Historic Approach to Quantum Mechanics and Relativity

Lecture Notes Compilation

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§1.1 The Problem of Atomic Spectra

J.J Thomson had discovered the cathode rays and subsequent discoveries have confirmed the existence of a charged particle called "electron" as well as precisely measured its (charge/mass) ratio. Later, Millikan-Fletcher's oil drop experiment gave its charge and mass separately. However, the emission of cathode rays from atoms is not by itself proof enough for us to conclude that the electrons, the cathode ray particles, are actually present inside the atom. Thus, the question remained as to how do we know whether atoms actually contains electrons or not until it was finally answered by the **Zeeman Effect**. Let us see what is it now.

We know that light emitted by the atom has a characteristic spectrum consisting of many lines. For the moment, we consider one of these lines. In some cases, close investigation reveals that, as is observed in the case of the well-known D line of the Na atom, an apparent single line consists of two or more lines but, for the sake of simplicity, we take the line which is really single, or stated more rigorously, one which belongs to a certain singlet term. We now place the atom in a magnetic field and let it emit light. The spectral line which is ordinarily single is now split into three lines; one has the same frequency as before and the other two are displaced from it in opposite directions but by equal amounts. The magnitude of this frequency displacement is found to be proportional to the strength of the applied magnetic field. This phenomenon was found by Zeeman in 1897 and is called the Zeeman effect.

Theoretically, this phenomenon is interpreted in the following manner. The charged particle in the atom responsible for the emission and absorption of light undergoes some periodic motion with a certain characteristic frequency determined by the intratomic forces. When the external magnetic field H is applied to this atom, there will be an **additional force**

$$F = \frac{-e}{v}.(v \times H)$$

acting on the charged particle whose charge and velocity are denoted by $-e$ and v, respectively. The problem of explaining the Zeeman effect is now reduced to finding the difference in the motion of the particles due to this additional force, especially the difference in the characteristic frequencies of motion before and after the application of H.

Let the cylindrical coordinates describing the charged particles in the atom be denoted by (r_n, ϕ_n, z_n), where the subscript n refers to the coordinates of the n-th particle. The equations of motion in the absence of the magnetic field for the n-th particle are given by

$$\ddot{r_n} - r\dot{\phi_n}^2 = -\frac{1}{m}\frac{\partial V}{\partial r_n}$$

$$2\dot{r_n}\dot{\phi_n} + r_n\ddot{\phi_n} = -\frac{1}{m}\frac{1}{r_n}\frac{\partial V}{\partial \phi_n}$$

$$\ddot{z_n} = -\frac{1}{m}\frac{\partial V}{\partial z_n}$$

where m stands for the mass of the particle and V, the potential of the force governing the interatomic world, is a function of $r_1, \phi_1, z_1, r_2, \phi_2, z_2, \ldots \cdot$ Since the atom is considered to be spherically symmetric, the simultaneous displacement of the angular coordinates, ϕ_n of all the particles leaves the potential V unchanged, i.e., $V(r_1, \phi_1 + \Delta, z_1; r_2, \phi_2 + \Delta, z_2; r_3, \phi_3 + \Delta, z_3 \ldots) = V(r_1, \phi_1, z_1; r_2, \phi_2, z_2; r_3, \phi_3, z_3 \ldots)$

When the external magnetic field H is applied in the direction of the z-axis, the equations of motion are obtained by adding the additional force to the right hand side of the previous equations and are given as,

$$\ddot{r_n} - r\dot{\phi_n}^2 = -\frac{1}{m}\frac{\partial V}{\partial r_n} - \frac{eH}{mc}r_n\dot{\phi_n}$$

$$2\dot{r_n}\dot{\phi_n} + r_n\ddot{\phi_n} = -\frac{1}{m}\frac{1}{r_n}\frac{\partial V}{\partial \phi_n} + \frac{eH}{mc}\dot{r_n}$$

$$\ddot{z_n} = -\frac{1}{m}\frac{\partial V}{\partial z_n}$$

If solutions in absence of magnetic field are r_n^o, ϕ_n^o and z_n^o, then the solutions in the presence of magnetic field are shown to be, ignoring terms in the order of H^2 and using the above stated property of potential

$$r_n = r_n^o$$

$$\phi_n = \phi_n^o + \frac{eH}{2mc}t$$

$$z_n = z_n^o$$

This implies the simple fact that the motion of a particle in the presence of the magnetic field H is obtained from its motion in the absence of the field by simply superposing a rotation with the angular velocity of $eH/2mc$ around the field direction. We call this rotation the Larmor precession and the angular velocity $\omega = eH/2mc$ the Larmor angular velocity. When the ratio e/m was measured from the slope of fit, then it gave the same values as that for an electron, proving that electrons are really inside atoms.

Immediately following this, Thomson himself and Nagaoka proposed models of the atom. Thomson's model was that of electrons embedded in a positively charged sphere with uniform positive charge density. Nagaoka's model was a Planetary one with positive charge at centre.

§1.1.i Before Bohr – Unanswered Questions

Rutherford studied Geiger-Marsden's experiments of α- particle scattering and found support for Nagaoka's model - which later came to be called Rutherford's model. Thus, now we have a heavy nucleus of positive charge at the center and light electrons of negative charge around this

nucleus. Since the attractive force, inversely proportional to the square of the relative distance, is acting between the nucleus and the electrons, the latter must revolve around the former in order that they not collapse to the center. The situation then closely resembles the solar system.

- What explains that a certain atom has size 10^{-10} m or in other words what would determine the size of the atom? The orbit of this micro-solar system can take any size depending on the initial conditions, and, accordingly, the size, the energy and the period of motion of the atom can take any value. What then will explain the fact that an atom of a given material has a unique size, unique spectrum and unique energy depending only on the material.

- Even if by some unknown law, like Bode's law for the solar system, the sizes of the electronic orbits are determined, the electrons in these orbits cannot help but emit electromagnetic waves in accordance with Maxwell's theory. Maxwell's theory requires that a charged particle in accelerated motion necessarily emits electromagnetic waves which carry away energy per unit time at the rate of

  $$S = \frac{2}{3}\frac{e^2}{c^3}|\dot{v}^2|$$

  where e, v and c are the charge of the particle, its velocity, and the velocity of light, respectively. Due to the energy loss resulting from this process, the electron should eventually collapse into the nucleus.

  Thomson avoided this type of model, an atom with a center nucleus, and, took instead, the expended sphere of positive charge so that he could get around this difficulty. In his theory, besides m and e, there is another quantity specifying the size of this sphere as the additional structure constant. Therefore, it is quite natural that a quantity with the dimension of length results from his theory. As a matter of fact, the size of atom is nothing but this third structure constant, i.e., the size of the sphere of positive charge. Furthermore, the second difficulty in Rutherford's model also disappears in this model, since there is an equilibrium state in which the electrons are at rest and hence emitting no electromagnetic waves.

- Say that the electron in an atom undergoes some multi-periodic motion with fundamental frequencies $v_l, v_2, \ldots, v_k$ the coordinates of the electron are given as a multiple Fourier series of terms like $\cos\{2\pi(\tau_1 v_1 + \tau_2 v_2 + \cdots + \tau_k v_k)t\}$ with $\tau_1, \tau_2, \ldots, \tau_k$, integers or zero. Consequently, in this case, these fundamental frequencies are to be accompanied by higher harmonics with the frequencies $(\tau_1 v_1 + \tau_2 v_2 + \cdots + \tau_k v_k)$. The actually observed spectrum of the emitted light, however, does not showe any regularity of this kind.

- In the fundamental equations of the theory in Rutherford's model as well as in Nagaoka's, the electric charge e and mass m naturally appear as the constants which determine the structure of the atom. The mass of the nucleus does not come into play since we assume that it is very large and hence the nucleus may be assumed to be at rest. Then any conclusion of our theory must be expressed in terms of combinations of these two quantities, e and m. However, as can be seen from their dimensions, it is impossible to construct a quantity having the dimension of length by combining the above two quantities. This explains why

these two models cannot allow a determination of the size of the atom. The removal of the assumption that the nucleus is at rest and hence the introduction of the nuclear mass M in the theory does not remedy the situation, for obvious dimensional reasons.

- Another unanswered question concerns the spectrum of light emitted by the atom. Let us calculate the frequency v of the electronic motion in the circular orbit considered above. Denoting the angular velocity of this circular motion by ω, we have

$$mr\omega^2 = \frac{e^2}{r^2}$$

expressing the balance of the centrifugal force $mr\omega^2$ and the attractive electric force e^2/r^2. The frequency v then, satisfies

$$\frac{1}{v^2} = \left(\frac{2\pi}{\omega}\right)^2 = \frac{4\pi^2}{e^2} mr^3$$

Thus v is proportional to $r^{-3/2}$, a result corresponding to Kepler's third law for the solar system. Accordingly, this frequency increases as r shrinks from a (radius of hydrogen atom) to zero. However, then the frequency of light emitted during this motion cannot be constant and we cannot understand at all why a hydrogen atom emits a line spectrum of light having a constant frequency.

Some other questions are why are not atoms of a given material not different in sizes? Why are they all the same size? how are atoms stable at all? because based on a simple calculation, 10^{-12} sec is how long it can be stable.

§1.2 Bohr's model of the atom

Neil's Bohr based his model on a few results that had been obtained earlier, namely

- The numerical expression for regularity observed in the spectrum of hydrogen was successfully obtained by Balmer. He observed that the four lines in the visible part, $H_\alpha, H_\beta, H_\gamma$ and H_δ, have wave lengths given, respectively, by

$$\frac{9}{5}\lambda_o, \frac{16}{12}\lambda_o, \frac{25}{21}\lambda_o \text{ and } \frac{36}{32}\lambda_o$$

where $\lambda_o == 3645.6A^o$ and furthermore that these wave lengths are given by the general formula

$$\lambda = \frac{n^2}{n^2 - 4}\lambda_o, \qquad n = 3, 4, 5, 6$$

- Following this finding by Balmer, Rydberg of Sweden investigated the spectra of other atoms and found the formulae for these more complex spectra. He found that, despite the

apparent complexities, the spectrum of any atom can be classified into several series and that the lines in each of these series are expressible by the formula

$$\frac{1}{\lambda} = \frac{1}{\lambda_\infty} - \frac{R}{(n+b)^2}$$

with n a positive integer, and λ_∞ signifying the limiting wave length of the series under consideration, i.e., the wave length toward which the lines of the series converge with ever increasing density. The constant R in his formula does not depend on the kind of atom but is a universal constant. This R is called Rydberg's constant and has the value $R = 109677.691\ \text{cm}^{-1}$. On the other hand, the constant b in Rydberg's formula takes different values for different substances, or for different series, but within a certain series it has an approximately constant value.

Rydberg pushed his experimental studies still further and found that the series-limits of various series had also a similar regularity. Thus the term $1/\lambda_\infty$ in the above formula can be expressed as $R/(m+a)^2$ where m is a positive integer. He thus found that the spectrum in general could be expressed by the following formula, which is now called Rydberg's formula.

$$\frac{1}{\lambda} = \frac{R}{(m+a)^2} - \frac{R}{(n+b)^2}$$

When Rydberg discovered the formula , he did not forget to stress at the same time a fact which was later found to be extremely important for the development of quantum mechanics. He noted that the frequencies of a spectrum were given as the difference of two terms each of which contained an integer. He called these terms the spectral terms. Since this is so, it is simpler, in classifying the spectral lines, to work with the terms rather than with the frequencies themselves, the latter being found by taking differences of two terms. Since Ritz in 1908 used this fact extensively in his analysis of spectral lines, this is generally called Ritz's Combination law. Hence, Rydberg's formula written in terms of frequencies becomes

$$\nu = \frac{Rhc}{(m+a)^2} - \frac{Rhc}{(n+b)^2}$$

Rydberg's formula for spectral lines is not only very simple and elegant, but is also firmly verified experimentally. However, as Ritz stressed, this formula cannot be understood at all in the realm of classical theories. For according to classical ideas, it is considered that the light from an atom is emitted by the atomic electrons which are in some sort of periodic motion and produce waves in the surrounding electromagnetic field. According to this point of view, the spectrum of light in general has to contain, together with the fundamental modes, the higher harmonics the frequencies of which have the form of a sum of integral multiples of these fundamental frequencies.

§1.2.i Bohr introduces Planck's constant into atomic spectra

The difficulties in Rutherford's model however arose because we assumed the validity of Newtonian mechanics for the motion of the electron and the validity of Maxwell's theory for the

emission of electromagnetic waves. On the other hand, since Planck's discovery of h, these classical theories have been shown to be merely approximate in nature. Now then, the difficulty in Rutherford's model might well be due to the neglect of this h and not due to some defect of the model itself.

If Planck's constant h enters in the law governing the atomic world, the situation becomes quite different. As was explained previously, we cannot construct a constant with the dimension of length from any combination of the two constants e and m. This was a clear-cut indication of the difficulty. But if the law contains h, it is possible for the results of the theory to contain some quantity involving this h together with e and m. There exists one quantity with the dimension of length derivable from the combination of these three constants, namely

$$l = \frac{h^2}{me^2}$$

It would then become possible for us to explain the size of atom theoretically without arbitrarily introducing a certain object of predetermined size in the theory such as was done in Thomson's theory. In fact, using the known numerical values of e, m and h, the above l becomes 2.1×10^{-7} cm, a value which is roughly of the order of atomic size. Then our expectation that Planck's constant enters is considerably strengthened, since, if a certain quantity of the dimension of length could be derived from such a theory, it would be the above constant l multiplied by some numerical factor not much different from unity such as π, 2, 3, $\sqrt{2}$ etc. This numerical factor, by the way, will later be shown to be $1/(2\pi)^2$.

Now that the introduction of Planck's, or Einstein's quantum concept seems to solve all the difficulties in our present problem, would it not be natural to proceed in the following manner? Planck considered that, in quantum theory, the energy, and hence the amplitude, of a dynamical system in sinusoidal oscillation, to be called hereafter simply a harmonic oscillator, is not allowed to take any values continuously but takes only a set of discrete values given by

$$E_n = nhv, \; n \in \mathbb{W}$$

Should it not then be that the energy of an atom also is allowed, in quantum theory, to take only a set of discrete values? Assuming this to be so, we designate the energy values by W_n, with n being integer. The discreteness of the energy requires that the electron orbits in the atom have discrete sizes, the smallest among which will then correspond to the size of the stable atom.

Meanwhile, Einstein showed that the photoelectric effect can be well understood by considering that the electron, on absorbing the energy of incident light of frequency v, increases its energy by hv. Though in the photoelectric effect the energy is transferred from the incident light to an electron, would not the quantum theoretical situation be the same also in the reverse process where an atom emits light? Thus, when an atom originally in a state of energy W_n, changes its state for some reason to that of energy W_m, where we assume $W_n > W_m$, can we expect that a light quantum of energy hv satisfying $hv = W_n - W_m$ will be emitted? If so, the frequency of the emitted light must satisfy the following condition, which we call Bohr's frequency condition.

$$v = \frac{W_n - W_m}{h}$$

Such an idea is entirely different from that of Maxwell. For now the emission of light is not considered as due to something like the acceleration of electrons in the state w_N but instead as due to an abrupt change of state, $W_n \to W_m$. As long as an atom is in one of the allowed energy states, it does not emit light at all. It was for this reason that Bohr called such states stationary states. Furthermore, such an abrupt change of state as $W_n \to W_m$ is entirely beyond comprehension within the framework of Newtonian mechanics. We call this abrupt change a quantum jump or transition. According to this new idea, the wave length of light emitted from an atom satisfies

$$\nu_{nm} = \frac{W_n - W_m}{h} = \frac{c}{\lambda_{nm}}$$

This result, $1/\lambda$ being given by the difference of two terms, is in fact the Rydberg-Ritz combination law itself.

§1.2.ii Bohr's Hypotheses about Atoms and Radiation

- **Hypothesis (I) :** *An atom can not take continuous energy values as in the classical theory, but instead it is allowed to take only certain discrete energy values, $W_1, W_2, \ldots$, characteristic of each atom. In these allowed states, the atom does not emit light.*

  We call the above allowed states and the allowed energy values, W_n, the " stationary states" and the " energy levels" of the atom, respectively.

- **Hypothesis (II) :** *Emission or absorption of light by an atom occurs when the atom makes a transition from one to another of its stationary states. When this happens, monochromatic light of the frequency given by $\nu = (W_n - W_m)/h$ is emitted or absorbed depending on whether $W_n > W_m$ or $W_n < W_m$.*

§1.2.iii Harmonicity at large n

It has already been stated that the generalized Balmer formula holds for the spectrum of hydrogen; i.e.,

$$\frac{1}{\lambda} = \frac{R}{m^2} - \frac{R}{n^2}$$

By comparing this with equation $\lambda = \nu/c = W_n/hc - W_m/hc$, we find that the allowed energy values W_m are given by

$$W_m = -\frac{Rhc}{m^2}$$

The negative sign for W_m is due to the fact that the electron in the hydrogen atom is bound, requiring then a certain amount of work in order to be separated from the atom. Let us consider the quantum expression for $n > m$,

$$\frac{1}{\lambda_{nm}} = \frac{R}{m^2} - \frac{R}{n^2}$$

Now, let n and m be both very large numbers ($n, m >> 1$) and $m = n - s$ where $n >> s$. Then, on simplification, we get to the first order in (s/n), which is a small quantity

$$\frac{c}{\lambda_{n,n-s}} = \frac{Rc}{(n-s)^2} - \frac{Rc}{n^2} = \frac{Rc}{n^2}\left[\left(1 - \frac{s}{n}\right)^{-2} - 1\right] = \frac{Rc}{n^2}\left[\cancel{1} - (-2).\frac{s}{n} - \cancel{1}\right]$$

$$\therefore \nu_{n,n-s} = \frac{2Rc}{n^3}.s = s.\nu_o$$

where $\nu_o = 2Rc/n^3$, can be interpreted as the orbital frequency of the electron in the n-th orbit. In other words, as m and n increase, the quantum formula for ν_{nm} does give rise to harmonics as in the classical case. One should bear in mind that the interpretation of the quantum formula as a quantum jump between states n and m, of course, does not have any classical analogy.

