conditions. We require that $\psi(0) = 0$ and $\psi(L) = 0$.

$0 = A\sin(0)+B\cos(0)\Rightarrow B=0$

$0 = A\sin(kL)+B\cos(kL)\Rightarrow \sin(kL)=0$, since $B = 0$.

If both A & B are zero, we have the trivial solution, $\psi = 0$.

d. Energy levels

Because $sin(kL) = 0$, there is a restriction on the energy of the particle in the well. Evidently, $kL = n\pi$, where n = 1, 2, 3, 4, 5, . . . Substitute for k in the total energy

$$E=\frac{\hbar^2k^2}{2m}=\frac{\hbar^2n^2\pi^2}{2mL^2}=n^2\frac{\pi^2\hbar^2}{2mL^2},\ n=1,2,3,4,5,\ldots$$

Note: i) the quantized energy levels arise from the boundary conditions and ii) the lowest possible energy is $E_1=\frac{\pi^2\hbar^2}{2mL^2}\neq 0$. This lowest possible energy is called the *zero-point energy*, even though it isn't zero.

e. Normalization

The wave functions corresponding to the energy levels are $\psi_n = A\sin\left(\frac{n\pi x}{L}\right)$. We evaluate A by setting $\int|\psi|^2\,dx=1$. $\int|\psi|^2\,dx=\int A^2\sin^2\left(\frac{n\pi x}{L}\right)dx=1$

Use the identity $2\sin^2\theta = 1-\cos 2\theta$.

$$\int_0^L \frac{A^2}{2}\left(1-\cos\left(\frac{n2\pi x}{L}\right)\right)dx = \frac{A^2}{2}(L-0) = 1 \text{; solve for } A = \sqrt{\frac{2}{L}}.$$

Because the wave function is zero outside the well, we integrate from 0 to *L* rather than $\pm\infty$.

Finally, we have $\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$. [See Fig. 5.7 and 5.9 in the text.]

2. Expectation Values

a. Weighted averages

When averaging a list of values, we say

$< A >= \frac{\sum_{i=1}^{N} p_i A_i}{\sum_{i=1}^{N} p_i}$, where p_i is the number of times the value A_i appears in the list having *N* different values.

b. Probability & expectation

Now, $|\Psi|^2$ is the probability density, giving the odds that the particle will be observed to be in the state described by $\Psi(x,t)$. Suppose we make many observations of the position of the particle. Then the average of our observations would be

$$< x >= \int \psi x \psi^* dx = \int x|\psi|^2 dx.$$

This is called the *expectation value* of *x*. The standard deviation of many observations of *x* is

$$\Delta x = \sqrt{\frac{\sum (x_i - < x >)^2}{N}}$$

$$\Delta x = \sqrt{\frac{\sum x_i^2 - 2 < x > \sum x_i + m < x >^2}{N}}$$

$$\Delta x = \sqrt{< x^2 > - < x >^2},$$

where we could calculate $< x^2 >= \int x^2|\psi|^2 dx$.

c. particle momentum

We *define* the expectation value of the particle momentum as $< p >= m\frac{d < x >}{dt}$. For macroscopic objects, this expression reduces to $p = mv$. Also, $\Delta p = \sqrt{< p^2 > - < p >^2}$.

C. Three-Dimensional Potentials

1. Three-dimensional Schrödinger Equation

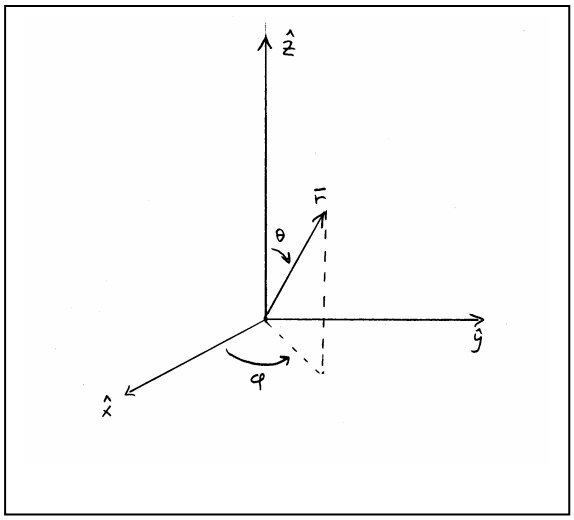
$$-\frac{\hbar^2}{2m}\nabla^2\Psi + U(\vec{r})\Psi = i\hbar\frac{\partial\Psi}{\partial t}\text{, where } \nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial x^2}$$

The solutions have the form $\Psi(\vec{r},t) = \psi(\vec{r})e^{-i\omega t}$.