This observation became the basis for Bohr's Correspondence principle, which is roughly stated as "the quantum theoretic expression involving the quantum numbers n must give the classical behaviour in the limit of large n or $n \to \infty$". Looked at differently, the quantum expressions seem to take a more fundamental colour with the classical expressions playing the subordinate role as a limiting case.

§1.2.iv Bohr's third hypothesis

In the case of an oscillator, the quantum of energy is given by $\epsilon = h\nu$. Since a spring-mass system is an oscillator, we first write down the expression for frequency of the oscillator as $2\pi\nu = \sqrt{k/m}$. In other words, the frequency is related to the constants in the equations of motion or Hamiltonian. However, in the atomic spectral formula, R is just an empirical constant.

Hence, Bohr asked the question if Rydberg's constant can be expressed in terms of e, h, m and c. To do this, he started by treating the electron classically when it is in a very large n state. By "behaving classically" we mean that the following relations hold :- Let r be the radius of a circular "orbit" of the electron of charge e moving under the influence of a positive charge $+e$. Then the centripetal force is :

$$\frac{mv^2}{r} = \frac{e^2}{r^2} \implies mr\omega_o^2 = \frac{e^2}{r^2}$$

$$\therefore \omega_o^2 = \frac{e^2}{mr^3} \implies \nu_o^2 = \frac{e^2}{4\pi^2 mr^3}$$

Also,

$$E = \frac{1}{2}mr^2\omega_o^2 - \frac{e^2}{r} = \frac{1}{2}\cancel{mr^2}.\frac{e^2}{\cancel{mr^2}.r} - \frac{e^2}{r} = -\frac{e^2}{2r} = -|K.E| = 2|P.E|$$

$$\therefore \frac{1}{r} = \frac{2|E|}{e^2}$$

Eliminating r,

$$\nu_o^2 = \frac{e^2}{4\pi^2 mr^3} = \frac{e^2}{4\pi^2 m}.\left(\frac{2|E|}{e^2}\right)^3 = \frac{2|E|^3}{\pi^2 me^4}$$

$$\therefore v_o = \frac{\sqrt{2}|E|^{\frac{3}{2}}}{\sqrt{\pi^2 me^4}}$$

However, from correspondence principle, when the electron is in the n-th stationary state, $v_o = 2Rc/n^3$. When written in terms of $W_n = -Rhc/n^2$ becomes

$$v_o = \frac{2Rc|W_n|^{\frac{3}{2}}}{(Rhc)^{\frac{3}{2}}}$$

Bohr identified W_n with E, the classical energy of the electron in the circular nth orbit to obtain the following expression for R:

$$\frac{2Rc}{(Rhc)^{\frac{3}{2}}} = \frac{\sqrt{2}}{\sqrt{\pi^2 me^4}} \implies \frac{\sqrt{2}}{R^{\frac{1}{2}} c^{\frac{1}{2}} h^{\frac{3}{2}}} = \frac{1}{\sqrt{\pi^2 me^4}}$$

$$\therefore R = \frac{2\pi^2 me^4}{ch^3}$$

This agrees remarkably well with the empirical value of R obtained from the line spectra indicating that the correspondence principle is on the right track. If we further extend this assumption that the electron follows classical dynamics in the state W_n, we can also get the quantised radius of the orbit r_n quantised.

$$W_n = -\frac{Rhc}{n^2} = -\frac{2\pi^2 me^4}{n^2 h^2}$$

$$r_n = \frac{e^2}{2|E|} = \frac{e^2}{2|W_n|} = \frac{n^2 h^2}{4\pi^2 me^2}$$

When $n = 1$, this gives the correct size of the Hydrogen atom also obtained independently from kinetic theory of gases. It is further to be noted that the introduction of the third hypothesis together with the assumption of a circular orbit allows a simplification of the relationship $W_n = -(2\pi^2 me^4)/(n^2 h^2)$. Namely, in terms of the angular momentum L of the electron's circular motion, its energy W is expressed as,

$$W = -|K.E| = -\frac{1}{2}mv^2 = -\frac{1}{2}m\left(\frac{L}{mr}\right)^2 = -\frac{L^2}{2mr^2}$$

$$\therefore L_n = \sqrt{2mr_n^2.|W_n|} = \sqrt{mr_n e^2} = \frac{nh}{2\pi}$$

All these successes suggested to Bohr that he was on the correct path to a full quantum theory. Note that in the above derivations, Bohr implicitly assumed that while in a stationary state the electron followed classical mechanics. This led to Bohr making the following hypothesis : Bohr's III hypothesis.

Hypothesis (III) : *The electron in a stationary orbit obeys the rule of classical mechanics.*

The Hypothesis III by Bohr is clearly not very consistent because the E.M. laws of Maxwell are not applicable, while the laws of mechanics can be applied to get some information of the microscopic dynamics. In fact, in the purely quantum regime, i.e., for small n, applying Maxwell's EM gives results that are very different from the measured frequencies of line spectra.

Example : The fundamental frequency of the periodic motion of an electron around the hydrogen nucleus is given by the classical expression :

$$v_o = \frac{\sqrt{2}|E|^{\frac{3}{2}}}{\sqrt{\pi^2 me^4}} = \frac{\sqrt{2}}{\sqrt{\pi^2 me^4}}.\left(\frac{2\pi^2 me^4}{n^2h^2}\right)^{\frac{3}{2}} = \frac{4\pi^2 me^4}{n^3h^3}$$

Since $W_n \propto 1/n^2 \propto 1/r \implies v_o \propto r^{-3/2}$. Therefore, the time period $T = 1/v_o \propto r^{3/2} \implies T^2 \propto r^3$. This is nothing but Kepler's III law for planetary orbits in a $1/r$ gravitational potential. Hence, radiation of frequencies $v_o, 2v_o, 3v_o, 4v_o, \ldots$ is expected classically. However, the quantum expression is

$$v_{nm} = \frac{c}{\lambda_{nm}} = Rc.\left(\frac{1}{m^2} - \frac{1}{n^2}\right) = \frac{2\pi^2 me^4}{h^3}\left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$

When $n = 5$, $m = 1, 2, 3\ldots$ one can verify that $v_{n\to m}$ is very different from the classical expression with $n = 5$! This inconsistency suggests that classical physics meets successes only partially. However, classical physics does play a role to an extent in quantum theory, and one has to make certain leaps – such as the purely non-classical idea of a quantum jump – to move into the quantum theory. After all, this idea of transition between states leading to radiation is the most drastic change introduced by Bohr and therefore the classical law of radiation is to be understood from now on as a limiting case. In fact, the modern recipe for writing a quantum equation of motion involves going through the classical Hamiltonian and Bohr recognised it intuitively before Dirac.

§1.2.v Ehrenfest's Adiabatic hypothesis

In the last section, we learned that the energy of a hydrogen atom in a stationary state is given as $W_n = -(2\pi^2 me^4)/(n^2h^2)$ while that of Planck's oscillator is given as $E_n = nhv = (nh/2\pi)\sqrt{k/m}$, where m is the mass oscillating under the influence of an elastic force with elasticity coefficient k . We now ask what law, if any, determines in general the quantum theoretically allowed states of a given dynamical system. Without such a general law we cannot treat atoms more complicated than the hydrogen atom, and cannot treat molecules. We have to know the recipe for selecting the quantum theoretically allowed states from the continuous manifold of states of a general dynamical system. Hereafter we call this recipe simply the quantum condition. The general quantum condition was obtained historically in the following manner.

The quantum laws are in their nature entirely different from the laws of classical mechanics or of electrodynamics and they cannot be understood in terms of classical ideas. We learned in the last section that the first two hypotheses could not take us beyond the law of spectral lines and the third hypothesis was introduced tentatively in order to treat the dynamical system in a stationary

state by classical mechanics. On the other hand, the transition, being a typically quantum effect, remained entirely inaccessible to treatment by classical methods.

In view of this feature of the theory, we have to rely on the classical theory in some parts of the problem while in the other parts we introduce quantum theoretical ideas. This attitude naturally is very unsatisfactory and is to be considered merely as a temporary one. It should at least be made clear at what point we have to make the switch over from the classical ideas to quantum theoretical ones. Our Hypothesis III was to meet this requirement. We now ask if it is possible to extend the domain of classical theory beyond the limit as specified by Hypothesis III. In partial response to this question, Ehrenfest introduced Hypothesis IV on the basis of considerations to be described in the following. This Hypothesis IV plays an important role in leading us to a quantum condition of more generality and is called Ehrenfest's adiabatic hypothesis.

Our derivation of Wien's displacement law was based entirely on Maxwell's classical idea that E/ν for a classical oscillator was invariant under slow adiabatic variations. We applied this to the normal coordinates of radiation inside a volume V . Then, by the same reasoning , ν/T was also found invariant under adiabatic volume compression. This led to Wien's guess

$$E_s = \frac{V.8\pi\nu^2}{c^3} h\nu e^{-\beta h\nu} d\nu$$

However most interestingly, Planck's hypothesis which treats light in a quantum theoretic way also satisfied this law. To see this, consider a general oscillator :

$$E = \alpha p^2 + \beta q^2$$

The average energy is according to Boltzmann's principle

$$< E >= A \int \int (\alpha p^2 + \beta q^2) e^{-E/kT} dpdq$$

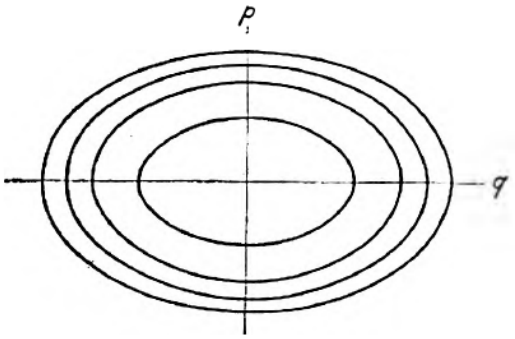
where A is given by

$$\frac{1}{A} = \int \int e^{-E/kT} dpdq$$

Since Planck considered that energy cannot take all the values continuously, p as well as q accordingly cannot assume every arbitrary value either. Denoting the amount of the energy quantum by ε, the energy E can take only those values which are integral multiples of ε and hence p and q can take only those values which satisfy

$$E = \alpha p^2 + \beta q^2 = n\varepsilon \qquad , n \in \mathbb{W}$$

Geometrically speaking, the points on a set of ellipses defined by the above equation on the $q - p$ plane, as shown in below figure, correspond to the allowed values for p and q.



Thus the integration is to be understood not as a surface integral over the whole $q - p$ plane but as a sum of the line integrals on these ellipses. In accordance with this understanding, the calculation proceeds as follows. We first change the variables from q and p to x and y by $q\sqrt{\beta} = x$ and $p\sqrt{\alpha} = y$, respectively. The energy E is then given by $E = x^2 + y^2$ and the integrations to be performed become

$$I_1 = \frac{1}{\sqrt{\alpha\beta}} \int\int (x^2 + y^2) e^{-(x^2+y^2)/kT} dxdy$$

$$I_2 = \frac{1}{\sqrt{\alpha\beta}} \int\int e^{-(x^2+y^2)/kT} dxdy$$

In order to carry out these integrations, we use as the integration variables the energy E itself and the angle θ, defined by $\theta = \tan^{-1}(y/x)$, instead of x and y. The Jacobian matrix is given as follows, from which we can see that $dEd\theta = 2dxdy$

$$J = \begin{pmatrix} \partial E/\partial x & \partial E/\partial y \\ \partial\theta/\partial x & \partial\theta/\partial y \end{pmatrix} = \begin{pmatrix} 2x & 2y \\ -y/(x^2+y^2) & x/(x^2+y^2) \end{pmatrix} \implies |J| = 2$$

The above integrals then become

$$I_1 = \frac{1}{2\sqrt{\alpha\beta}} \int\int E e^{-E/kT} dEd\theta$$

$$I_2 = \frac{1}{2\sqrt{\alpha\beta}} \int\int e^{-E/kT} dEd\theta$$

Since θ can take any value from zero to 2π, whereas E has to satisfy the condition $E = n\varepsilon,\ n \in \mathbb{W}$, we first integrate with respect to θ and obtain

$$I_1 = \frac{\pi}{\sqrt{\alpha\beta}} \int E e^{-E/kT} dE$$

$$I_2 = \frac{\pi}{\sqrt{\alpha\beta}} \int e^{-E/kT} dE$$

$$\therefore \quad < E >= \frac{\int E e^{-E/kT} dE}{\int e^{-E/kT} dE}$$

where the integration with respect to E is to be understood as the sum of the integrand for those values of E satisfying $= n\varepsilon,\ n \in \mathbb{W}$. Thus,

$$< E >= \frac{\sum_{n=0}^{\infty} n\varepsilon\, e^{-n\varepsilon/kT}}{\sum_{n=0}^{\infty} e^{-n\varepsilon/kT}}$$

The summation of these series is not difficult. Since

$$\sum_{n=0}^{\infty} n\varepsilon\, e^{-n\varepsilon/kT} = -\frac{\partial}{\partial\left(\frac{1}{kT}\right)} \sum_{n=0}^{\infty} e^{-n\varepsilon/kT}$$

We have only to calculate $\sum_{n=0}^{\infty} e^{-n\varepsilon/kT}$, which in turn is nothing but a geometrical series the sum of which is readily given as

$$\sum_{n=0}^{\infty} e^{-n\varepsilon/kT} = \frac{e^{\varepsilon/kT}}{e^{\varepsilon/kT-1}}$$

From this result we obtain

$$\sum_{n=0}^{\infty} n\varepsilon\, e^{-n\varepsilon/kT} = \frac{\varepsilon e^{\varepsilon/kT}}{(e^{\varepsilon/kT-1})^2}$$

The substitution of these results gives,

$$< E >= \frac{\varepsilon}{e^{\varepsilon/kT-1}}$$

If we define function $P(x) = x/(e^x - 1)$, then

$$< E >= kTP\left(\frac{\varepsilon}{kT}\right)$$

This agrees with **Planck's interpolation formula** which is stated as follows : *The amount of energy actually distributed to a degree of freedom of frequency v is*

$$< E_v >= kTP\left(\frac{hv}{kT}\right)$$

if we take hv as the energy quantum i.e., $\varepsilon = hv$, v being the frequency of the oscillating system under consideration. Hence, we find that the requirement ε = *a universal constant times v* was necessary and sufficient for the derivation of a formula which satisfies the displacement law despite the existence of the energy quantum ε : with this substitution for ε the function $P(\varepsilon/kT)$ became a function of v/T as required by the displacement law. Thus we can conclude that if, following Planck, we accept the existence of the elementary unit of energy for electromagnetic oscillations, the **necessary and sufficient** condition for the derived result to satisfy the displacement law is that this elementary unit is proportional to the frequency, say $\varepsilon = hv$, and that the energy of each proper oscillation is an integral multiple of this unit : $E = nhv$.

While proving Wein's law, we used the procedure of compressing the hollow cavity adiabatically

and at the same time infinitely slowly. During this compression, the energy as well as the frequency of each proper oscillation of the light varies continuously. Since, however, the ratio E_s/v_s is an adiabatic invariant, the quantum condition $E_s = hv_s n_s$, $(n_s = 0, 1, 2, 3, \dots)$ for each proper oscillation, once satisfied initially, will be satisfied at all times during and after the process of this compression. Thus, the quantum condition being always satisfied during the compression, our proof of Wien's law can naturally be expected to be valid also in quantum theory. This is the very origin of the above connection between the energy unit and the displacement law.

In this argument, however, a basic assumption is tacitly made. Namely that the results of classical mechanics on infinitely slow adiabatic variations, especially the result about adiabatic invariants, hold also in quantum theory and, in addition, if the system is in one of the quantum theoretically allowed states before the variation, it will stay there during as well as after the variation. This assumption which led to Wien's law in the case of the black body radiation has been explicitly extended by Ehrenfest to include dynamical systems in general.

§1.2.vi Bohr's fourth hypothesis - the quantum condition

Hypothesis (IV) : *When a variation is given externally to a dynamical system, and if this variation is performed infinitely slowly, then the behavior during the variation of this dynamical system can be described by conventional mechanics and, in this case, the system which is initially in a quantum theoretically allowed state will remain there during as well as after the variation.*

Let the Hamiltonian function be given as $H = H(p, q, a)$ where the parameter a is given as a slowly varying function of time, $a(t)$. The existence of such a time varying parameter in the Hamiltonian function does not alter the fact that $q(t)$ and $p(t)$ are determined by Hamilton's equations of motion, i.e.,

$$\dot{q} = \frac{\partial H}{\partial p} \qquad , \qquad \dot{p} = -\frac{\partial H}{\partial q}$$

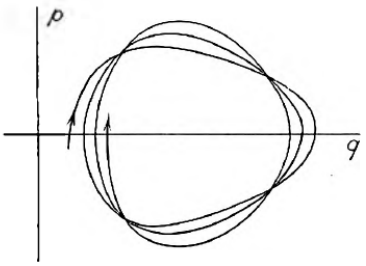
If we introduce the q and p determined by these equations as functions of time into H, the value of H thus obtained gives the instantaneous energy of the system in this state of motion. The energy is not a constant but a function of time which we denote by E. Namely we have $H(p, q, a) = E$ which can be solved for p as $p = p(q, E, a)$.

We now consider the hypothetical dynamical system which would result if the parameter a were fixed at the value which it has at a certain instant τ. It is further assumed that the values of p and q of this system coincides at the time τ with $p(\tau)$ and $q(\tau)$ of the original dynamical system, respectively. We denote this motion of the hypothetical system by $p_\tau(t)$ and $q_\tau(t)$. The energy of this system E_τ which is naturally a constant, is to coincide with E of the original system at time τ, i.e., $E_\tau = E(\tau)$. In the meantime, since this hypothetical system is completely periodic, its trajectory is a closed curve and is obviously given by the equation $p_\tau = p(q_\tau, E_\tau, a_\tau)$.

We shall now show that the area under the curve enclosed in the case of periodic oscillatory

motion, say J is the adiabatic invariant itself. In other words, we prove that

$$J = \oint pdq = \oint p(q, a(\tau), E)dq = J(\tau) \implies \frac{dJ}{d\tau} = 0$$



Adiabatic deformation of a trajectory

The area, J, enclosed by this curve is a function of τ and is calculated by

$$J = 2\int_{q_\tau^{(2)}}^{q_\tau^{(1)}} p(q_\tau, E_\tau, a_\tau)dq_\tau$$

where $q_\tau^{(1)}$ and $q_\tau^{(2)}$ are the two roots of the equation $p(q_\tau, E_\tau, a_\tau) = 0$. Let the total change of J due to the change of the parameter a be denoted by ΔJ. Then our aim is to prove $\Delta J = 0$ for a sufficiently slow variation of a as a function of time. The proof goes as follows. First of all,

$$\frac{dJ}{d\tau} = 2\left[p(q_\tau^{(2)}, E_\tau, a_\tau)\frac{dq_\tau^{(2)}}{d\tau} - p(q_\tau^{(1)}, E_\tau, a_\tau)\frac{dq_\tau^{(1)}}{d\tau}\right] + 2\int_{q_\tau^{(1)}}^{q_\tau^{(2)}}\left[\left(\frac{\partial p}{\partial E}\right)_\tau \frac{dE_\tau}{d\tau} + \left(\frac{\partial p}{\partial a}\right)_\tau \frac{da_\tau}{d\tau}\right]dq_\tau$$

where the symbol $(\,)_\tau$ implies that the variables q, E, a (and sometimes p, too) inside the bracket assume their respective values at time τ, i.e., q_τ, E_τ, a_τ (and p_τ). The first term on the right hand side of the above equation vanishes since $q_\tau^{(1)}$ and $q_\tau^{(2)}$ are both solutions of $p(q_\tau, E_\tau, a_\tau) = 0$. In the meantime, $p(q, E, a)$ has been obtained by solving $H(p, q, a) = E \implies E = H(p(E, q, a), q, a)$.

Now partially differentiating $E = H(p(E, q, a), q, a)$ with respect to E, we get

$$1 = \left(\frac{\partial H}{\partial p}\right)\left(\frac{\partial p}{\partial E}\right) \implies \left(\frac{\partial p}{\partial E}\right)_\tau = \frac{1}{(\partial H/\partial p)_\tau}$$

and partially differentiating $E = H(p(E, q, a), q, a)$ with respect to a, we get

$$\left(\frac{\partial E}{\partial a}\right) = \left(\frac{\partial H}{\partial a}\right) + \left(\frac{\partial H}{\partial p}\right)\left(\frac{\partial p}{\partial a}\right) \implies \left(\frac{\partial p}{\partial a}\right)_\tau = -\frac{(\partial H/\partial a)_\tau}{(\partial H/\partial p)_\tau}$$

Furthermore, $(\partial H/\partial p) = \partial q/\partial t$ by Hamiltonian's equation of motion. We finally obtain,

$$\frac{dJ}{d\tau} = \int\left[\frac{dE_\tau}{d\tau} - \left(\frac{\partial H}{\partial a}\right)_\tau \frac{da_\tau}{d\tau}\right]dt$$

where the integration with respect to t is to be carried out over one period of the hypothetical system like from $\tau - 1/(2\nu_\tau)$ to $\tau + 1/(2\nu_\tau)$, $1/\nu_\tau$ being this period. We notice here that $(\partial H/\partial a)_\tau$ as a function of t, is

$$\left(\frac{\partial H}{\partial a}\right)_\tau = \frac{\partial H(p_\tau(t), q_\tau(t), a_\tau)}{\partial a_\tau}$$

In the meantime, for the motion of the actual dynamical system, not the hypothetical one, we have the relationship

$$\frac{dE}{dt} = \frac{\partial H}{\partial a}\frac{da}{dt}$$

where

$$\frac{\partial H}{\partial a} = \frac{\partial H(p(t), q(t), a(t)}{\partial a(t)}$$

Then we get

$$\frac{dE_\tau}{d\tau} = \frac{\partial H(p(\tau), q(\tau), a_\tau)}{\partial a_\tau}\frac{da_\tau}{d\tau}$$

$$\therefore \frac{dJ}{d\tau} = \int_{\tau-\frac{1}{2\nu_\tau}}^{\tau+\frac{1}{2\nu_\tau}} \frac{\partial H(p(\tau), q(\tau), a_\tau)}{\partial a_\tau}\frac{da_\tau}{d\tau}dt - \int_{\tau-\frac{1}{2\nu_\tau}}^{\tau+\frac{1}{2\nu_\tau}} \frac{\partial H(p_\tau(t), q_\tau(t), a_\tau)}{\partial a_\tau}\frac{da_\tau}{d\tau}dt$$

In order to express mathematically the fact that the change of a occurs infinitely slowly, we replace $a(t)$ by $a(t/T)$ and let T tend to infinity. Then $a(t/T)$ varies from $a(0)$ to $a(1)$ as t changes from 0 to T. If the values of $a(0)$ and $a(1)$ are fixed, then the change is quick when T is small and is slow when T is large. Now the total change of J caused by changing a from $a(0)$ to $a(1)$ is given by integrating $dJ/d\tau$i.e.,

$$\Delta J = \int_0^T d\tau \int_{\tau-\frac{1}{2\nu_\tau}}^{\tau+\frac{1}{2\nu_\tau}} \frac{\partial H(p(\tau), q(\tau), a_\tau)}{\partial a_\tau}\frac{da_\tau}{d\tau}dt - \int_{\tau-\frac{1}{2\nu_\tau}}^{\tau+\frac{1}{2\nu_\tau}} \frac{\partial H(p_\tau(t), q_\tau(t), a_\tau)}{\partial a_\tau}\frac{da_\tau}{d\tau}dt$$

where a_τ is replaced with $a_{\tau/T}$. Our task is to show that ΔJ vanishes for infinitely large T. For proving this it is convenient to use new integration variables defined by $\tau/T = \sigma$ and $t/T = s$. Then ΔJ becomes,

$$\Delta J = T\left[\int_0^1 d\sigma \int_{\sigma-\frac{1}{2T\nu_\sigma}}^{\sigma+\frac{1}{2T\nu_\sigma}} \frac{\partial H(p(T\sigma), q(T\sigma), a_\sigma)}{\partial a_\sigma}\frac{da_\sigma}{d\sigma}ds\right]$$

$$-T\left[\int_0^1 d\sigma \int_{\sigma-\frac{1}{2T\nu_\sigma}}^{\sigma+\frac{1}{2T\nu_\sigma}} \frac{\partial H(p_{T\sigma}(Ts), q_{T\sigma}(Ts), a_\sigma)}{\partial a_\sigma}\frac{da_\sigma}{d\sigma}ds\right]$$

The domain of the double integration is a narrow band-shaped region along the straight line $s = \sigma$ in the σs-plane extending from $\sigma = 0$ to $\sigma = 1$, the width being of the order $1/T\nu_\sigma$. We now change the order of integration in the first integral and replace the integration variable σ by s and s by σ. Then we see that the first integral becomes,

$$\int_0^1 d\sigma \int_{\sigma-\frac{1}{2T\nu_\sigma}}^{\sigma+\frac{1}{2T\nu_\sigma}} \frac{\partial H(p(Ts), q(Ts), a_s)}{\partial a_s}\frac{da_s}{ds}ds$$

Strictly speaking the domain of integration indicated in this expression is not exact, but the error is negligibly small, of the order of $(1/Tv)^2$. In carrying through the integration over s we may replace a_s and da_s/ds in the integrand by a_σ and $da - \sigma/d\sigma$ respectively, since the integration interval is very small, of the order of $1/Tv$. The correction to this approximation is a small quantity of the order of $1/Tv$. We may further replace $p(Ts)$ and $q(Ts)$, the motion of the actual system, by $p_{T\sigma}(Ts)$ and $q_{T\sigma}(Ts)$ of the hypothetical system. The correction is here again of the order of $1/Tv$. After integration over s these correction terms will give rise to a term of the order of $(1/Tv)^2$, the order of the integrand multiplied by the order of the area of the integration domain.

Having made these approximations it is now clear that in [] portion of ΔJ, the main term of the first integral is cancelled by the second integral and the remaining correction term is of the order of $(1/Tv)^2$. We get then

$$\Delta J = T\left[(\text{finite term})\left(\frac{1}{Tv}\right)^2\right]$$

which vanishes for infinite T. It can be proved that the area enclosed by a trajectory is invariant with respect to canonical transformations of coordinates and momenta. This quantity J is occasionally referred to as the action variable. The general definition of J can be written as $J = \oint pdq$ where the small circle on the integral sign indicates that the integra tion should be performed over one cycle of the motion.

The Hamiltonian function of a dynamical system making a sinusoidal motion, for example an oscillator, is given in general by $H = \alpha p^2 + \beta q^2$ with frequency of motion $v = \sqrt{\alpha\beta}/\pi$. The Hamiltonian, of course, has the physical meaning of the energy of the system. We now consider the motion where the value of the energy H is E. In this motion, both q and p are functions of time and they describe a curve, $q = q(t)$ and $p = p(t)$ on the $q - p$ plane. We call this curve the trajectory of the motion. In the present case where H is given as $\alpha p^2 + \beta q^2$, the trajectory is an ellipse given by $E = \alpha p^2 + \beta q^2$. Comparing with standard equation of ellipse, $1 = (x/a)^2 + (y/b)^2$, we get semi-major axis $a = \sqrt{E/\alpha}$ and semi-minor axis $b = \sqrt{E/\beta}$. Hence, the area J, inside this ellipse on the $q - p$ plane is readily calculated to be $J = \pi ab = \pi E/\sqrt{\alpha\beta}$. Thus, we obtain the relationship $J = E/v$. With $E = nhv$, $J = nh$ for a stationary state. We, hence, can conclude that, for one-dimensional periodic systems, the quantum theoretically allowed states are characterized by

$$J = \oint pdq = nh,\ n \in \mathbb{I}$$

This is the Bohr's quantisation condition, which now being for true an oscillator, can be generalised to any dynamical system. When the dynamical system under consideration has many degrees of freedom, the situation becomes quite complicated. Let the coordinates of the dynamical system and their conjugate momenta be $q_1, q_2, \ldots, q_f$ and $p_1, p_2, \ldots, p_f$, respectively. One of the simplest is the case where the Hamiltonian function of the dynamical system under consideration consists of a sum of terms each depending on only one of the coordinates and its conjugate momentum as follows :

$$H(q_1 q_2, \ldots, q_f; p_1, p_2, \ldots, p_f) = \sum_{s=1}^{f} H_s(p_s, q_s)$$

Such a choice of coordinates that makes the Hamiltonian separable is called the normal mode coordinates. We encountered them in the context of the modes of oscillation of a string. In this case, we can consider each degree of freedom of the whole system as an independent dynamical system and consequently the calculation of J can be carried out for each degree of freedom separately and this is nothing but the one-dimensional system whose treatment we have just seen. Thus, each individual H_s above is conserved. Hence, the equations

$$H_s(p_s, q_s) = E_s, \ s = 1, 2, \ldots, f$$

give separate trajectories for each degree of freedom and by solving these equations for the p_s's we obtain

$$p_s = p_s(q_s, E_s), \ s = 1, 2, \ldots, f$$

The calculation of $J_s = \oint p_s dq_s$ together with the quantum condition $J_s = n_s h$, $n_s \in \mathbb{I}$, for each degree of freedom, $s = 1, 2, \ldots, f$ will determine the stationary states of the dynamical system under consideration. Such a choice of coordinates that makes the Hamiltonian separable is called the normal mode coordinates. We encountered them in the context of the modes of oscillation of a string.

§1.3 Bohr discovers a correspondence between classical radiation and quantum transitions

Bohr's theory is thus supported by the experimental results but it cannot be considered as a completed theory. It does explain how the discontinuous elements of nature discovered by Planck can be incorporated into the laws governing the atomic world, but the essential point of the problem is left still untouched; for in this theory we do not yet know about the fundamental quantum phenomenon of " transitions" . Without knowledge of the mechanism by which these transitions occur, Bohr's theory can determine only the frequencies but neither the intensity nor the polarization of light emitted by the atom. The same is true for the absorption of light by the atom.

The classical theory was complete in this sense, if we put aside the problem of agreement with experimental results. For Newtonian mechanics together with Maxwell's electrodynamics allows us to calculate not only the frequency but also the intensity and the polarization of light emitted by an electron in motion. The interaction being small between the electron and the electromagnetic field of the light, the calculation can simply be carried out in the following manner. The motion of the electron is primarily governed by Newtonian mechanics and the weak interaction with the field of the light can be neglected without seriously affecting the motion. The electron then describes a multiply-periodic motion and the dipole moment of the electron system accordingly undergoes a multiply-periodic variation.

The dipole moment, denoted by P, is then as a function of time to be expressed as a multiple Fourier series such as

$$P(t) = \sum_{n_1,n_2,n_3,\ldots,n_k=-\infty}^{+\infty} C_{n_1,n_2,n_3,\ldots,n_k} e^{2\pi i(n_1\nu_1+\ldots n_k\nu_k)t}$$

where in order to make $P(t)$ real the coefficients $C_{n_1,n_2,\ldots,n_k}$ have to satisfy the relationship

$$C^*_{n_1,n_2,\ldots,n_k} = C_{-n_1,-n_2,\ldots,-n_k}$$

At this stage Maxwell's electrodynamics is introduced and it tells us that electromagnetic waves are emitted from this oscillating dipole moment. This electromagnetic wave then consists of waves of various frequencies corresponding to each term; i.e. of frequencies given by

$$\nu_{n_1,n_2,\ldots,n_k} = |n_1\nu_1 + n_2\nu_2 + \ldots n_k\nu_k|$$

where $n_1, n_2, \ldots, n_k$ can be zero, or positive or negative integers. When one of the n's is equal to unity while all the others are zero, the wave corresponding to the fundamental mode appears, and when the n's have any other set of values waves of higher harmonics are obtained. Each of these waves, according to Maxwell's theory, can be considered as being emitted independently by the appropriate terms of the dipole moment. For example, the wave with frequency $\nu_{n_1,n_2,\ldots,n_k}$ is equal to the wave emitted by the dipole moment of the corresponding harmonic oscillator

$$P_{n_1,n_2,\ldots,n_k}(t) = C_{n_1,n_2,\ldots,n_k} e^{2\pi i\nu_{n_1,n_2,\ldots,n_k}t} + C_{-n_1,-n_2,\ldots,-n_k} e^{-2\pi i\nu_{n_1,n_2,\ldots,n_k}t}$$

Now, using the condition obtained for $P(t)$ to be real, we have

$$P_{n_1,n_2,\ldots,n_k}(t) = 2\Re(C_{n_1,n_2,\ldots,n_k})\cos(2\pi\nu_{n_1,n_2,\ldots,n_k}t) + 2\Im(C_{-n_1,-n_2,\ldots,-n_k})\sin(2\pi\nu_{n_1,n_2,\ldots,n_k}t)$$

Therefore, when one wants to obtain the intensity of this wave, one simply substitutes the above equation into

$$\frac{dE}{dt} = \frac{2}{3c^3} < \ddot{P}^2 >$$

which gives the energy radiated per unit time in the form of waves. The symbol $< >$ means that the time average over one period of the enclosed quantity is to be taken. We hence obtain for the intensity of the wave,

$$\frac{dE_{n_1,n_2,\ldots,n_k}}{dt} = \frac{2}{3c^3} < \ddot{P}^2_{n_1,n_2,\ldots,n_k} >$$

$$\implies \frac{dE_{n_1,n_2,\ldots,n_k}}{dt} = \frac{4(2\pi\nu_{n_1,n_2,\ldots,n_k})^4}{3c^3} < \mathrm{Re}(C_{n_1,n_2,\ldots,n_k})^2 + \mathrm{Im}(C_{n_1,n_2,\ldots,n_k})^2 >$$

$$\therefore \frac{dE_{n_1,n_2,\ldots,n_k}}{dt} = \frac{(2\pi\nu_{n_1,n_2,\ldots,n_k})^4}{3c^3}|C_{n_1,n_2,\ldots,n_k})^2|$$

The Fourier series expansion tells us the intensity of radiation emitted by an oscillating dipole. The classical Electrodynamics theory can similarly predict the polarisation of the emitted light based on the Fourier component $C_{n_1,n_2,\ldots,n_k}$. While in Bohr's theory, there is no way of determining either the intensity or polarisation. However, a mathematical similarity between the classical frequency and the quantum frequency solves the riddle.