2. Central Forces; polar coordinates

The Coulomb force is spherically symmetric, so it's convenient to use spherical polar coordinates.

a. Wave equation in polar coordinates



$$-\frac{\hbar^2}{2m}\left\{\frac{\partial^2}{\partial r^2}+\left(\frac{2}{r}\right)\frac{\partial}{\partial r}+\frac{1}{r^2}\left[\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\csc^2\theta\frac{\partial^2}{\partial\varphi^2}\right]\right\}\psi(\vec{r})+U(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

For central potentials, $U(\vec{r}) = U(r)$ and we can separate the variables by assuming that $\psi = R(r)\Theta(\theta)\Phi(\varphi)$.

$$-\frac{\hbar^2}{2m}\left\{\frac{\partial^2}{\partial r^2}+\left(\frac{2}{r}\right)\frac{\partial}{r}+\frac{1}{r^2}\left[\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\csc^2\theta\frac{\partial^2}{\partial\varphi^2}\right]\right\}\psi(\vec{r})+(U(\vec{r})-E)\psi(\vec{r}) = 0$$

Multiply through by $-\dfrac{2mr^2}{\hbar^2}$

$$\left(r^2\frac{\partial^2}{\partial r^2}+2r\frac{\partial}{\partial r}\right)\psi+\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\csc^2\theta\frac{\partial^2}{\partial\varphi^2}\right)\psi-\frac{2mr^2}{\hbar^2}(U(r)-E)\psi = 0$$

Collect the terms depending on r and divide through by ψ.

$$\frac{r^2}{R}\frac{\partial^2}{\partial r^2}R+\frac{2r}{R}\frac{\partial}{\partial r}R-\frac{2mr^2}{\hbar^2}(U(r)-E)+\frac{1}{\Theta}\frac{\partial^2}{\partial\theta^2}\Theta+\frac{\cot\theta}{\Theta}\frac{\partial}{\partial\theta}\Theta+\frac{\csc^2\theta}{\Phi}\frac{\partial^2}{\partial\varphi^2}\Phi = 0$$

We'll have to solve this thing one piece at a time.

b. Angular momentum—the angular parts

$$\frac{1}{\Theta}\frac{\partial^2}{\partial\theta^2}\Theta+\frac{\cot\theta}{\Theta}\frac{\partial}{\partial\theta}\Theta+\frac{\csc^2\theta}{\Phi}\frac{\partial^2}{\partial\varphi^2}\Phi=-C$$

-C is the separation constant.

Multiply by $\sin^2\theta$

$$\frac{\sin^2\theta}{\Theta}\frac{\partial^2}{\partial\theta^2}\Theta+\frac{\cos\theta\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\Theta+\frac{1}{\Phi}\frac{\partial^2}{\partial\varphi^2}\Phi=-C\sin^2\theta$$

Separate again

$\frac{\sin^2\theta}{\Theta}\frac{\partial^2}{\partial\theta^2}\Theta+\frac{\cos\theta\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\Theta+C\sin^2\theta=-\frac{1}{\Phi}\frac{\partial^2}{\partial\varphi^2}\Phi=m^2$, another separation constant.

Set $-\frac{1}{\Phi}\frac{\partial^2}{\partial\varphi^2}\Phi=m^2$, which equation has familiar solutions

$$\Phi=e^{\pm im\varphi}.$$

Substitute this into the θ-equation

$$\frac{\sin^2\theta}{\Theta}\frac{\partial^2}{\partial\theta^2}\Theta+\frac{\cos\theta\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\Theta+C\sin^2\theta=m^2,\text{ rearrange}$$

$$\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\Theta\right)+\left(C\sin^2\theta-m^2\right)\Theta=0.$$

This is a standard, "well known" differential equation—the Associated Legendre Equation. The solutions are bounded and differentiable (the physical requirements) if

$$C=\ell(\ell+1)\text{ and }m=-\ell,-\ell+1,...,\ell-1,\ell.$$

We identify m with the angular momentum about the $\hat{z}$-axis, which is quantized:

$$L_z=m_\ell\hbar,\ m_\ell=0,\pm1,\pm2,\pm3,...,\pm\ell$$

The other constant is identified with the magnitude of the total angular momentum

$$L^2=\ell(\ell+1)\hbar^2,\ \ell=0,1,2,3,...$$

Note: $C\sin^2\theta-m_\ell^2\Rightarrow$ combination of angular momentum about the $\hat{x}$- and $\hat{y}$-axes.