§1.3.i Classical orbital frequencies

Let $q_1, q_2, \ldots, q_s; p_1, p_2, \ldots, p_s$ be the canonical variables, then $J_s = \oint p_s dq_s$. We assume that $H(q_1, \ldots, q_s; p_1, \ldots, p_s)$ is constant and the motion is periodic. The abbreviated action integral $\int \sum_i p_i dq_i$ generates a new canonical variable θ_s such that $H(J_1, \ldots, J_s)$ and all the θ's are cyclical coordinates.

$$\therefore \dot{\theta_s} = \frac{\partial H}{\partial J_s} = \nu_s \implies \theta_s = \nu_s t + k$$

where ν_s is the frequency of oscillation of the s-th coordinate and k is a constant. To see this, we consdier the simplest case when

$$H(q_1 q_2, \ldots, q_f; p_1, p_2, \ldots, p_f) = \sum_{s=1}^{f} H_s(p_s, q_s) \text{ where } H_s = E_s = \alpha p_s^2 + \beta q_s^2$$

From Hamiltonian equation of motion, we have

$$\dot{q_s} = \frac{\partial H_s}{\partial p_s} = 2\alpha p_s = 2\alpha \sqrt{\frac{E_s - \beta q_s^2}{\alpha}} = 2\sqrt{\alpha.(E_s - \beta q_s^2)}$$

We can hence show that, if $T = T(E_s)$ is the period of motion

$$\frac{\partial J_s}{\partial H} = \frac{dJ_s}{dE_s} = \frac{d}{dE_s} \oint p_s dq_s = \frac{d}{dE_s} \oint \sqrt{\frac{E_s - \beta q_s^2}{\alpha}}.dq_s = \oint \frac{1}{2\sqrt{\alpha.(E_s - \beta q_s^2)}}.dq_s$$

$$\therefore \frac{\partial J_s}{\partial H} = \oint \frac{dq_s}{\dot{q_s}} = \oint dt = T = \frac{1}{\nu_s}$$

In general, lets denote the energy of a dynamical system in its n-th stationary state by W_n. Our problem is to obtain the energy W of the system as a function of J, but we first calculate the inverse function $J(W)$. Since the Hamiltonian function has the physical meaning of the energy, p and q have to satisfy, in the motion with energy W : $H(p, q) = W$ which describes a curve on the $q - p$ plane which is the trajectory of the motion with energy W. The system being a periodic one, the trajectory is a closed curve. The area enclosed by this closed curve is equal to J. Then, we have

$$J = 2 \int_{q_1}^{q_2} p(W, q) dq$$

where $p(W, q)$ is the momentum as a function of W and q obtained as the solutions of $H(p, q) = W$ while q_1 and q_2 are the solutions of $p(W, q) = 0$. The integration gives J as a function of W.

$$\frac{dJ(W)}{dW} = 2\left[p(W, q_2)\frac{dq_2}{dW} - p(W, q_1)\frac{dq_1}{dW}\right] + 2\int_{q_1}^{q_2} \frac{\partial p(W, q)}{\partial W} dq$$

The first term of this expression vanishes according to the definition of q_1 and q_2, while the second term can be transformed to a simpler form. By the use of the relation,

$$\frac{\partial p(W, q)}{\partial W} = \left(\frac{\partial H(p, q)}{\partial p}\right)^{-1}$$

which is a consequence of the fact that $p(W,q)$ is the solution of $H(p,q) = W$. Together with the equation of motion $\dot{q} = \partial H/\partial p$, we finally arrive at

$$\frac{dJ(W)}{dW} = 2\int \frac{dq}{\dot{q}} = \int_0^T dt = T$$

In this result, t is the time it takes for the system to make one revolution of the trajectory; that is, it is the period of the motion. However, T is the reciprocal of the frequency v appearing in the Fourier series, thereby resulting in the important relation

$$v = \left(\frac{\partial J(W)}{\partial W}\right)^{-1} = \frac{\partial W}{\partial J(W)}$$

§1.3.ii Correspondence to quantum transitions - Selection Rules

The frequencies of light emitted by the dynamical system under consideration in the last section, in n-th stationary state are given by Bohr's frequency condition

$$v_{n\to n-\tau} = \frac{W_n - W_{n-\tau}}{h}$$

The W_n's, in turn, are determined by imposing the quantum condition $J = nh$ where $n \in \mathbb{I}$ on the allowed motions of the system. More specifically, when the energy W is obtained as a function of J , the substitution of nh for J in this expression gives W_n i.e., $W_n = W(nh)$. Now, we can approximate the numerator in the limit of very large n and of negligibly small τ compared with n, by

$$W_n - W_{n-\tau} = W(nh) - W((n-\tau)h) = \tau h\left(\frac{W(nh) - W((n-\tau)h)}{\tau h}\right) = \tau h\left(\frac{dW}{dJ}\right)_{J=nh}$$

and accordingly

$$v_{n\to n-\tau} = \tau\left(\frac{dW}{dJ}\right)_{J=nh} = \tau v$$

where v is the fundamental frequency, in the sense of classical theory, in the state of motion of $J = nh$.

This similarity can be interpreted as a correspondence between classical and quantum theoretical frequencies: For very large n, the frequency of the quantum transition from the stationary state n to $n-\tau$, when τ is small, is nothing but the τ-th harmonic of the frequency of the "orbital motion" in the state $J = nh$ classically. Clearly this does not hold for small n as seen earlier.

For a general transition from a state given by $W(J_1 = n_1h, \ldots, J_s = n_sh)$ to one by $W(J_1^{'} = (n_1 - k_1)h, \ldots, J_s^{'} = (n_s - k_s)h$, we get

$$v_{(n_1,\ldots,n_s)\to(n_1-k_1,\ldots,n_s-k_s)} = \frac{W(n_1h,\ldots,n_sh) - W((n_1-k_1)h,\ldots,(n_s-k_s)h)}{h}$$

which, for sufficiently large n's and for sufficiently small k' s , reduces approximately to

$$v_{(n_1,\ldots,n_s)\to(n_1-k_1,\ldots,n_s-k_s)} = k_1\frac{\partial W}{\partial J_1} + \cdots + k_s\frac{\partial W}{\partial J_s} = k_1v_1 + \cdots + k_sv_s$$

This is the same as the frequency term in the classical Fourier series,

$$P(t) = \sum_{k_1,k_2,k_3,\ldots,k_s} C_{k_1,k_2,k_3,\ldots,k_s} e^{2\pi i(k_1 v_1 + \ldots k_s v_s)t}$$

§1.4 Correspondence Principle codified

In the last section it was stated that, in the limit of large quantum number, the frequency, intensity, and polarization of the quantum theoretically emitted light agree with the corresponding quantities for the light emitted according to the classical theory.

As has been repeatedly remarked, this does not at all imply that the emission mechanisms in the two theories are the same. In the classical theory, the atomic electrons emit the light in their process of orbital motion and they emit both the fundamental mode and the higher harmonics simultaneously. In the quantum theory, on the contrary, the light is emitted at the instant of the transition and the emitted light is a monochromatic one. Therefore, when only a single transition of an atom is involved, one obtains, in a vague sense, only an instant flash of one of the spectral lines of the atom and the energy emitted thereby is exactly equal to hv. Under these circumstances, we cannot define the intensity of a spectral line. Since the intensity means the amount of energy emitted per unit time, knowledge of the rate of occurrence of such a transition is essential for the definition of intensity.

It is, then, necessarily concluded that we should be referring to the overall effect of a large number of atoms and not to a single transition of an atom when we say that the correspondence principle relates the quantum theoretical frequency or intensity to the respective counterpart in the classical theory. Physically the context of the correspondence principle primarily claims that when the intensity of a spectral line of an atom calculated in the classical theory is strong, or weak, the corresponding quantum transition should occur frequently, or rarely, in the aggregate of a large number of atoms of the kind under consideration. Namely, the correspondence can be realized only through the introduction of statistical considerations.

What mechanism then makes the transition occur? And what determines the rate of occurrence when some of the transitions occur more frequently and some others less frequently? Or, tracing the problem still further back, what is the reason why an atom cannot indefinitely stay in one of its stationary states but instead makes a transition to some other state? What factors then influence the atom in choosing a particular one of the many possible final states? Suppose that a number of atoms of the same kind are initially in the same stationary state; some of them will make transitions at time t_A to a state A while some others at time t_B to a state B. What difference in the two atoms of the same kind make them behave differently? We have, for the time being, no answer at all to these questions.

Under these circumstances, it seems advisable that with Einstein, we give up any inquiry into the causal structure of the transition and proceed with the assumption that they are governed by a certain probability law. That is, we assume that an atom in a stationary state has a prob-

ability of falling spontaneously in a given time interval to another state of lower energy. This probability may and will be determined by yet unknown laws of interaction between the atom and radiation, but here we just assume that this probability, like the one governing the decay of radioactive elements, is proportional to the time interval and that the proportionality constant, or the probability of occurrence per unit time of the transition, is characteristic of the transition process under consideration. This constant is called the transition probability.

By $A_{n\to n-k}$ we denote the transition probability for an atom to make the transition from a state n to a state $n-k$. The amount of energy released by the atom is $hv_k = W_n - W_{n-k}$. Accordingly, when an ensemble of a large number of atoms is considered, the intensity of the light emitted from this ensemble per one atom is given by

$$\frac{dE_k}{ct} = hv_k.A_{n\to n-k}$$

Although the laws of interaction between the atom and radiation are not known, Bohr's correspondence principle furnishes a method of calculating the transition probability. Namely, the principle requires that the quantum theoretical intensity obtained above should agree with the one obtained from classical theory via Fourier series. By comparing these two equations we find that the transition probability is to be given by

$$A_{n\to n-k} = \frac{(2\pi)^4 v_k^3 |C_k|^2}{3hc^3}$$

Conversely,if any transition $n \to n-k$ is possible, we require that the classical Fourier series have a component $C_k.e^{2\pi i v_k t}$. This correspondence also throws light on why only some transitions are possible. In other words, the correspondence principle led to the discovery of selection rules !

Example : As a simple illustration of the correspondence principle, we take, in this section, the case of Planck's oscillator. The motion of the mass point in the case of the harmonic oscillator is quite simple and the Fourier series consists only of two terms, namely,

$$x = X_1 e^{2\pi i v t} + X_{-1} e^{-2\pi i v t}$$

where the x-axis is taken in the direction of the oscillation. When the point mass has an electric charge e, the dipole moment of this harmonic oscillator is given by

$$P = C_1 e^{2\pi i v t} + C_{-1} e^{-2\pi i v t} = -e(X_1 e^{2\pi i v t} + X_{-1} e^{-2\pi i v t})$$

Since the Fourier series of the dipole moment has only terms with $k = \pm 1$, all but the transitions $n = n \pm 1$ are forbidden and, in the emission of light, only the transition $n = n - 1$ is allowed (since we have $W_n > W_{n-1}$).

§1.4.i How do we calculate using Bohr's theory ?

As a simple example, we consider Planck's oscillator, the Hamiltonian of which is

$$H = \frac{p^2}{2m} + \frac{1}{2}kq^2$$

In the state of energy E, the equation

$$\frac{p^2}{2m} + \frac{1}{2}kq^2 = E$$

holds, and, as has been stated previously, this determines an elliptic trajectory in the $q - p$ plane. The area, enclosed by this trajectory, J, is given by

$$J = \oint pdq = 2\int_{q_1}^{q_2} \sqrt{2m\left(E - \frac{1}{2}kq^2\right)}.dq$$

where q_1 and q_2 are the two solutions of the equation,

$$E - \frac{1}{2}kq^2 = 0 \implies q_1 = -\sqrt{\frac{2E}{k}},\ q_2 = \sqrt{\frac{2E}{k}}$$

The result of the integration is

$$J = 2\pi\sqrt{\frac{m}{k}}E$$

The same result can also be obtained directly from the consideration

$$J = (\text{area of ellipse}) = \pi \times (\text{semi-major axis}) \times (\text{semi-minor axis}) = \pi \times \sqrt{2mE} \times \sqrt{\frac{2}{k}E}$$

In any case, the application of the quantum condition $J = nh$, $n \in \mathbb{W}$ gives

$$E = \frac{1}{2\pi}\sqrt{\frac{k}{m}}.nh,\ n \in \mathbb{W}$$

$$\because v = \frac{1}{2\pi}\sqrt{\frac{k}{m}} \implies E = nhv,\ n \in \mathbb{W}$$

We can also determine the motion of the oscillator in these stationary states. The system naturally makes a sinusoidal motion, then for some amplitude a and phase δ.

$$q = a.\cos(2\pi vt + \delta) \implies p = m\dot{q} = -a.2\pi mv.\sin(2\pi vt + \delta)$$

$$\therefore E = \frac{1}{2}ka^2 + 2\pi mv^2a^2$$

$$\because k = (2\pi)^2mv^2 \implies 2\pi mv^2a^2 = nhv,\ \ \therefore a^2 = \frac{nh}{(2\pi)^2mv},\ n \in \mathbb{W}$$

The oscillator, therefore, can assume only a set of discrete values for the amplitude of its motion.

Summary of Correspondence Principle

- The quantum formula for an $m \to m - k$ transition gave the k-th harmonic of the orbital frequency in the m-th orbit.
- The existence of the k-th harmonic of v_m in the Fourier series meant the $V_{m\to m-k}$ was allowed.

§1.5 Correspondence principle as a guiding principle

Summarizing the procedure, we first solve the given problem by the classical approach and then reinterpret the results by replacing the concept of the frequency of orbital motion (or of the Fourier component) with the corresponding concept of the quantum frequency (or the probability) of the transition; i.e., the classical frequency $\nu_{k_1,k_2,\ldots,k_s}$ is replaced by the quantum theoretical one of the transition $n_1 \to n_1 - k_1, n_2 \to n_2 \bar{} k_2, \ldots, n_k \to n_s \bar{} k_s$ and the square of the Fourier component, $|C^2_{k_1,k_2,\ldots,k_s}|$, of the dipole moment by the corresponding transition probability $A_{n_1,n_2,\ldots,n_s \to n_1-k_1,n_2-k_2,\ldots,n_s-k_s}$.

In this way Bohr's theory is supplemented and a useful method for calculating various processes is obtained. Nevertheless, this procedure is to be considered as merely a convenient recipe for calculating quantum theoretical quantities such as transition probabilities, since we still do not know the cause of a quantum transition. When we arrive at the true theory, the first thing to be clarified is the mechanism through which only a certain discrete set of states can occur in nature and then to understand what determines why some atoms jump from A to B at time t_B while some others jump from A to $B^{'}$ at t_B, and so on. We would then be able to calculate the frequency of occurrences of such transitions and presumably would find that it actually is in harmony with the correspondence principle result in the limit of large n.

§1.6 Heisenberg's discovery - How numbers became matrices - Birth of Matrix mechanics

According to the correspondence principle, there is a close correspondence between the quantum transitions of an atomic system on the one hand and the Fourier components of the electron's orbital motion in the sense of classical mechanics on the other. That is, for instance, to the transition $n \to n - k$ of the quantum theory there corresponds the k-th higher harmonic of the motion of the electron in the state n. When the quantum number n is very large, the light resulting from the transition $n \to n - k$ has the same frequency as that of this higher harmonic and, furthermore, they have the same intensity as well as the same polarization. Although a number of considerations were successfully guided by this principle, the principle itself gives correct answers only in these cases of very large values of the quantum number n. Should it be possible at all to obtain a theory which can give correct answers also in the cases of small n-values ?

Heisenberg took up the task of extending the correspondence principle to all n. In other words, he started with the premise that the observed spectral frequencies are the only measurable quantities and therefore, any hope of measuring the position or momentum of an electron in an atom should be given up. In this philosophy, his belief was that a true quantum theory would emerge if quantum theoretic quantities are defined in correspondence with the classical counterparts. With this aim he went about constructing a dictionary to translate classical quantities into quantum theoretic counterparts.

- A classical quantity such as the position of the electron in an atom would have a Fourier series representation given as follows, with the subscript c explicitly indicating classical

quantities,

$$x(t) = \sum_k X_c(n,k)e^{2\pi i \nu_c(n,k)t}$$

- In the classical Fourier term $X_c(n,k)e^{2\pi i \nu_c(n,k)t}$, the notation used is $\nu_c(n,k) \equiv k\nu_n \equiv k\nu_c(n,1)$. We now require, by correspondence principle, that a corresponding quantum theoretic quantity, say Transition component be defined. Let it be denoted as follows, with $\nu_q(n \to n-k) \equiv (W_n - W_{n-k})/h$ and the subscript q explicitly indicating quantum quantities,

$$X_q(n \to n-k)e^{2\pi i \nu_q(n \to n-k)t}$$

- We note that for classical frequencies

$$\nu_c(n,k) = -\nu_c(n,-k) \because \nu_c(n,k) = k\nu_c(n,1)$$

and for quantum theoretical frequencies

$$\nu_q(n \to n-k) = -\nu_q(n-k \to n) \because \nu_q(n \to n-k) = \frac{W_n - W_{n-k}}{h}$$

This fact implies that the correct translation of $\nu_c(n,k) = -\nu_c(n,-k)$ into the quantum theoretical language is not a simple change of sign of k, such as $\nu(n \to n-k) = -\nu(n \to n+k)$, but rather the interchange of the initial and final states. Furthermore, for the coordinate x to be real, it is required in the classical and quantum theory respectively that

$$X_c(n,k) = X_c^*(n,-k),\ X_q(n \to n-k) = X_q^*(n-k \to n)$$

$$\therefore X_c(n,-k) \leftrightarrow X_q(n \to n+k)$$

- Classically, we have the following relation

$$\nu_n = \frac{\partial W(J)}{\partial J} = \frac{1}{h}\left(\frac{\partial W(n)}{\partial n}\right) \because J = nh$$

$$\therefore \nu_c(n,k) = k\nu_c(n,1) = \frac{k}{h}\left(\frac{\partial W(n)}{\partial n}\right)$$

While quantum theoretically, we have

$$\nu_q(n \to n-k) = \frac{W(n) - W(n-k)}{h}$$

$$\therefore \nu_c(n,k) \leftrightarrow \nu_q(n \to n-k) \because \frac{\partial W(n)}{\partial n} = \frac{W(n) - W(n-k)}{k}$$

This is just a restatement of the correspondence principle. The *LHS* of this correspondence is the k-th harmonic of the orbital frequency in the nth orbit. Whereas, the *RHS* represents a transition between two states. In other words, mathematically, we are moving from derivatives (continuous variables) to differences (discrete variables).

- If we have an arbitrary dynamical variable $F(\theta, J)$ defined classically in terms of the canonical variables - action variables $J_s = n_s h$ and their corresponding coordinates, angle variables, we extend the last case to replace :

$$k\frac{\partial F}{\partial n} = F(n) - F(n-k)$$

- Further, we often encounter in the classical theory a differential of the following kind which we shall interpret as follows, in conformity with the definition of second differentiation

$$\begin{aligned}\frac{d^2 f}{dx^2} &= \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{(\Delta x)^2} \\ &= \lim_{\Delta x \to 0} \frac{(f(x+\Delta x) - f(x)) - (f(x) - f(x-\Delta x))}{(\Delta x)^2}\end{aligned}$$

$$\begin{aligned}\therefore k\left(\frac{\partial v_c(n,k)}{\partial n}\right) &= \frac{1}{h}\left(k\frac{\partial}{\partial n}\left(k\frac{\partial W(n)}{\partial n}\right)\right) \\ &\leftrightarrow \frac{1}{h}\left(k\frac{\partial}{\partial n}(W(n) - W(n-k)\right) \\ &= \frac{1}{h}[(W(n+k) - W(n)) - (W(n) - W(n-k))] \\ &\leftrightarrow v_q(n+k \to n) - v_q(n \to n-k)\end{aligned}$$

We shall see that a sign change of k leaves $k.(\partial v_c(n,k)/\partial n)$ invariant because

$$k\left(\frac{\partial v_c(n,k)}{\partial n}\right) \quad \xrightarrow{k \to -k} \quad -k\left(\frac{\partial v_c(n,-k)}{\partial n}\right) = k\left(\frac{\partial v_c(n,k)}{\partial n}\right)$$

However, $v_q(n \to n-k) - v_q(n-k \to n-2k)$, is not invariant under sign change of k. Since corresponding principle requires such an argument for large n, we instead choose $v_q(n+k \to n) - v_q(n \to n-k)$. Analogously, we can say that any $k.(\partial X_c(n,k)/\partial n)$ (derivatives of Fourier coefficient) is to be replace by $X_q(n+k \to n) - X_q(n \to n-k)$ where $X_q(n+k \to n)$ is a quantum transition component i.e.,

$$k\left(\frac{\partial X_c(n,k)}{\partial n}\right) \leftrightarrow X_q(n+k \to n) - X_q(n \to n-k)$$

- We have that $x = \sum_k X_c(n,k)e^{2\pi i \nu_c(n,k)t}$. Lets now compute x^2,

$$\begin{aligned}x^2 &= \sum_k \left[\sum_{k'} X_c(n,k')e^{2\pi i \nu_c(n,k')t}.X_c(n,k-k')e^{2\pi i \nu_c(n,k-k')t}\right] \\ &= \sum_k \left[\sum_{k'} X_c(n,k')X(n,k-k')\right]e^{2\pi i \nu_c(n,k)t}\end{aligned}$$

This shows that, while the Fourier coefficients may be different, x^2 has the same frequency components in its Fourier series as $x(t)$. One can show this for x^3 etc and in the limit.

Any function of $x(t)$ can be written as a Taylor series $f(x) = a_0 + a_1 x + a_2 x^2 + \dots$ in $x(t)$. Using the same reasoning as above, we can say that while some elements may be zero etc, but, over all, the series is harmonic as $x(t)$ is. Therefore, according to Bohr's correspondence principle, the quantum theoretical analogue of $x^2(t)$ should have the same "transition components" as $x(t)$.

- Classically, we have $v_c(n,k) + v_c(n,k') = v_c(n,k+k') \leftrightarrow v_c(n,k) + v_c(n,k'-k) = v_c(n,k)$. We have shown that $\sum_{k'} X_c(n,k')X(n,k-k')$ is the coefficient of $e^{2\pi i v_c(n,k)t}$ in $x^2(t)$. Now, we try to find the coefficient of $e^{2\pi i v_q(n\to n-k)t}$ in quantum theory for X_q^2. Naively, using

$$X_c(n,k')e^{2\pi i v_c(n,k')t} \leftrightarrow X_q(n \to n-k')e^{2\pi i v_q(n\to n-k')t}$$

$$X_c(n,k-k')e^{2\pi i v_c(n,k-k')t} \leftrightarrow X_q(n \to n-(k-k'))e^{2\pi i v_q(n\to n-(k-k'))t}$$

won't work, because then for the $n \to (n-k)^{\text{th}}$ transition,

$$\sum_{k'} X_q(n \to n-k')e^{2\pi i v_q(n\to n-k')t}.X_q(n \to n-(k-k'))e^{2\pi i v_q(n\to n-(k-k'))t}$$

which must have frequency $v_q(n \to n-k)$, has frequency $v_q(n \to n-(k-k')) + v_q(n \to n-k') \neq v_q(n \to n-k)$. However, $v_q(n \to n-k') + v_q(n-k' \to n-k) = v_q(n \to n-k)$. Therefore, thanks to correspondence principle, we realise that we need to have the $v_q(n \to n-k)$ component as,

$$\sum_{k'} X_q(n \to n-k')X_q(n-k' \to n-k)e^{2\pi i v_q(n\to n-k)t}$$

Similarly, for x^3 component, we have

$$\sum_{k'}\sum_{k''} X_q(n \to n-k')X_q(n-k' \to n-k'')X_q(n-k'' \to n-k)e^{2\pi i v_q(n\to n-k)t}$$

- In other words, if x has quantum transition components given by $X_q(n \to n-k)$, then we also have

$$x^2 \leftrightarrow \sum_{k'} X_q(n \to n-k')X_q(n-k' \to n-k)$$

$$x^3 \leftrightarrow \sum_{k'}\sum_{k''} X_q(n \to n-k')X_q(n-k' \to n-k'')X_q(n-k'' \to n-k)$$

By redefining $n-k = n'$, $n-k' = n''$, ... we have

$$x \to \left[X_q\right]_{nn'} \equiv \hat{X}_q$$

$$x^2 \to \sum_{n''} \left[X_q\right]_{nn''} \left[X_q\right]_{n''n'} \equiv \hat{X}_q.\hat{X}_q$$

$$x^3 \to \sum_{n''}\sum_{n'''} \left[X_q\right]_{nn''} \left[X_q\right]_{n''n'''} \left[X_q\right]_{n'''n'} \equiv \hat{X}_q.\hat{X}_q.\hat{X}_q$$

Here, $\hat{X}_q$ is an infinite dimensional matrix in mathematical sense having matrix element between the stationary states indexed by n, n', n'' etc and explicitly follows the rules of matrix multiplication. This is how a number in classical physics became a matrix in quantum theory.

This really doesn't cause any problem to correspondence principle because the language of transitions and transition components can never be fully translated into the language of Fourier series and intensities and orbital motion. Also, by construction, these quantum theoretic quantities X_q oscillate at the correct frequencies $X_q(n \to n-k)e^{2\pi i \nu_q (n \to n-k)t}$ and combine as per Rydberg-Ritz combination rules of $\nu_{n\to m} = (E_n - E_m)/h$ to give the correct correspondence relation.

§1.7 Bohr's Quantum Condition becomes the canonical commutation relation

Bohr's quantum condition expressed as $\oint pdq = nh$ is not very satisfactory because it takes classical quantities on the *LHS* and imposes an integer quantum number on the *RHS* on the classical trajectory. Heisenberg thought that in the true quantum theory, such a relation should contain only the quantum theoretic quantities. To do this, we first need to express $\oint pdq = nh$ in terms of Fourier series of $p(t), q(t)$. Hence, $p = \sum_k p_c(n,k)e^{2\pi i \nu_c(n,k)t}$ and $q = \sum_k q_c(n,k)e^{2\pi i \nu_c(n,k)t}$. Now, $\oint pdq = \oint p(dq/dt)dt = \int_0^T p\dot{q}dt$. Hence, we have the following integration, where t runs from 0 to $T = (\nu_c(n,1))^{-1}$ i.e., one full period.

$$\begin{aligned} nh &= 2\pi i \sum_k \sum_{k'} \int_0^T p_c(n,k)q_c(n,k')\nu_c(n,k')e^{2\pi i(\nu_c(n,k)+\nu_c(n,k'))t}dt \\ &= 2\pi i \sum_k \sum_{k'} p_c(n,k)q_c(n,k')\nu_c(n,k') \int_0^{\frac{1}{\nu_c(n,1)}} e^{2\pi i(\nu_c(n,k)+\nu_c(n,k'))t}dt \end{aligned}$$

The integral can be evaluated by noting that

$$\int_0^{\frac{1}{\nu_c(n,1)}} e^{2\pi i(k+k')\nu_c(n,1)t}dt = \frac{e^{2\pi i(k+k')} - 1}{2\pi i(k+k')\nu_c(n,1)} = \begin{cases} 0 & , \ k+k' \neq 0 \\ (\nu_c(n,1))^{-1} & , \ k+k' = 0 \end{cases}$$

Therefore, only $k + k' = 0$ term contributes, giving us

$$nh = 2\pi i \sum_k \sum_{-k} p_c(n,k)q_c(n,-k)\frac{\nu_c(n,-k)}{\nu_c(n,1)}$$

$$\implies nh = -2\pi i \sum_k \sum_{-k} p_c(n,k)q_c^*(n,k)k$$

Bohr imposed the integer nature of n onto the orbit is phase space and thereby got the discreteness of energy levels / stationary states. However, we want the discreteness to follow from the correspondence principle, from the discreteness of the harmonics in the limit of large n and Heisenberg's goal is to extend the definition of quantum theoretical quantities to all n (including

small n). So it is important that a general version of Bohr's quantum condition not have any explicitly rule that n be an integer.

Physically this requirement means that we formulate fundamental quantum behaviour in terms of transitions and transition components and classical trajectories and orbital frequencies appear only in the correspondence limit. In such a scenario, the discreteness of the energy levels, or more precisely the discreteness of the labels of the energy levels will automatically give rise to integer harmonics in the usual harmonic Fourier series of classical multiperiodic systems. Differentiation of the above equation on both sides with respect to n, we get using the equivalences between classical and quantum quantities from the previous section,

$$
\begin{aligned}
\implies \frac{h}{2\pi i} &= \sum_k -k\frac{\partial}{\partial n}(p_c(n,k)q_c^*(n,k)) \\
&= \sum_k \left[-k\left(\frac{\partial p_c(n,k)}{\partial n}\right).q_c^*(n,k) + p_c(n,k)\left(-k\left(\frac{\partial q_c^*(n,k)}{\partial n}\right)\right)\right] \\
&= \sum_k [-(p_q(n+k\to n) - p_q(n\to n-k)).q_q^*(n+k\to n) \\
&\qquad - p_q(n\to n-k)(q_q^*(n+k\to n) - q_q^*(n\to n-k))] \\
&= \sum_k \left[-p_q(n+k\to n)q_q^*(n+k\to n) + p_q(n\to n-k)q_q^*(n\to n-k)\right] \\
&\qquad - \sum_k \left[p_q(n\to n-k)q_q^*(n+k\to n) - p_q(n\to n-k)q_q^*(n\to n-k)\right] \\
&= \sum_k -p_q(n+k\to n)q_q^*(n+k\to n) + \sum_k p_q(n\to n-k)q_q^*(n+k\to n) \\
&\qquad - p_q(n\to n-k)q_q^*(n+k\to n) + \sum_k p_q(n\to n-k)q_q^*(n\to n-k) \\
&= \sum_k -p_q(n+k\to n)q_q(n\to n+k) + \sum_k p_q(n\to n-k)q_q(n-k\to n) \\
&= \sum_k -q_q(n\to n+k)p_q(n+k\to n) + \sum_k p_q(n\to n-k)q_q(n-k\to n) \\
&= -\hat{q}_q.\hat{p}_q + \hat{p}_q.\hat{q}_q
\end{aligned}
$$

$$
\therefore \boxed{i\hbar = [\hat{q}_q, \hat{p}_q]}
$$

This condition is the equivalent of the Bohr quantum condition and does not suffer from the inexplicable ad hoc requirement that $\oint pdq$ has to be an integer multiple of the quantum of action (h). Moreover, since it has been expressed using quantum theoretic quantities q_Q, p_Q (commonly denoted as $\hat{q}$ and $\hat{p}$ where the hats signify that we are not dealing with classical dynamical quantities q and p, but their matrix analogues which necessarily do not "commute" always), it now extends the Bohr correspondence principle to any quantum stationary states. The operation $AB - BA$ for two matrices A and B is called its commutator product. Therefore $[\hat{q}, \hat{p}] = i\hbar$ is the canonical/ fundamental commutation relations. How do we know this is equivalent to the Bohr

quantisation condition ?

If we apply it to the simple harmonic oscillator, we get $E_n = (n + 1/2)hv$ (analysis skipped for now). Bohr's theory gives $E_n = nhv$ for the oscillator. While Heisenberg's theory agrees with this assertion, it also predicts an additional term. This term $1/2hv$ is termed the zero-point energy of an oscillator and has been experimentally verified conclusively. Physically it means that there is no "rest" position for a quantum oscillator, and this is because of the fundamental commutation relation $i\hbar = [\hat{q}_q, \hat{p}_q]$. Thought of differently, the oscillator does not, in its ground or lowest energy state have a fixed position or momentum and exhibits a fluctuation. This means there is a certain uncertainty in its position and momentum and the equation. $i\hbar = [\hat{q}_q, \hat{p}_q]$ is a mathematical expression of this fundamental uncertainty. The discovery of an uncertainty relation is one of Heisenberg's fundamental contributions and ultimately set limits on the accuracy with which a position and its conjugate momentum can be measured, which is the very subject of this course!

II

Modern Quantum Mechanics

2 Heisenberg, Schrödinger and Dirac's "Quantum Mechanics"

§2.1 Born-Jordan-Heisenberg's Matrix Mechanics

Following Heisenberg's successful formulations of the "quantum transition-component" analogue to the classical Fourier series of a generally multi-periodic quantity, Born identified that the mathematical structure of the aggregate /collection of the transition components was that of a matrix. The indices of the matrices were to begin with the indices or quantum numbers marking the stationary states of Bohr. Moreover, Bohr quantum condition was reformulated as $\sum_{n'} P_{nn'}Q_{n'n} - Q_{nn'}P_{n'n} = -i\hbar = [\hat{P}\hat{Q} - \hat{Q}\hat{P}]_{nn'}$. Bohr - Jordan and Heisenberg gave the following recipe to "quantise" a system.

- **Recipe (I) :** *Consider that each quantity is a matrix and that, when the quantity is real-number-like, the matrix is hermitian*
- **Recipe (II) :** *Assume that the (n, n') element of the matrix of a physical quantity oscillates, as a function of time, as $e^{2\pi i \nu_{nn'} t}$*
- **Recipe (III) :** *For the frequencies there is the Ritz-Rydberg combination law which states that $\nu_{nn'} + \nu_{n'n''} = \nu_{nn''}$, from which it results that $\nu_{nn} = 0$ and $\nu_{nn'} = -\nu_{n'n}$*

$$X = \begin{bmatrix} x_{11} & x_{12} & \dots \\ \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots \\ \vdots & \vdots & \vdots \end{bmatrix} \implies \frac{dX}{dt} = \begin{bmatrix} \dot{x}_{11} & \dot{x}_{12} & \dots \\ \vdots & \ddots & \vdots \\ \dot{x}_{n1} & \dot{x}_{n2} & \dots \\ \vdots & \vdots & \vdots \end{bmatrix}$$

- **Recipe (IV) :** *The time derivative of a physical quantity should be defined by the matrix whose elements are the time derivatives of the corresponding elements of the matrix representing the original quantity.*
- **Recipe (V) :** *Assume that the momentum P, conjugate to the coordinate Q, satisfies the following relationship, known as the canonical commutation relation.*

$$\hat{Q}\hat{P} - \hat{P}\hat{Q} = i\hbar\hat{\mathbb{I}}$$

Here, $\hat{\mathbb{I}}$ is the identity matrix. In other words, $\left[\hat{P}\hat{Q} - \hat{Q}\hat{P}\right]_{nn} = -i\hbar$ and $\left[\hat{P}\hat{Q} - \hat{Q}\hat{P}\right]_{nn'} = 0$ for $n \neq n'$.

To shed more light on this recipe, note that we have already proven the following relation in the last section, in which we apply a sign change of k in the first summation to arrive at the second equation,

$$\begin{aligned}\frac{h}{2\pi i} &= \sum_k -q_q(n \to n+k)p_q(n+k \to n) + \sum_k p_q(n \to n-k)q_q(n-k \to n) \\ &= \sum_k p_q(n \to n-k)q_q(n-k \to n) - \sum_k q_q(n \to n-k)p_q(n-k \to n)\end{aligned}$$

Now, by the definition of matrix multiplication, we have that $\sum_k p_q(n \to n-k)q_q(n-k \to n)$ is the (n,n) element of the product $\hat{p}\hat{q}$ while $\sum_k q_q(n \to n-k)p_q(n-k \to n)$ is that of product $\hat{q}\hat{p}$. Hence, $i\hbar = (\hat{p}\hat{q})_{nn} - (\hat{q}\hat{p})_{nn}$. We now add to this relationship derived from the quantum condition $\oint pdq = nh$, a new hypothesis $0 = (\hat{p}\hat{q})_{nn'} - (\hat{q}\hat{p})_{nn'}$ for $n \neq n'$.

- **Recipe (VI) :** *For a general dynamical system with many degrees of freedom namely, the momenta $p_1, p_2, p_3, \ldots, p_f$ conjugate to the coordinates $q_1, q_2, q_3, \ldots, q_f$ respectively, should satisfy the relations for $s \neq s'$*

$$q_s q_{s'} - q_{s'} q_s = 0$$

$$p_s p_{s'} - p_{s'} p_s = 0$$

$$p_s q_{s'} - q_{s'} p_s = 0$$

$$p_s q_s - q_s p_s = i\hbar$$

Hence, $\left[\hat{Q}_s, \hat{Q}_{s'}\right] = \left[\hat{P}_s, \hat{P}_{s'}\right] = \left[\hat{P}_s, \hat{Q}_{s'}\right] = 0$ and $\left[\hat{Q}_s, \hat{P}_s\right] = i\hbar$ or $\left[\hat{Q}_s, \hat{P}_{s'}\right] = i\hbar\delta_{ss'}$ where $\delta_{ss'}$ is 1 for $s = s'$ and 0 for $s \neq s'$.

In other words, any two coordinates, any two momenta, and a coordinate with one of the momenta conjugate to other coordinates, all commute, while a coordinate and its conjugate momentum do not commute but satisfy the canonical commutation relation.