Define: $\ell\equiv$ *orbital quantum number* and $m_\ell\equiv$ *magnetic quantum number*.

c. Spherical harmonics

The "well known" solutions to the Associate Legendre Equation are the *Spherical Harmonics*:

$$\Theta(\theta)\Phi(\varphi) = Y_\ell^m(\theta,\varphi)$$

$$Y_0^0 = \frac{1}{2\sqrt{\pi}}$$

$$Y_1^0 = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$$

$$Y_1^{\pm 1} = \mp\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta\cdot e^{\pm i\varphi}$$

etc. [see Table 8.3 in the text]

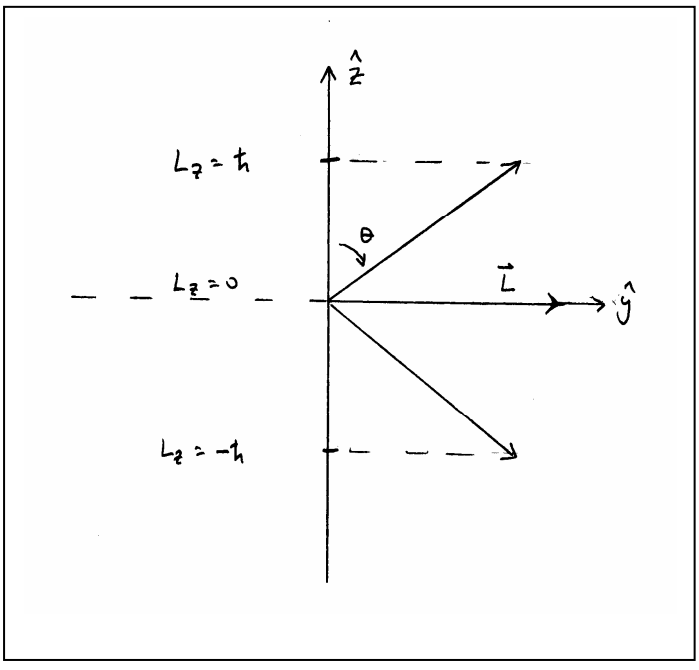
d. Radial equation

The radial part of the wave equation remains.

$$-\frac{\hbar^2}{2m}\left[\frac{d^2}{dr^2}R + \left(\frac{2}{r}\right)\frac{d}{dr}R\right] + \frac{L^2}{2mr^2}R + U(r)R = ER\,.$$

The allowed energy levels are obtained from the boundary conditions applied to *R(r)*; this will give the *principle quantum number*, *n*. The details depend on the exact form of *U(r)*. In the case of the Hydrogen atom, $U(r) = -\frac{ke^2}{r}$.

e. Angular momentum vectors



L_z is the projection of $\vec{L}$ on the *z*-axis. Not only is the $\vec{L}$ quantized, but so is the L_z. For instance, for $\ell = 1$, $L^2 = \ell(\ell+1)\hbar^2 = 2\hbar^2$, and $m = -1,0,+1$, so $L_z = -\hbar,0,+\hbar$. The vector $\vec{L}$ precesses around the *z*-axis. The condition $\cos\theta = \frac{L_z}{L} = \frac{m_\ell}{\sqrt{\ell(\ell+1)}}$ gives the allowed projections on the *z*-axis. For $\ell = 1$, $\cos\theta = -\frac{1}{\sqrt{2}},0,\frac{1}{\sqrt{2}}$. Fig. 7.7 in the text shows the case of $\ell = 2$.

D. The Hydrogen Atom

$$U(r) = -\frac{ke^2}{r}$$

So far we have $\Psi(r,\theta,\varphi,t) = R(r)Y_\ell^{m_\ell}(\theta,\varphi)e^{-i\omega t}$. Given $U(r)$, we have to find $R(r)$. Notice that many ℓ, m_ℓ combinations may apply to the same energy state, $R(r)$—degeneracy.

1. Radial Equation

$$-\frac{\hbar^2}{2m}\left[\frac{d^2}{dr^2}R + \left(\frac{2}{r}\right)\frac{d}{dr}R\right] + \frac{L^2}{2mr^2}R - \frac{ke^2}{r}R = ER$$

The whole equation is multiplied by r. Then the second derivative term can be collapsed to

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}(rR) + \left(\frac{L^2}{2mr^2} - \frac{ke^2}{r}\right)(rR) = E(rR).$$

A standard method of solution is to try a power series: $R = \sum_j a_j r^j$. The boundary conditions will require that $R(0) = 0$ and that $R \to 0$ as $r \to \infty$. The latter condition restricts the series to be a finite polynomial with the highest $j = n > \ell$. This is what determines the allowed energy levels. See Table 7.4 in the textbook.

$$E_n = -\frac{mk^2e^4}{2\hbar^2}\frac{1}{n^2},\ n = 1, 2, 3, 4, \ldots$$

Commonly, we write E_n in terms of the Bohr radius

$$E_n = -\frac{ke^2}{2a_o}\frac{1}{n^2}.$$

It follows that the allowed orbital (angular momentum) states are ℓ=0, 1, 2, 3, . . ., n-1.