- **Recipe (VII) :** *Classically for a system with Hamiltonian $H(q_1, q_2, \ldots; p_1, p_2, \ldots)$, we have the Canonical equations of motion :*

$$\dot{q}_s = \frac{\partial H}{\partial p_s}\ ,\ \dot{p}_s = -\frac{\partial H}{\partial q_s}$$

Theorem : *When a matrix $f(q,p)$ is given as a function of the coordinate q and the momentum p which satisfy $pq - qp = i\hbar$, then we have*

$$\frac{\partial f}{\partial q} = \frac{i}{\hbar}(pf - fp) = \frac{i}{\hbar}\left[\hat{p}, f\right]$$

$$\frac{\partial f}{\partial p} = \frac{i}{\hbar}(qf - fq) = \frac{i}{\hbar}\left[\hat{q}, f\right]$$

Proof : If we first itself take f as p, then the equations are easily verified as the first equation gives $\partial p/\partial q = 0$ while the second equation gives $\partial p/\partial p = 1$ and these are what we should have for the derivatives. The validity of the theorem for the case of f as q can be verified in an analogous manner.

The next step is to show that when the theorem holds for two functions f_1 and f_2 separately it holds also for their sum $(f_1 + f_2)$. This can readily be done by making use of the fact that the distribution law holds also for the multiplication of matrices, i.e., $p(f_1 + f_2) = pf_1 + pf_2$ and $(f_1 + f_2)p = f_1p + f_2p$ so that

$$\begin{aligned}\frac{\partial}{\partial q}(f_1 + f_2) &= i\hbar(p(f_1 + f_2) - (f_1 + f_2)p) \\ &= i\hbar(pf_1 - f_1p) + i\hbar(pf_2 - f_2p) \\ &= \frac{\partial f_1}{\partial q} + \frac{\partial f_2}{\partial q}\end{aligned}$$

By a similar argument we can also prove $-i\hbar(q(f_1 + f_2) - (f_1 + f_2)q) = \partial(f_1 + f_2)/\partial p$. We now prove that if the theorem holds for f_1 and f_2 separately, then it also holds for their product f_1f_2. Namely,

$$\begin{aligned}\frac{\partial f_1}{\partial q}f_2 + f_1\frac{\partial f_2}{\partial q} &= i\hbar((pf_1 - f_1p)f_2 + f_1(pf_2 - f_2p)) \\ &= i\hbar(pf_1f_2 - f_1pf_2 + f_1pf_2 - f_1f_2p) \\ &= i\hbar(p[f_1, f_2] - [f_1, f_2]p) \\ &= \frac{\partial(f_1f_2)}{\partial q}\end{aligned}$$

Similarly, the second equation also can be verified in this case. Summarising the proof, the theorem holds for the choice of q or p as f , and also for the sum $(f_1 + f_2)$ and the product (f_1f_2) provided that it is valid both for f_1 and f_2 separately. This implies that the theorem holds for any polynomials of q and p or more generally that it holds for any power series of q and p provided that uniform convergence is guaranteed. We have hence arrived at the result that the theorem function f of q and p.

Now that quantum mechanical analogues of physical quantities are Hermitian matrices, the entire mathematical theory concerning Hermitian matrices comes into play. We state certain theorems concerning unitary matrices.

- **Theorem (I) :** *If X is a Hermitian matrix and U is any matrix such that $U^\dagger = U$ or $U^\dagger U = UU^\dagger = \hat{\mathbb{I}}$, then $X' = U^\dagger XU$ and $X'' = UXU^\dagger$ are also Hermitian*
- **Theorem (II) :** *When a matrix $f(X, Y, Z, \dots)$ is given as a function of a number of matrices $X, Y, Z, \dots$ then the transformed function $f' = U^\dagger fU$ is equal $f(X', Y', Z', \dots)$ or more specifically,*

$$U^\dagger f(X, Y, Z, \dots)U = f(U^\dagger XU, U^\dagger YU, U^\dagger ZU, \dots)$$

- **Theorem (III) :** *If two matrices X and P satisfy the canonical commutation relation $\left[\hat{X}, \hat{P}\right] = i\hbar$, then $X' = U^\dagger XU$ and $P' = U^\dagger XU$ also satisfy $\left[\hat{X}', \hat{P}'\right] = i\hbar$*
- **Theorem (IV) :** *If H is a Hermitian matrix, there always exists a Unitary matrix U such that $H' = U^\dagger HU$ is diagonal. The diagonal elements of H' are the eigenvalues of the matrix H, which can also be obtained by solving the equation $det(H - \lambda I)$.*
- **Theorem (V) :** *The sum of eigen values of a matrix is invariant under Unitary transformations.*
- **Theorem (VI) :** *The sum of diagonal elements of a matrix is equal to the sum of eigen values and is therefore invariant under unitary transformations.*

§2.2 Limitations of Matrix Mechanics

The above recipe was applied by Born, Heisenberg, Pauli and Dirac to simple problems. Even a problem like the Hydrogen atom proved too complicated to deal with using purely matrix mechanics, apart from the mathematical inconvenience there were other problems namely - (a) The theory is rooted in periodic systems, hence a simple system like a free electron in space has no formulation, (b) Matrices mean there are vectors in the picture. Heisenberg's approach shone no light or provided no physical intuition about what they meant, (c) Physical significance of the relation $\hat{P}\hat{Q} - \hat{Q}\hat{P} = -i\hbar$ has not been given.

§2.3 Louis de Broglie and Wave theory of particles

Historically, light was first studied in the realm of geometric optics. Subsequently, upon observing the interference effects of light, Huygens, Young , Fresnel, Fraunhofer and others successfully formulated its behaviour using wave optics. Thereafter, geometric optics became a limiting case of wave optics. Newton and others noticed a similarity in the formulation of Geometrical optics and particle mechanics.

Example : When a ray of monochromatic light passes through the boundary between two media of refractive indices n_1 and n_2, its path should obey Snell's Law which is stated as follows,

$$\frac{n_2}{n_1} = \frac{\sin\theta_1}{\sin\theta_2}$$

where θ_1 and θ_2 are the angles of incidence and refraction, respectively. Now, consider a point particle moving from one region with potential V_1 to another with potential V_2 with total energy E. Then, if v_1 are v_2 are the velocities in regions with potentials V_1 and V_2 respectively, we have

$$\frac{1}{2}mv_1^2 = E - V_1\ ,\ \frac{1}{2}mv_2^2 = E - V_2$$

Let θ_1 and θ_2 be the angles made by the velocity vectors v_1 and v_2 in regions with potentials V_1 and V_2 respectively. Then, ff the force acting at the interface is normal to the surface, the

tangential momentum remains constant i.e.,

$$v_1 \sin\theta_1 = v_2 \sin\theta_2$$

$$\therefore \frac{n_2}{n_1} = \frac{\sin\theta_1}{\sin\theta_2} = \frac{v_2}{v_1} = \sqrt{\frac{E - V_2}{E - V_1}}$$

Hence, in some sense, we can say that $n \propto \sqrt{E - V}$. In fact, principle of least action for a free particle says $\int_A^B p dq$ is extremised or $\int_A^B \sqrt{2m(E - V)} dq$ is extremised. This is the very heart of a wave theory for matter.

§2.3.i de Broglie - Einstein Relation

In his quantum theory of light, Einstein concluded that the following relations -

$$E = h\nu \,,\; p = \frac{h\nu}{c} = \frac{h}{\lambda}$$

Now de Broglie assumed that these Einstein relations should also hold in the wave theory of electrons. Namely, cathode rays, which were pictured as a stream of electrons with energy E and momentum p, are now to be pictured as the propagation of a wave with the frequency ν and wave length λ as determined by the above equations. The direction of the wave propagation is naturally the direction of the stream.

If we introduce Einstein's relation here, it becomes clear what corresponds, in the wave theory, to the presence of a potential $V(x, y, z)$ in the particle theory. The phase velocity of the wave, $u = \nu\lambda$, is given as

$$u = \frac{E}{p} = \frac{E}{[2m(E - V(x, y, z))]^{\frac{1}{2}}} = \frac{\nu}{[2(m/h).(\nu - V(x, y, z)/h)]^{\frac{1}{2}}}$$

Here we see that m, V etc are particle dynamics terminology while u, ν, λ etc are wave dynamics terminology. So, he set about describing the dynamics of massive particles using wave theory. More precisely, he sought to write down a wave equation – in other words a differential equation – which does not explicitly contain the frequency and phase velocity in it, and instead has "particle" properties such as a mass of the particle and the potential in which the particle is moving. Such a differential equation should then represent the wave equation for a particle.

§2.3.ii Bohr's quantum condition in wave theory

It was noticed by de Broglie that Bohr's quantum condition, $\oint p dq = nh$, $n = 1, 2, 3, \ldots$ could be very simply and naturally understood from the wave theoretical point of view, provided that Einstein's relation is valid. For the sake of simplicity let us consider an electron which is in a circular orbit inside a hydrogen atom. When we look at this phenomenon from the wave theoretical standpoint, we can visualize a de Broglie wave as propagating along this circular orbit inside the atom. If the radius of this circle is r, the circumference is $2\pi r$. In order for a wave propagating around this circle to be in a stable condition, the ratio of the circumference to the wave length should be an integer, since otherwise the front of the wave, after completing

one circle, cannot meet its tail smoothly i.e., when the circumference of the circle is an integral multiple of the wave length, the wave is continuous and smooth all over. In this way, the condition, $2\pi r = n\lambda$, $n \in \mathbb{N}$ follows quite naturally in the wave theory. Then, by making use of the relation between the particle momentum p and the wave length λ, we can translate this condition to that in the particle theory, namely $2\pi rp = nh = \oint pdq$.

This is the relation which was previously derived from the Bohr condition. According to this new interpretation, the quantum number in Bohr's theory is nothing but the number of nodes specifying each proper oscillation of the wave system. From this view-point, we may conclude that Bohr's quantum condition is the manifestation of the wave nature of the electron inside the atom. The wave nature of the electron is not restricted to intra-atomic phenomena. This fact was actually shown by the famous experiment by Davisson and Germer in 1927. This is one of the most important discoveries of the century.

§2.4 Experiments of Davison and Germer - evidence for matter waves

Scattering of cathode rays / electrons from metal showed patterns similar to X ray diffraction. Initially it was believed to be due to the internal structure of the electrons inside atoms. However, when the metal was annealed (heated to a high temperature and cooled down again), the recrystallisation into a different crystal phase of the metal resulted in a different pattern. X-ray diffraction had already been established as a technique to study the structures of solids and comparison of the "electron beam diffraction" showed stark similarities. Assuming a wave nature of the electron in free space, following de Broglie's simple model gave accurate results for the crystal structure which agreed with the X-ray method.

It is important to note that the wave nature of light was essential in describing X ray diffraction. And behind this phenomenon of interference / diffraction is the principle of superposition. This observation gave big support to the claims that e's behaved as waves in this experiment. Eventually it was established that de Broglie "waves" existed not just inside atoms but also in free space. This gave a big clue on how to proceed to describe system that were not very feasible with matrix mechanics. However, we need a general wave equation for particles – one that does not explicitly contain "wave parameters".

§2.5 Derivation of de Broglie's equation

we shall assume that the de Broglie wave can be described by a single scalar function. We shall denote this scalar quantity by ψ and call it the wave function. In 3-D space, When the phase velocity u is given as a function of x, y, z at every point of space,wave equation is given by

$$\nabla^2\psi - \frac{1}{u^2}\frac{\partial^2\psi}{\partial t^2} = 0$$

The usual way to solve it is using the "variables separable method". First, the time part of the equation is solved. For a monochromatic wave i.e., of constant frequency v, we have

$$\frac{\partial^2\psi}{\partial t^2} = -(2\pi v)^2\psi \implies \nabla^2\psi + \left(\frac{2\pi v}{u}\right)^2\psi = 0$$

From de Broglie, for a particle we associate the phase velocity given as

$$u = \frac{v}{[2\mu(v - D(x,y,z)]^{\frac{1}{2}}}\ , E = hv, \mu = \frac{m}{h}, D = \frac{V(x,y,z}{h}$$

Substituting the expression for wave velocity, we obtain

$$\implies \nabla^2\psi + 8\pi^2\mu(v - D(x,y,z))\psi = \nabla^2\psi + 4\pi\mu(2\pi v - 2\pi D(x,y,z))\psi = 0$$

$$\therefore (2\pi v)\psi = \left(-\frac{\nabla^2}{4\pi\mu} + 2\pi D\right)\psi$$

This equation still has a wave property v in it. We now eliminate v while maintaining that the overall equation should be linear, then we obtain

$$\begin{aligned}
\frac{\partial^2\psi}{\partial t^2} &= -(2\pi v)^2\psi \\
&= -(2\pi v)(2\pi v\psi) \\
&= -(2\pi v)\left(-\frac{\nabla^2}{4\pi\mu} + 2\pi D\right)\psi \\
&= -\left(-\frac{\nabla^2}{4\pi\mu} + 2\pi D\right)\psi(2\pi v\psi) \\
&= -\left(-\frac{\nabla^2}{4\pi\mu} + 2\pi D\right)^2\psi
\end{aligned}$$

$$\therefore \left(-\frac{\nabla^2}{4\pi\mu} + 2\pi D\right)^2\psi + \frac{\partial^2\psi}{\partial t^2} = 0$$

This equation is, however, too complicated. First of all, it is of the fourth order in the space differentiation of ψ. Secondly, it has redundant solutions, which are superposition of monochromatic waves not satisfying the original ($\nabla^2\psi + 8\pi^2\mu(v - D(x,y,z))\psi = 0$). Namely, this equation allows also those monochromatic waves which satisfy the equation obtained by changing v to $-v$. For these reasons one can hardly believe that the equation is the true one. This situation arises from the fact that in deriving it, the original equation which is linear in v, was coupled with $\partial^2\psi/\partial t^2 = -(2\pi v)^2\psi$ which is of the second order in v.

This leads one to assume that the equation to be satisfied by the de Broglie wave has to be of the first order in the time differentiation. The simplest assumption leading to such an equation turns out to be that, for a given frequency v, there exists only one wave of the form $e^{-2\pi ivt}$; we may

alternatively choose the positive sign in the exponential, and the following argument proceeds in quite an analogous way. On the basis of this assumption, we use, instead

$$\frac{\partial\psi}{\partial t} = -(2\pi iv)\psi \implies i\frac{\partial\psi}{\partial t} = 2\pi v\psi$$

$$\because 2\pi v\psi = \left(-\frac{\nabla^2}{4\pi\mu} + 2\pi D\right)\psi \implies i\frac{\partial\psi}{\partial t} = \left(-\frac{\nabla^2}{4\pi\mu} + 2\pi D\right)\psi$$

$$\therefore \nabla^2\psi - 8\pi^2\mu D\psi + 4\pi i\mu\frac{\partial\psi}{\partial t} = 0$$

We see that the de Broglie wave equation is deceptively similar to Schrödinger equation because if we replace $\mu = m/h$ and $D = V/h$, then we get

$$\nabla^2\psi - \frac{2mV}{\hbar^2}\psi + i\frac{2m}{\hbar}\frac{\partial\psi}{\partial t} = 0 \implies i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

This is exactly the form of Schrödinger's equation, but one should not already make that identification. All we can say at this point is that this equation looks deceptively similar to the Schrödiger equation which we will discuss later. However, we will also see that the physical meaning of the two equations is very different.

In Maxwell's field theory, the electromagnetic wave is considered to have energy and momentum. Namely, in the space where the electromagnetic wave exists, the energy and momentum are distributed in space and they are expressed by bilinear forms of the field quantities, E and H. The conservation of energy and momentum is guaranteed by the Maxwell equations. We also expect that the energy and momentum are distributed in the space in which the de Broglie wave exists. Furthermore, since the de Broglie wave is considered to describe the presence of matter, say the electron, we anticipate that the matter is distributed in the space in which the wave exists. Obviously, we have to consider matter not as a particle but as a continuum. By making an analogy with the case of an electromagnetic wave, we may expect that the densities of these quantities would be of second order in ψ, and also that the conservation laws for them would be guaranteed by the de Broglie wave equation However, since ψ is a complex function, the conjugate complex function ψ^* is to appear together with ψ in the expressions for these quantities in order that they may be real.

One of the quantities which satisfies the conservation law is the mass density denoted as $\rho_m = K\psi^*\psi$ where K is a constant. The conservation law for this quantity can be derived in the following way. Multiplying both sides of de Broglie wave equation by ψ^*, we obtain

$$\psi^*.\nabla^2\psi - 8\pi^2\mu D\psi.\psi^* + 4\pi i\mu\psi^*.\frac{\partial\psi}{\partial t} = 0$$

Subtracting this equation from its complex conjugate, which is

$$\nabla^2\psi^*.\psi - 8\pi^2\mu D\psi.\psi^* - 4\pi i\mu\frac{\partial\psi^*}{\partial t}.\psi = 0$$

We obtain the following relation

$$4\pi i\mu\left(\psi^*.\frac{\partial\psi}{\partial t}+\frac{\partial\psi^*}{\partial t}.\psi\right)+(\psi^*.\nabla^2\psi-\nabla^2\psi^*.\psi)=0$$

The following notation shows that ρ_m is conserved if we integrate the below equation over a certain domain of space. (We consider K to be μ subsequently)

$$\implies \frac{\partial\rho_m}{\partial t}+\mathrm{div}(j_m)=0\ ,\ j_m=\frac{K}{4\pi im}(\psi^*.\nabla\psi-\nabla\psi^*.\psi)$$

Similarly for energy density U, if D is independent of time and K' is another constant subsequently considered as $(8\pi^2\mu)^{-1}$ for convenience, is

$$U=K^{'}(\nabla\psi^*.\nabla\psi+8\pi\mu^2D\psi^*\psi)$$

If we consider S to be the vector defined as follows, it can then be showed that $\partial U/\partial t+\mathrm{div}S=0$.

$$S=\frac{K'}{4\pi i\mu}(\nabla\psi^*.\Delta\psi-\Delta\psi^*\nabla\psi+8\pi\mu D(\psi^*.\nabla\psi-\nabla\psi^*.\psi))$$

Then the total energy W is obtained as follows,

$$W=\frac{1}{8\pi^2\mu}\int(\nabla\psi^*.\nabla\psi+8\pi\mu^2D\psi^*\psi)dV$$

If ψ tends to zero sufficiently strongly at infinity, the expression for W can be written by a partial integration as

$$W=\frac{1}{8\pi^2\mu}\int\psi^*(-\nabla^2\psi+8\pi\mu^2D\psi)dV=\frac{i}{2\pi}\int\psi^*\frac{\partial\psi}{\partial t}dV$$

In the case of monochromatic waves, that is, when ψ has a definite frequency ν, we have

$$W=\nu\int\psi^*\psi dV$$

One can then apply this to various problems: It was applied successfully to free particle, oscillator, hydrogen atom and in all cases, the problem reduced to solving a differential equation (much easier than solving matrix equation for infinite dimensional matrices) and discreteness came as a result of boundary conditions. All the simple results agreed with those calculated using Matrix methods of Heisenberg and therefore a correspondence had to be there.