2. Spectroscopic Notation

For a specified n, the allowed values of ℓ and m_ℓ label states having the same energy, E_n. These states are said to form a *shell*; the allowed values of m_ℓ for a specified ℓ form a *subshell*. We still use the naming scheme created by the preModern spectroscopists who measured atomic spectra in the 19th century. As shown in the following table, the letter K stands for the n = 1 shell, while a lower case d stands for an ℓ = 2 subshell.

***n*(shells)**	**symbol**	**ℓ (subshells)**	**symbol**
1	K	0	s
2	L	1	p
3	M	2	d
4	N	3	f
5	O	4	g
6	P	5	h

We see that the quantum numbers (n, ℓ, m_ℓ) arise from *physical* restrictions placed on the *mathematical* solutions to the Schrödinger equation. Further, there is one quantum number for each degree of freedom.

3. Probability Densities

$$\psi_{n,\ell,m_\ell} = R_{n,\ell}(r) Y_\ell^{m_\ell}(\theta, \varphi)$$

a. Ground state

$$\psi_{1,0,0} = R_{1,0} Y_0^0 = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_o} \right)^{\frac{3}{2}} e^{-\frac{r}{a_o}}$$

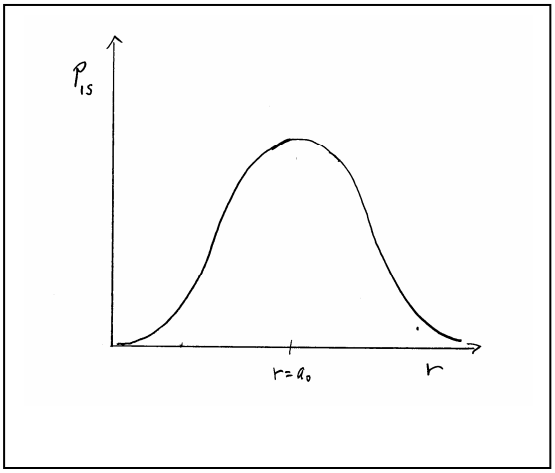
This function is spherically symmetric, since $\ell = 0$ --i.e., it's an s-state. In fact, all states with $\ell = 0$ are spherically symmetric. The probability density is

$$\left| \psi_{1,0,0} \right|^2 = \frac{e^{-\frac{2r}{a_o}}}{\pi a_o^3},$$

which is also spherically symmetric.

We define the Radial Probability Distribution, *P(r)* such that $P(r)dr = \left| \psi \right|^2 4\pi r^2 dr$.

For ψ_{100}, $P(r) = P_{1s}(r) = \frac{e^{-\frac{2r}{a_o}}}{\pi a_o^3} 4\pi r^2 = \frac{4}{a_o^3} r^2 e^{-\frac{2r}{a_o}}$.



Note that $P(r) = r^2 \left| R(r) \right|^2$ and that $\int_0^\infty P(r)dr = 1$.

We can calculate the expectation value of *r*, the distance of the electron from the atomic nucleus.

$$< r >= \int_0^\infty r P(r) dr$$

$$< r >_{1s} = \int_0^\infty r \frac{4}{a_o^3} r^2 e^{-\frac{2r}{a_o}} dr = \int \frac{4}{a_o^3} r^3 e^{-\frac{2r}{a_o}} dr$$

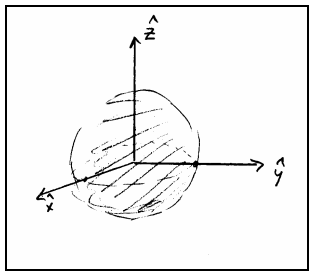
$$< r >_{1s} = \frac{4}{a_o^3} \frac{3!}{\left(\frac{2}{a_o}\right)^4} = \frac{24}{16} a_o = 1.5 a_o$$

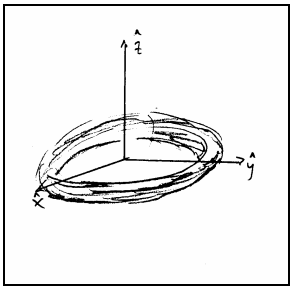
Notice: While $r = a_o$ is the *most probable* radius, the *expectation value* of the radius is <r> = $1.5a_o$, that is, averaged over a large number of observations of *r*.

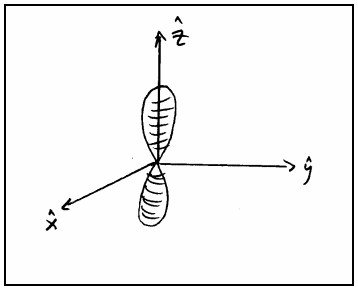
b. First excited state

In the first excited state, $n = 2$. The orbital quantum number, ℓ, may be 0 or 1. If $\ell = 1$, then m_ℓ = -1, 0, or +1. Therefore, there are 4 states with the same energy, E_2. We say that the degeneracy is *4-fold*. According to the spectroscopic notation, the *2s state* is $\psi_{2,0,0}$; the *2p states* are $\psi_{2,1,1}$, $\psi_{2,1,0}$, and $\psi_{2,1,-1}$.