Tunnelling came out as a natural consequence of the wave theory and therefore as the theory of matter became more and more believable due to experimental confirmation, Tunnelling had to be believed

§2.5.i 1-D: de Broglie wave in a box

We now consider the de Broglie wave contained in a box in which there is no force field. In order to simplify the problem further, we will assume that the box is a cube with side L. Let us take the coordinate origin at one corner of the box and three orthogonal axes along the three sides of the box. Then each of the variables x, y and z in the wave function ϕ has a value between 0 and L. As boundary conditions for ϕ, we should require it to vanish on the walls of the box. Thus, de broglie's wave equation becomes in this case

$$\frac{\partial^2\psi}{\partial t^2} + 4\pi i\mu\frac{\partial\psi}{\partial t} = 0$$

Since, we are seeking monochromatic solutions, we have

$$\frac{\partial^2\phi}{\partial t^2} + 8\pi^2\mu\nu\phi = 0 \implies \frac{\partial^2\phi}{\partial t^2} = k_x^2\phi$$

This second order differential equation has the standard solution - $\phi = a\sin k_x x + b\cos k_x x$. Since, we require that $\phi(0) = 0$, we have $\phi_n(x) = a\sin(k_n x)$ where $k_n = n\pi/L = (8\pi^2\mu\nu_n)^{1/2}$

$$\therefore \phi_n(x) = A_n\sin(\frac{n\pi x}{L}) \implies \psi(x) = \sum_n A_n\sin(\frac{n\pi x}{L})$$

The mass density in the n-th eigen wave is then given as,

$$\rho_{\mu,n}(x) \equiv \mu|\phi_n|^2 = \mu|A_n|^2\sin^2\left(\frac{n\pi x}{L}\right)$$

$$\therefore M_n = \int_0^L \rho_{\mu,n}dl = \frac{\mu L|A_n|^2}{2}$$

The energy density of the n-th eigen wave is then given as,

$$U_n(x) = \frac{1}{8\pi^2\mu}(\nabla\psi^*.\nabla\psi) = \frac{|A_n|^2}{8\mu L^2}\left(n^2\cos^2\frac{n\pi x}{L}\right)$$

By integrating this over L, we get the total energy stored as, or directly from $W = \nu\int\psi^*\psi dV$. Here, ν_n is the frequency of oscillation.

$$\therefore W_n = \frac{\nu_n L|A_n|^2}{2} = \frac{M_n\nu_n}{\mu} = \frac{M_n h\nu_n}{m}$$

So far the amplitudes A_n of de Broglie waves have been assumed to take arbitrary values as in the ordinary wave theory of light. Then, the mass M_n and the energy W_n can assume any positive value continuously. This means that the electron does not exhibit any particle nature. Recalling that the Planck condition led to the particle nature of light waves, we may expect that a similar procedure applied to the de Broglie wave will reveal its particle aspect. Just as in the case of a light wave, the energy of a de Broglie wave of frequency ν will be an integral multiple of $h\nu$. This implies that the amplitude A_n cannot assume arbitrary values.

$$W_n = N_n h\nu_n \implies M_n = N_n m\ ,\ N_n \in \mathbb{W}$$

$$\because v_n = \frac{k_n^2}{8\pi^2\mu} = \frac{n^2}{8\mu L^2} = \frac{hn^2}{8mL^2} \implies hv_n = \frac{h^2n^2}{8mL^2} = \varepsilon_n$$

The last relation shows its agreement with quantum theory. Thus, in Bohr Heisenberg model, N is an integer to begin with and the energy levels are quantised to give:

$$E = \sum_{n=1}^{\infty} N_n \varepsilon_n$$

for each ε_i level having N_i non-interacting particles In de Broglie case, the particle number N comes out as naturally due to boundary value problem. Therefore the exact context where quantisation is applied is different in the two cases. The need for quantisation arises because de Broglie wave needs to be quantised separately to result in particle behaviour.

§2.6 de Broglie's Wave Theory - Unanswered questions

We are still not sure as to why $M = Nm$ holds true for N particles of mass m. Hence, the topic to be addressed is the quantisation of the de Broglie wave. Lets see this in a bit detail as follows.

The wave function of a de Broglie field satisfies the wave equation

$$\nabla^2\psi - 8\pi^2\mu D\psi + 4\pi i\mu\frac{\partial\psi}{\partial t} = 0$$

Now denoting the eigenvalues and the eigen functions of the wave equation for monochromatic wave by $v_1, v_2, \ldots, v_s, \ldots$ and $\phi_1, \phi_2, \ldots, \phi_s, \ldots$, we can expand the solution of $\psi(x, y, z, t)$ in terms of these functions.

$$\nabla^2\phi + 8\pi^2\mu(v - D)\phi = 0$$

We here assume that the functions ϕ_s are normalized and are orthogonal to each other. Since the ϕ's do not have time dependence, the expansion coefficients will be functions of time, i.e.,

$$\psi(xyzt) = \sum_{s=1}^{\infty} A_s(t)\phi_s(xyz)$$

We introduce the above equation in the de Broglie wave equation, multiply by $\phi_s^*(x, y, z)$ and integrate over the entire space. The result is then

$$\frac{dA_s}{dt} = -2\pi i v_s A_s$$

Since our function $\psi(x, y, z, t)$ is in general complex, these A's are also complex and are specified by two real numbers each. We shall introduce two sets of real numbers, Q's and P's, by

$$\Re(A_s) = \frac{1}{2}(A_s + A_s^*) = \sqrt{\pi}Q_s$$

$$\Im(A_s) = \frac{1}{2i}(A_s - A_s^*) = \sqrt{\pi}P_s$$

From the fact that A_s satisfies $dA_s/dt = -2\pi i \nu_s A_s$, it follows immediately that Q_s and P_s have to satisfy

$$\frac{dQ_s}{dt} = 2\pi i \nu_s P_s$$
$$\frac{dP_s}{dt} = -2\pi i \nu_s Q_s$$

In the meantime, the energy of the de Broglie field can be expressed in terms of Q's and P's. Namely, starting with the expression for the energy

$$W = \frac{i}{2\pi} \int \psi^* \frac{\partial \psi}{\partial t} dV$$

we transform it by making use of the relation $\psi(xyzt) = \sum_{s=1}^{\infty} A_s(t)\phi_s(xyz)$ together with the facts that the set ϕ_s is orthonormal and that A_s satisfies $dA_s/dt = -2\pi i \nu_s A_s$. We obtain

$$W = \sum_s \nu_s A_s^* A_s = \frac{1}{2} \sum_s 2\pi \nu_s (P_s^2 + Q_s^2)$$

This expression of the energy and relation between Q_s, P_s tells us that we can bring the theory into canonical form by assuming a Hamiltonian of the form

$$H = \frac{1}{2} \sum_s 2\pi \nu_s (P_s^2 + Q_s^2)$$

since, then the earlier relations become the Hamiltonian equations of motion i.e.,

$$\frac{dQ_s}{dt} = \frac{\partial H}{\partial P_s}, \frac{dP_s}{dt} = -\frac{\partial H}{\partial Q_s}$$

In the meantime, if express the amount of matter M in terms of Q's and P's and observing the quantum condition $\oint P_s dQ_s = N_s h$ where $N_s = 0, 1, 2, \ldots$, we find that

$$M = \mu \int \psi^* \psi dV = \frac{1}{2} \sum_s 2\pi\mu (P_s^2 + Q_s^2) = m \sum_s N_s$$

Here we can clearly see how particle number N_s has to be imposed later through a quantum condition. Therefore, like in the case of Maxwell's equations requiring the Planck hypothesis to result in particle behaviour, de Broglie's wave is actually a classical wave equation (for a complex wave) and needs an explicit quantisation. In addition to this deficiency, there are other deeper mathematical difficulties.

§2.6.i System of interacting electrons – Breakdown of superposition principle

de Broglie wave equation gives the equation for the matter field in the presence of the potential $V(xyz)$. Let us take a system consisting of a number of electrons in an external electric field. The total electric potential at (xyz) consists of two terms,

$$V(xyz) = V_{ex}(xyz) + V_{el}(xyz)$$

where V_{ex} is the contribution of the externally applied electric field and V_{el} is that due to the electric field produced by the electrons themselves. Correspondingly, we must split the D in wave equation into two terms, namely

$$D(xyz) = D_{ex}(xyz) + D_{el}(xyz)$$

where

$$D_{ex} = \frac{1}{h}V_{ex} \; , \; D_{el} = \frac{1}{h}V_{el}$$

In the meantime, $V_{el}(xyz)$ in the particle theory is given as the sum of the Coulomb potential of all the electrons. That is, denoting the locations of these electrons by $r_1, r_2, \ldots, r_l, \ldots$, we have

$$V_{el}(r) = e^2 \sum_l \frac{1}{|r - r_l|}$$

However, in our wave theory, we do not accept the notion, at least before quantization, of discrete and localized electrons, but instead we consider that the electricity is continuously spread over the space, where the electric density is,

$$\rho_e = \tilde{e}\psi^*\psi \; , \; \tilde{e} = \frac{e}{h}$$

The charge density being given as above, the potential energy at r due to this charge distribution is then given by,

$$V_{el}(r) = e \iiint \frac{\rho_e(r')}{|r - r'|} d^3r'$$

and hence,

$$B_{el}(r) = \tilde{e} \iiint \frac{\rho_e(r')}{|r - r'|} d^3r'$$

Accordingly, the $D(r)$ to be used in the wave equation is

$$D(r) = D_{ex}(r) + \tilde{e} \iiint \frac{\rho_e(r')}{|r - r'|} d^3r'$$

and the wave equation itself becomes,

$$\nabla^2\psi(r) + 4\pi i\mu \frac{\partial\psi(r)}{\partial t} - 8\pi^2\mu \left(D_{ex}(r) + \tilde{e} \iiint \frac{\rho_e(r')}{|r - r'|} d^3r' \right) \psi(r) = 0$$

using expression for $\rho_e(r)$, it becomes

$$\nabla^2\psi(r) + 4\pi i\mu \frac{\partial\psi(r)}{\partial t} - 8\pi^2\mu \left(D_{ex}(r) + \tilde{e}^2 \iiint \frac{\psi^*(r')\psi(r')}{|r - r'|} d^3r' \right) \psi(r) = 0$$

This equation is quite complicated. First of all, this is an integro-differential equation. Furthermore, it is not linear. As a result of the non-linearity, we cannot speak of proper oscillations. Furthermore, the principle of superposition does not apply. This latter fact can be expected from the physical point of view; for instance, two streams of cathode ray will repel each other by electric force and the streams will be bent accordingly. Therefore, the propagation of two streams of cathode ray cannot be reproduced by the superposition of the propagation of each stream separately. This is a violation of the principle of superposition. Hence, arose the motivation to go from de Broglie's wave theory to Schrödinger's equation.

§2.6.ii Deficiencies of de Broglie's approach

de Broglie's wave equation needs separate quantisation and therefore we have to take recourse to Bohr / Heisenberg quantum condition and therefore reconnect with matrix theory at some stage. Moreover, many particle systems with mutual interactions give non - linear integro-differential equations which violate the principle of superposition and are very difficult to solve and quantise.

§2.6.iii Advantages of de-Broglie's Approach

Bohr's quantum condition has a very elegant formulation in terms of a standing wave for an electron and electrons in free space can also be described. Moreover, discreteness of energy levels comes out a solution to the differential equation with relevant boundary conditions and is much easier to solve then infinite dimensional matrix eigen value equations. Moreover, Schrödinger noticed that there was a connection between functions (as solutions to differential equations) and vector (as solutions of Matrix equations). By establishing this connection firmly, one can use the easier wave equation approach to solve problems. In the process he also discovered that the incomplete formulation. He went about rectifying all these defects as follows.

§2.7 Schrödinger's wave theory – inherently quantum

Agreement of results between de Broglie method and Heisenberg method means there has to be a mathematical correspondence between the two. On the one hand, the quantisation had a very clear physical picture in matrix mechanics. However, mathematically de Broglie's method is more convenient. In addition, the latter approach had an ability to describe free particle and non-periodic systems. It also gave a better definition of the state of a quantum system. Therefore, Schrödinger's approach was to construct a one-to-one correspondence between functions and vectors, matrices and differential operators.

Let us recapitulate the procedure of obtaining the solution of the equation in matrix mechanics for the simple case of a one dimensional problem. The given dynamical system is described in terms of the coordinate q and momentum p and has the Hamilton function $H(p, q)$. In solving the problem, we first take time-independent Hermitian matrices P^0 and Q^0 which are arbitrary so far as they satisfy $[P^0, Q^0] = -i\hbar$ and then substitute p and q in $H(p, q)$ by these P^0 and Q^0, respectively. Then we obtain the Hamiltonian matrix $= H(P^0, Q^0)$. Using the matrix elements $H_{nn'}$ of this matrix, we write down the simultaneous linear equations for the unknowns $\xi_1, \xi_2, \ldots$ to solve $|H - WI| = 0$,

$$\sum_{n'} H_{nn'}\xi_{n'} - W\xi_n = 0, \qquad n, n' \in \mathbb{N}$$

Using matrix definitions, if ξ_n are the components of a vector ξ, then the above equations can be summarised as $H\xi - W\xi = 0$ where H is a matrix, W is its eigenvalue and ξ is its eigen vector.

Example : We have the following equations for a harmonic oscillator, namely

$$\text{Classical} : H = \frac{p^2}{2m} + \frac{1}{2}kq^2$$
$$\text{Matrix} : H(P,Q) = \frac{P^2}{2m} + \frac{1}{2}kQ^2$$

We also know that $QP - PQ = i\hbar \implies (QP - PQ)\eta = i\hbar\eta$ for any vector η.

$$H(P,Q)\xi - W\xi = 0 \implies \left[\frac{P^2}{2m} + \frac{1}{2}kQ^2\right]\xi - W\xi = 0$$

We have from wave theory,

$$\nabla^2\phi + 8\pi^2\mu\left(v - \frac{1}{2}\frac{kx^2}{h}\right)\phi = 0$$
$$\implies \nabla^2\phi + \frac{8\pi^2\mu}{h}\left(E - \frac{1}{2}kx^2\right)\phi = 0$$
$$\implies \left[\frac{1}{2m}(-i\hbar\nabla)^2 + \frac{1}{2}kx^2\right]\phi - E\phi = 0$$

If we compare it with the matrix equation, we immediately find the following remarkable correspondences :

- The vector ξ is replaced by the function ϕ
- The matrix Q^2 is replaced by x^2
- The matrix P^2 is replaced by $(-i\hbar\nabla)^2$
- The eigenvalue W is replaced by the eigenvalue E

This correspondence is not merely of a formal nature but, as we shall see subsequently, it has a more profound mathematical significance. In fact, there is a firm mathematical correspondence between "linear operator" acting on functions and matrices acting on vectors. The coincidence of E and W is a necessary consequence of this fact.

§2.7.i Functions and Vectors

Schrodinger's idea is based on the fact that, by means of a set of ortho-normal functions, a one-to-one correspondence can be established between functions and vectors, and between linear operators and matrices. The mathematical basis for the coincidence of W and E is provided by this correspondence. First, we take a complete set of ortho-normal functions : $\chi_1(q), \chi_2(q), \ldots, \chi_n(q), \ldots$ For simplicity, we shall assume that all the χ's vanish for $|q| \to \infty$. Since this set is complete, a function $f(q)$ can be expanded in terms of these ortho-normal functions as $f(q) = \sum_n \eta_n\chi_n(q)$. This determines uniquely the function when $f(q)$ a set of numbers $\eta_1, \eta_2, \ldots, \eta_n, \ldots$ is given. If we regard the set of numbers $\eta_1, \eta_2, \ldots, \eta_n, \ldots$ as the components of a vector η, we can say that there is a one-to-one correspondence between functions

and vectors. The ortho-normal set of functions $\chi_1, \chi_2, \ldots, \chi_n, \ldots$ served as an intermediary in this correspondence.

$$\therefore f(q) \leftrightarrow \begin{pmatrix} \eta_1 \\ \eta_2 \\ \vdots \end{pmatrix} \equiv \vec{\eta}$$

§2.7.ii Linear Operators

We now introduce a new terminology. The result of applying the operation d/dx to an arbitrary function $f(x)$ will be referred to simply as the product of the function $f(x)$ by the operator d/dx. Similarly, the function $xf(x)$ obtained from $f(x)$ by multiplying it by x will be referred to as the product of the function $f(x)$ by the operator x. We shall now investigate the properties of the operators $(h/2\pi i)(d/dx)$ and x. We multiply an arbitrary function $f(x)$ first by x and then by d/dx and the result is,

$$\frac{d(xf(x))}{dx} = f(x) + x\frac{df(x)}{dx}$$

$$\implies \left(\frac{d}{dx}.x - x.\frac{d}{dx}\right) f(x) = f(x)$$

Then, we have

$$\implies \left[\left(-i\hbar\frac{d}{dx}\right).x - x.\left(-i\hbar\frac{d}{dx}\right)\right] f(x) = -i\hbar f(x)$$

Since this equation holds for an arbitrary function $f(x)$, we may also write it simply as

$$\left(-i\hbar\frac{d}{dx}\right).x - x.\left(-i\hbar\frac{d}{dx}\right) = -i\hbar$$

If we compare these equations with the commutation relation of matrices, we find the characteristic correspondence i.e., the vector η, matrices P and Q are replaced by the function $f(x)$ and the operators $(-i\hbar d/dx)$ and x respectively.