$|\psi_{200}|^2$ $|\psi_{211}|^2$ or $|\psi_{21-1}|^2$ $|\psi_{210}|^2$



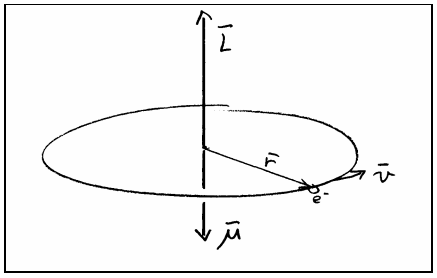




4. Normal Zeeman Effect

a. Magnetic moments

Viewed in preModern terms, in circulating about the proton, the orbiting electron creates a magnetic dipole field. The dipole moment is $\vec{\mu}$, having a magnitude of $\mu = jA$, where *j* is the time-averaged electrical current and *A* is the area of the closed orbit. If *T* is the orbital period, then $j = \frac{-e}{T}$. On the other hand, the magnitude of the orbital angular momentum, according to Kepler, is $L = \frac{2m_e A}{T}$. The magnetic moment *vector* becomes $\vec{\mu} = \frac{-e}{T}\frac{\vec{L}T}{2m_e} = \frac{-e\vec{L}}{2m_e}$.



It's convenient to define the quantity called the *Bohr Magneton*, thus:

$$\mu_B = \frac{e\hbar}{2m_e} = 9.274x10^{-24}\frac{Jouls}{Tesla} = 5.788x10^{-9}\frac{eV}{Gauss}.$$

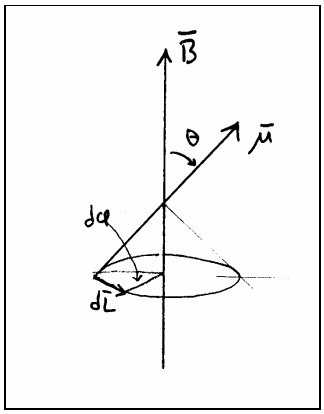
Notice the charge-to-mass ratio: e/m_e. The quantity that appears in the magnetic moment is ½ the charge-to-mass ratio. For any charged particle, we define the *geomagnetic ratio* to be $\frac{q}{2m}$,

where q is the particle charge and m is the particle mass. The z-component of $\vec{\mu}$, like L_z, is quantized: $\mu_z = -\mu_B \cdot m_\ell$.

b. Larmor precession

In an externally applied magnetic field, a magnetic dipole will experience a torque,

$$\vec{\tau} = \vec{\mu} \times \vec{B} = \frac{d\vec{L}}{dt}.$$



The $\vec{\mu}$ vector precesses around an axis aligned along the $\vec{B}$, since the $\frac{d\vec{L}}{dt} \perp \vec{\mu}$ and $\vec{B}$.

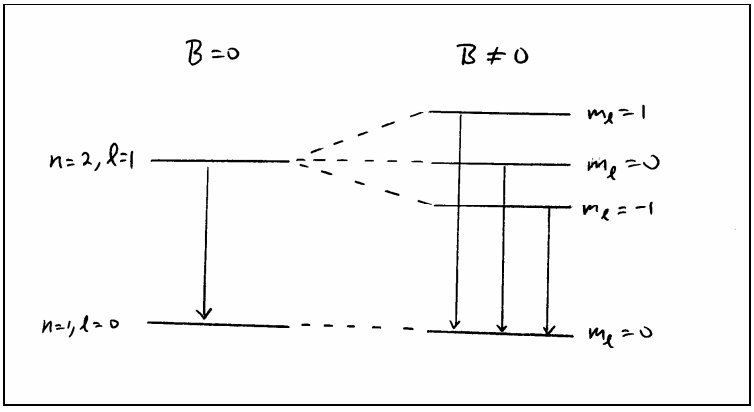
$$\left|d\vec{L}\right| = L\sin\theta d\varphi = \left|\vec{\tau}\right| dt = \left|\frac{e}{2m_e}\right| LB\sin\theta dt.$$

$$\omega_L = \frac{\left|d\vec{L}\right|}{L\sin\theta} = \frac{e}{2m_e}\frac{LB\sin\theta}{L\sin\theta} = \frac{eB}{2m_e}$$

This precession rate is called the *Larmor Frequency*.

c. Normal Zeeman effect

With no external B-field, all the $n = 2$ states have the same energy, E_2. In the presence of a strong magnetic field, the interaction of the orbital magnetic dipole with the externally applied magnetic field leads to a change in the energy. $\Delta E = -\vec{\mu} \cdot \vec{B} = \frac{e}{2m_e}\vec{L} \cdot \vec{B} = \frac{eB}{2m_e}L_z$, where we have assumed that $\vec{B} = B\hat{z}$. Thus, if E_2 is the state energy without the B-field, then $E = E_2 + \hbar\omega_L m_\ell$ is the energy with the B-field. Since $m_\ell = 0$, ± 1, ± 2, ± 3, . . ., $\pm\ell$, the formerly degenerate energy levels are separated by $\pm m_\ell \hbar\omega_L$. We call this *lifting the degeneracy*. The higher the value of n, the more m_ℓ values there are. The *Normal Zeeman Effect*, then, is characterized by the splitting of spectral lines into sets of several uniformly spaced lines in the presence of a strong magnetic field.



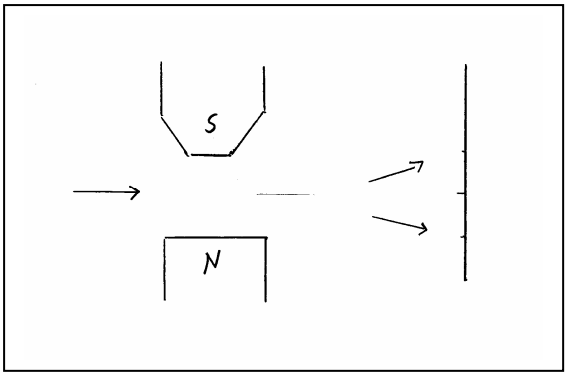
5. Fine Structure

a. Anomalous Zeeman effect

In addition to the uniformly split lines due to the normal Zeeman effect, there are often nonuniform splittings of spectral lines. These are called the anomalous Zeeman splittings. These are not accounted for by the orbital $\vec{\mu}$.

b. Stern –Gerlach experiment

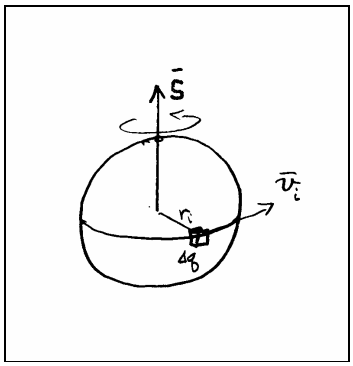
Atoms passing through a *nonuniform* magnetic field: any net magnetic dipole possessed by the atoms will cause them to be deflected. The observed result is that the atomic beam is divided into two beams with equal but opposite deflections.



Interpretation: i) the effect is not due to the orbital magnetic moment, else there would be either $2\ell+1$ or zero spots on the screen and ii) the deflections are due to a magnetic moment that has only two possible values.

c. Electron spin

We propose that a magnetic moment is produced by the electron itself, visualized as spinning. In analogy to orbital angular momentum, we define a *spin quantum number*, s, such that the number of possible angular momentum z-components is $2s+1$.



Since Stern & Gerlach obtained $2s+1=2$, we infer that for the electron $s=\frac{1}{2}$ and that $m_s=\pm\frac{1}{2}$. The z-component of the spin angular momentum is $S_z=m_s\hbar$, while $S^2=s(s+1)\hbar^2$. This S^2 is constant, so this thing called spin is an intrinsic property of the electron as much as are its mass and electric charge.

The spin magnetic moment is $\vec{\mu}_s=g\frac{e}{2m_e}\vec{S}$. The quantity g is called the *g-factor*, which is a kind of a fudge factor. For electrons, the g-factor is found experimentally to be $g=2$. This value indicates that the electric charge is not uniformly distributed in a tiny solid rotating sphere as our classical visualization depicts it.

d. Total magnetic moment of an electron

With these two contributions, the total magnetic moment of an electron in an orbit about a proton is $\vec{\mu}=\vec{\mu}_\ell+\vec{\mu}_s=\frac{-e}{2m_e}\left(\vec{L}+g\vec{S}\right)$.

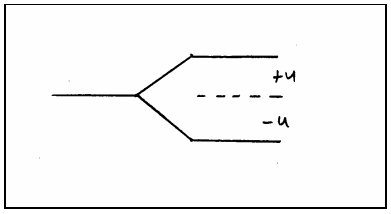
6. Spin-Orbit Interaction

a. Potential energy of two magnetic dipoles

The orbital angular momentum gives rise to a magnetic moment. Call the B-field due to this moment $\vec{B}_\ell$, where $B_\ell = \frac{\mu_o(-e)vR^2}{2R^3} = -\frac{\mu_o ev}{2R}$ and $\vec{B}_\ell = -\frac{\mu_o e}{2m_e R}\vec{L}$. With the electron in the first Bohr orbit, $R = a_o$. $\vec{B}_\ell = -\frac{\mu_o e}{2m_e a_o}\vec{L}$. This $\vec{B}_\ell$ exerts a torque on the spin magnetic moment, $\vec{\mu}_s$: $\vec{\tau} = \vec{\mu}_s \times \vec{B}_\ell$

The potential energy contribution is

$U = -\vec{\mu}_s \cdot \vec{B}_\ell = -\frac{\mu_o e^2 g}{2m_e a_o}\vec{L}\cdot\vec{S}$, since $\vec{\mu}_s = \frac{-eg}{2m_e}\vec{S}$. $\vec{S}$ has two possible orientations, so U may raise or lower the energy level. What was once a single electron level becomes two. This is called *fine structure doubling*.



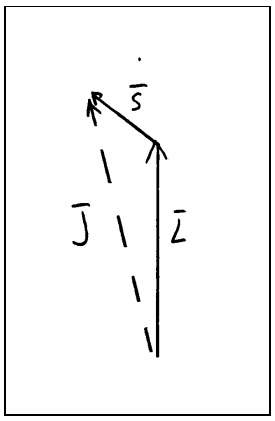
b. Total angular momentum, $\vec{J}$

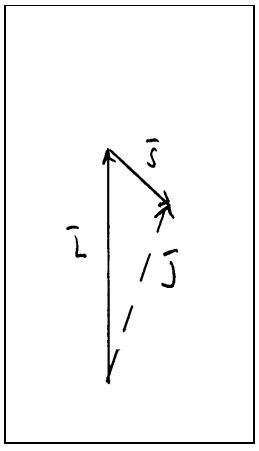
The total angular momentum of the isolated Hydrogen atom is conserved: $\vec{J} = \vec{L} + \vec{S}$. Let us examine the possible values $\vec{J}$ can have, based on the quantum restrictions on $\vec{L}$ and on $\vec{S}$.

By analogy (again), we introduce a new quantum number, such that $J^2 = j(j+1)\hbar^2$ and $J_z = m_j\hbar$, with $m_j = j, j\text{-}1, \ldots, -j+1, -j$. What is the range of j? $\vec{J}$ is the sum of $\vec{L}$ and $\vec{S}$, so j takes on the values $\ell \pm \frac{1}{2}$ for atomic electrons.

e.g. $\ell = 2$, $s = \pm\frac{1}{2}$

then $j = 2 + \frac{1}{2} = \frac{5}{2}$ and $j = 2 + \frac{1}{2} - 1 = \frac{3}{2}$





e.g. $\ell = 4,\ s = \pm\frac{1}{2}$

then $j = 4 + \frac{1}{2} = \frac{9}{2}$ and $j = 4 + \frac{1}{2} - 1 = \frac{7}{2}$

The number of m_j values is $2j + 1$. In terms of ℓ, $j = \ell \pm \frac{1}{2}$, so there are $2\left(\ell \pm \frac{1}{2}\right) + 1$ values of m_j—the projection of $\vec{J}$ on the z-axis.

e.g. $j = \frac{1}{2} \Rightarrow \ell = 0 \Rightarrow m_j = \pm\frac{1}{2}.\ [2 \cdot \frac{1}{2} + 1 = 2]$

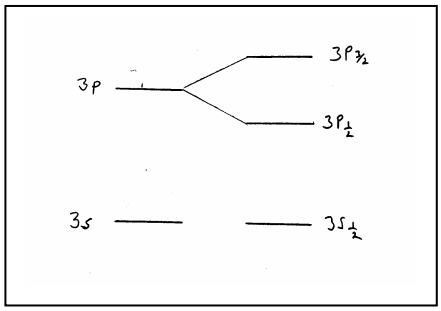
$j = \frac{3}{2} \Rightarrow \ell = 1 \Rightarrow m_j = \pm\frac{3}{2}, \pm\frac{1}{2}.\ [2 \cdot \frac{3}{2} + 1 = 4]$

$j = \frac{3}{2} \Rightarrow \ell = 2 \Rightarrow m_j = \pm\frac{3}{2}, \pm\frac{1}{2}.$

$j = \frac{9}{2} \Rightarrow \ell = 4 \Rightarrow m_j = \pm\frac{9}{2}, \pm\frac{7}{2}, \pm\frac{5}{2}, \pm\frac{3}{2}, \pm\frac{1}{2}.\ [2 \cdot \frac{9}{2} + 1 = 10]$

Each m_j level has *slightly* different energy since the angle between $\vec{\mu}_s$ and $\vec{B}_\ell$ is different---*fine structure*.

e.g. the Sodium doublet



c. Spectroscopic notation
number for *n*
capital letter for *orbital* angular momentum
subscript for *total* angular momentum

e.g. $\left\{\begin{matrix} n = 2 \\ \ell = 0 \\ j = \frac{1}{2} \end{matrix}\right\} \Rightarrow 2S_{1/2}$ $\qquad$ $\left\{\begin{matrix} n = 3 \\ \ell = 2 \\ j = \frac{5}{2} \end{matrix}\right\} \Rightarrow 3D_{5/2}$

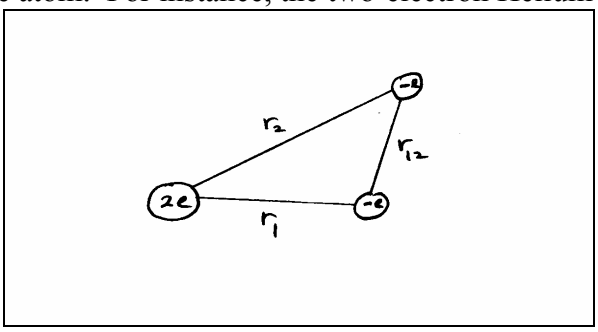
The usages of the 2 schemes of spectroscopic notation goes as follows: for orbital subshells we use the lower case letters s, p, d, f, etc; for the energy states we use the capital letters S, P, D, etc.

E. Multi-electron Atoms

Two effects are important: i) screening of the nucleus and ii) the exclusion principle.

1. Nuclear Screening

In a multi-electron atom, each electron interacts not only with the atomic nucleus, but also with every other electron in the atom. For instance, the two-electron Helium atom:



The net effect is that electrons farther from the nucleus "see" a nuclear charge of something less than *Ze*. The energy states are not simply the same ones found for the H-atom. This means in practice that it is practically impossible to solve for the multi-electron energy states exactly—they have to be approximated to some degree.

2. Exclusion principle

It turns out that no two electrons within an atom can be in exactly the same quantum state. This is a property of a class of subatomic particles called *fermions*. That is, no two electrons in an atom can have exactly the same set of values for their quantum numbers. This has implications for the electronic structure of multi-electron atoms and the periodic table of elements. Namely, no more than 2 electrons can occupy an atomic subshell, with $m_s = \pm\frac{1}{2}$.

3. Electronic Configurations of the Elements

a. Shells & subshells

We envision the atomic energy levels to be labeled by quantum numbers n and ℓ --1s, 2p, 3s, 4f, etc. These are called shells, since their probability densities are spherically symmetric around the nucleus. The shells are divided into $2\ell+1$ subshells, or *orbitals*, according to m_ℓ. With electron spin, each subshell has two levels. According to the exclusion principle, one electron may occupy each level, so each shell may be occupied by up to $2(2\ell+1)$ electrons.

In the atomic ground states, the subshells are filled in order of increasing energy. Commonly, the outermost subshell is partially filled. These are the valance electrons.

b. Hund's Rule

Each orbital (subshell) holds two electrons, spin up and down. However, within a shell, lower energy is usually obtained if the spins are aligned, but in different subshells.

e.g. for Carbon 2p shell

this		
↑	↑	
rather than		
↑↓		
$m_\ell = -1$	0	+1

This is Hund's Rule: a shell is filled first with one electron in each orbital, spins aligned. Then the second electron, with opposite spin, is placed in each orbital.

e.g. Oxygen & Fluorine 2p shell

Oxygen	↑↓	↑	↑
Fluorine	↑↓	↑↓	↑

c. Notation

The electronic configuration is written out by listing the occupied orbitals, and the number of electrons in each orbital. See Table 8.2 for the ground states of the elements. e.g.,

atom	**config**	**1s**	**2s**	**2p**			**3s**
H	$1s^1$	↑					
He	$1s^2$	↑↓					
Li	$1s^2 2s^1$	↑↓	↑				
Na	$1s^2 2s^2 2p^6 3s^1$	↑↓	↑↓	↑↓	↑↓	↑↓	↑

As *n* increases, the spacing between levels decreases. So there are quirks in the order in which shells are filled up.

e.g. see the elements 18 – 30. K is not [Ne] $3s^2 3p^6 3d^1$, but [Ne] $3s^2 3p^6 4s^1$. The 4s level is of lower energy than 3d, so the 4s level fills before the 3d level is occupied.

e.g. worse, look at V, Cr, and Mn. The outer most shells are $3d^3 4s^2$ for V; $3d^5 4s^1$ for Cr; $3d^5 4s^2$ for Mn.

Evidently, the energy levels are ordered thusly:

1s<2s<2p<3s<3p<4s~3d<4p<5s<4d<5p<6s<4f~5d<6p<7s<6d~5f. . . . where "4s~3d" means these states have nearly the same energy.