§2.8 Operators and Matrices in Quantum Theory

The next problem is to find the vector which corresponds to $Af(q)$ the product of a function $f(q)$ by a linear operator A. Let us denote the vector which corresponds to $f(q)$ by η, and the vector which corresponds to $Af(q)$ by ζ. It can be shown from expansion theorem and orthogonality of

eigenvalues that if $f(q) = \sum_n \eta_n \chi_n(q)$, then $\eta_n = \int \chi_n^*(q) f(q) dq$. Hence,

$$\begin{aligned}
\zeta_n &= \int \chi_n^*(q) A f(q) dq \\
&= \int \chi_n^*(q) A \sum_{n'} \eta_{n'} \chi_{n'}(q) dq \qquad \because f(q) = \sum_n \eta_n \chi_n(q) \\
&= \int \chi_n^*(q) \sum_{n'} \eta_{n'} A \chi_{n'}(q) dq \qquad \because A \text{ is a linear operator} \\
&= \sum_{n'} \left(\int \chi_n^*(q) A \chi_{n'}(q) dq \right) \eta_{n'} \qquad \text{Interchanging the summation and integration} \\
&= \sum_{n'} A_{nn'} \eta_{n'} \qquad \text{Define } A_{nn'} = \int \chi_n^*(q) A \chi_{n'}(q) dq
\end{aligned}$$

This indicates that the vector ζ is given by the product of the vector η by the matrix A, whose elements are given above i.e.,

$$\zeta = A\eta$$

This gives a recipe as to how to construct a matrix for a linear operator. Thus, we have shown that when a linear operator is given, there is a definite matrix which corresponds to the operator.

Conversely, we can show that when a matrix is given, there is a definite linear operator which corresponds to the matrix. Suppose that a matrix A and two vectors η and ζ are related by $\zeta = A\eta$ and let the functions which correspond to η and ζ be denoted by $f(q)$ and $g(q)$ respectively. Note that $\zeta = A\eta \implies \zeta_n = \sum_{n'} A_{nn'} \eta_{n'}$. Hence, the function $g(q)$ corresponding to ζ is written as

$$\begin{aligned}
g(q) &= \sum_n \sum_{n'} \chi_n(q) A_{nn'} \eta_{n'} \\
&= \sum_n \sum_{n'} \chi_n(q) A_{nn'} \int \chi_{n'}^*(q') f(q') dq' \qquad \because (\eta_{n'} = \int \chi_{n'}^*(q') f(q') dq') \\
&= \int \sum_{nn'} \chi_n(q) A_{nn'} \chi_{n'}^*(q') f(q') dq' \qquad \text{(Interchanging the summation and integration)} \\
&= \int G(q, q') f(q') dq' \qquad \text{(Define } G(q, q') = \sum_{nn'} \chi_n(q) A_{nn'} \chi_{n'}^*(q'))
\end{aligned}$$

Thus G is determined solely by A and χ's where χ_n's themselves are solutions of differential equation. Now, we return to Hamiltonian. We have already obtained the algebraic relation

$$\left(-i\hbar \frac{d}{dx}\right).x - x.\left(-i\hbar \frac{d}{dx}\right) = -i\hbar$$

Taking a complete set of ortho-normal functions $\chi_1(q), \chi_2(q), \ldots$, we construct the matrices P and Q, which correspond respectively to the operators $-i\hbar(d/dq)$ and q respectively. From $A_{nn'} = \int \chi_n^*(q) A \chi_{n'}(q) dq$, we construct the matrices whose matrix elements are respectively given by

$$P_{nn'} = \int \chi_n^*(q) \left(-i\hbar \frac{d}{dq}\right) \chi_{n'}(q) dq$$

$$Q_{nn'} = \int \chi_n^*(q) q \chi_{n'}(q) dq$$

Hence, by construction $PQ - QP = -i\hbar$. We shall further prove that these matrices P and Q are Hermitian i.e., $P_{nn'} = P^*_{n'n}$ and $Q_{nn'} = Q^*_{n'n}$. The proof for the matrix P goes as follows. First, take the complex conjugate and interchange the indices n, n'. Then, we obtain

$$P^*_{n'n} = \int \chi_{n'}(q) \left(i\hbar \frac{d}{dq} \right) \chi_n^*(q) dq$$

Applying the partial integration and making use of the fact that the function χ_n goes to zero as $|q| \to \infty$, we find that

$$\begin{aligned} P^*_{n'n} &= -\int \left(i\hbar \frac{d}{dq} \chi_{n'}(q) \right) \chi_n^*(q) dq \\ &= \int \chi_n^*(q) \left(-i\hbar \frac{d}{dq} \right) \chi_{n'}(q) dq \\ &= P_{nn'} \end{aligned}$$

which shows that the matrix P is Hermitian. The proof that the matrix Q is also Hermitian is quite easy. Now the central problem in matrix mechanics is to solve the equation $H(P, Q)\xi - W\xi = 0$ where H is the Hamiltonian matrix of the dynamical system. The matrices P and Q can be chosen arbitrarily as long as they are Hermitian and satisfy the canonical commutation relation. With the proven results, the matrix $H(P, Q)$ corresponding to the linear operator $[-i\hbar(d/dq), q]$ is

$$H(P, Q) = \int \chi_n^*(q) \left[-i\hbar \frac{d}{dq}, q \right] \chi_{n'}(q) dq$$

Define the function $\phi(q)$ which corresponds to the vector ξ as

$$\phi(q) = \sum_n \xi_n \chi_n(q), \ \xi_n = \int \phi(q) \chi_n^*(q) dq$$

we can conclude that a relation of the same form $H(P, Q)\xi - W\xi = 0$ holds for the linear operator $-i\hbar(d/dq)$ and the function $\phi(q)$ and we have

$$H\left(-i\hbar \frac{d}{dq}, q \right) \phi(q) - W\phi(q) = 0$$

§2.8.i Extension to many degrees of freedom

We have so far discussed the dynamical systems which have only one degree of freedom. It is not difficult to generalize the argument to make it applicable to systems with many degrees of freedom. Let the coordinate matrices be denoted by $Q_1, Q_2, \ldots, Q_f$ and the momentum matrices by $P_1, P_2, \ldots, P_f$ where / is the number of degrees of freedom. Then the canonical commutation relations are as follows where $s, s' = 1, 2, \ldots, f$.

$$\begin{aligned} P_s P_{s'} - P_{s'} P_s &= 0 \\ Q_s Q_{s'} - Q_{s'} Q_s &= 0 \\ P_s Q_{s'} - Q_{s'} P_s &= -i\hbar \delta_{ss'} \end{aligned}$$

We now consider a function $f(q_1, q_2, \ldots, q_f)$ of variables $q_1, q_2, \ldots, q_f$ together with the differential operators $-i\hbar(\partial/\partial q_1), -i\hbar(\partial/\partial q_2), \ldots, -i\hbar(\partial/\partial q_f)$ as well as the multiplication operators $q_1, q_2, \ldots, q_f$. It is readily seen that they satisfy

$$\left(i\hbar\frac{\partial}{\partial q_s}\right)q_s - q_{s'}\left(i\hbar\frac{\partial}{\partial q_s}\right) = -i\hbar\delta_{ss'}$$
$$\left(i\hbar\frac{\partial}{\partial q_s}\right)\left(i\hbar\frac{\partial}{\partial q_{s'}}\right) - \left(i\hbar\frac{\partial}{\partial q_{s'}}\right)\left(i\hbar\frac{\partial}{\partial q_s}\right) = 0$$
$$q_s q_{s'} - q_{s'} q_s = 0$$

The correspondence between vectors and functions and that between matrices and linear operators can be established by the use of a complete ortho-normal set of functions now containing f variables

$$\chi_1(q_1, q_2, \ldots, q_f), \chi_2(q_1, q_2, \ldots, q_f), \ldots$$

The correspondence between function f and the vector η is defined by

$$f(q_1, q_2, \ldots, q_f) = \sum_n \eta_n \chi_n(q_1, q_2, \ldots, q_f)$$

and η is given by the following relation

$$\eta_n = \iint\cdots\int \chi_n^*(q_1, q_2, \ldots, q_f) f(q_1, q_2, \ldots, q_f) dq_1 dq_2 \ldots dq_f$$

Furthermore, the correspondence between matrix and operator is given by

$$A_{nn'} = \iint\cdots\int \chi_n(q_1, q_2, \ldots, q_f) A \chi_{n'}(q_1, q_2, \ldots, q_f) dq_1 dq_2 \ldots dq_f$$

When the Hamiltonian matrix of the dynamical system is $H(P_1, P_2, \ldots, P_f, Q_1, Q_2, \ldots, Q_f)$, the matrix equation is $H(P_1, P_2, \ldots, P_f; Q_1, Q_2, \ldots, Q_f)\xi - W\xi = 0$ which has the following corresponding Schrodinger equation of the form

$$H\left(-i\hbar\frac{\partial}{\partial q_1} - i\hbar\frac{\partial}{\partial q_2}, \ldots, -i\hbar\frac{\partial}{\partial q_1 f}; q_1, q_2, \ldots, q_f\right)\phi(q_1, q_2, \ldots, q_f) - W\phi(q_1, q_2, \ldots, q_f) = 0$$

§2.8.ii Difference Between de Broglie Equation and Schrödinger Equation

For one particle, both the de Broglie and Schrödinger equations look the same. However, we saw that the de Broglie equation was nonlinear for interacting systems. It is on this count that Schrödinger's equation is vastly different. Apart from this, there are some very important differences between the two equations, namely

- Schrödinger's wavefunction ϕ is a function of generalised coordinates – for an N dimensional space with N generalised coordinates, $\phi(q_1, \ldots, q_N, t)$. On the other hand, de Broglie's wavefunction $\psi(x, y, z, t)$ is always a function only of the three spatial coordinates and time. In other words, the Schrödinger wavefunction lives in a higher dimensional space.

- For many particle systems Schrödinger's equation remains linear therefore principle of Superposition holds.
- The Schrodinger function always has an arbitrary numerical factor ϕ because of the linearity of the Schrodinger equation. However, as mentioned if the Schrodinger function is to correspond to the vector ξ appearing in the matrix equation, it must be normalized according . Primarily only the normalized Schrodinger function has a physical meaning and the numerical factor has nothing to do with physics. On the other hand, in the case of the field quantity ψ in the de Broglie theory, the situation is completely different. For the sake of simplicitv, let us consider the caseof no mutual interaction. Here the de Broglie equation is linear, so that ψ also has an arbitrary numerical factor. But, in this case, this factor plays an essential role in physics, because the density of various physical quantities defined all depends essentially on this factor.
- In the Schrödinger equations, no separate quantisation is necessary because the Heisenberg canonical commutation relation holds for any ϕ in the incorporation itself.

§2.8.iii Connection between Schrödinger Equation and Hamiltonian Jacobi equation

The Hamiltonian Jacobi equation is classical physics for time invariant Hamiltonian looks like

$$H\left(\frac{\partial W}{\partial q}, q\right) = E$$

Here we solve for W and in the process solve the problem of system evolution. While in the time varying case it reads

$$H\left(\frac{\partial S}{\partial q}, q\right) + \frac{\partial S}{\partial t} = 0$$

Here we solve for S and in the process solve system evolution.

§2.8.iv Schrödinger's equation in time independent case

In this case, we have the following relation, wherein we solve for ϕ. Also, the connection with the Hamiltonian Jacobi equation for time invariant Hamiltonian is fairly clear. Similarly in the time dependent case.

$$H\left(-i\hbar\frac{d}{dq}, q\right)\phi = E\phi$$

§2.8.v Time dependent Schrödinger equation

If we want to study systems evolving in time, we can write down a general time-dependent version for the Schrödinger equation as follows,

$$\begin{aligned}\frac{\partial\phi}{\partial t} &= -(2\pi i\nu)\phi \\ &= -\left(\frac{2\pi E}{h}\right)\phi \\ &= -i\frac{E}{\hbar}\phi\end{aligned}$$

$$\therefore i\hbar\frac{\partial\phi}{\partial t} = E\phi \implies H\left(-i\hbar\frac{d}{dq}, q\right)\phi - i\hbar\frac{\partial\phi}{\partial t} = 0$$

In either case, if we set up the Hamilton-Jacobi equation in classical physics, moving to Schrödinger's equation involves going from $\partial/\partial q \to -i\hbar\partial/\partial q$ and $\partial/\partial t \to -i\hbar\partial/\partial t$

§2.9 Recipe to write down the equations of motion for quantum systems

- Select a set of appropriate generalised coordinates that best describe the dynamics of the classical system. This step is usually by trial and error. One goes by symmetry conditions to choose the right set of coordinates.

  Example :

  - Spherical polar coordinates for an electron in coloumbic force field.
  - Cylindrical polar coordinates for an atom in a uniform magnetic or electric field

  Note : For a system of coupled oscillators or in general for interacting systems one has to choose a set of normal mode coordinates that often decouple the system into several uncoupled components.

- Write down the classical Lagrangian $\mathcal{L}(q_i, \dot{q}_i, t)$
- Define the canonical momenta $p_i = \partial\mathcal{L}/\partial\dot{q}_i$
- Solve for $\dot{q}_i$ as a function of p_i's
- Construct the classical Hamiltonian $H = \sum_i p_i\dot{q}_i - \mathcal{L}(q_i, \dot{q}_i, t)$. Note that the q_i in this should be written in terms of p_i, then the Hamiltonian is a function entirely in terms of the coordinates and momenta.
- Promote the canonical variables to "operators", and all dynamical quantities become "Hermitian operators". This arises from the only extra ingredient that Bohr in- troduced to extend classical physics to the atomic world – the quantum jump between discrete quantum levels.

- The classical canonical variables – the coordinates and the corresponding conjugate momenta then satisfy the commutation relation $[\hat{q}, \hat{p}] = i\hbar$
- At this point, we identify differential operators corresponding to each momentum $p \leftrightarrow -i\hbar\partial/\partial q$
- Schrödinger's method of constructing matrices from linear operator means that when we say operators, we also mean matrices.
- Schrödinger's equation for a quantum state denoted by the wavefunction ψ can then be written as :

$$H\left(-i\hbar\frac{\partial}{\partial q_1} - i\hbar\frac{\partial}{\partial q_2}, \ldots, -i\hbar\frac{\partial}{\partial q_1 f}; q_1, q_2, \ldots, q_f\right)\phi = i\hbar\frac{\partial\phi}{\partial t}$$

- The Heisenberg equations of motion for operators can be written as $[\hat{q}, \hat{H}] = i\hbar\dot{\hat{q}}$, $[\hat{p}, \hat{H}] = i\hbar\dot{\hat{p}}$ or in general $[\hat{A}, \hat{H}] = i\hbar\dot{\hat{A}}$

Note that Heisenberg's approach is closer in physical meaning to the classical formalism where $q(t)$ and $p(t)$ are the end goals of solving the equations of motion. However, which is a function of all the generalised coordinates of the system in the Schrödinger approach gives a better picture of the "state" of a quantum system. Certain problems (Harmonic oscillators and oscillating system) are easier in the Heisenberg approach while H atom etc are easier in the Schrödinger method. Of course we showed that the two methods are equivalent in the end!

§2.9.i Heisenberg equations and Poisson Brackets

We have in classical physics that,

$$[q, p]_{P,B} \equiv \frac{\partial q}{\partial q}\frac{\partial p}{\partial p} - \frac{\partial q}{\partial p}\frac{\partial p}{\partial q} = 1$$

While in Heisenberg formulation, we have that

$$\frac{[\hat{q}, \hat{p}]}{i\hbar} = 1$$

Similarly, when $\partial g/\partial t = 0$, we have

$$\frac{dg}{dt} = [g, H]_{P.B}$$

While in the quantum case, when $\partial\hat{g}/\partial t = 0$, we have

$$\frac{d\hat{g}}{dt} = \frac{[\hat{g}, \hat{H}]}{i\hbar} = \hat{g}, \hat{H} - \hat{H}, \hat{g}$$

One therefore sees that every classical Poisson bracket equation becomes a commutation equation in quantum physics i.e.,

$$[\,]_{P.B} \leftrightarrow \frac{[\,]}{i\hbar}$$

In fact, the Jacobi identity is $[A,[B,C]] + [C,[A,B]] + [B,[C,A]] = 0$. This is also valid for commutators. It is also much easier to prove using commutators that in the classical case !! Therefore, the formulation of quantum mechanics has very close relations to the Lagrange. Hamiltonian formalism of classical mechanics. This indicates our study of this early on in the course and also the statement that the Hamiltonian formalism describes the underlying dynamical structure of physical systems almost completely!

3 Theory of representation of Quantum States

§3.1 What does the wave function represent?

The wave function in the de-Broglie case was interpreted as a smeared out density of the corresponding properties such as mass and charge in space. But this approach needed an additional quantisation step to reconcile with the particle behaviour. This was, in fact, how we began our quest for a quantised wave theory which resulted in the Schrodinger equation ultimately. In loose terms, Schrodinger succeeded in casting Bohr-Heisenberg's particle quantum mechanics into the form of a wave equation. More precisely the matrix eigenvalue equation for finding the eigenvalues of the Hamiltonian became the eigenvalue equation for a wave equation. In form, the wave function of Schrodinger wave represents a smeared out mass or charge density, but not in real 3 dimensional space, but in configuration space. It was then interpreted as a "probability amplitude "(complex valued), the absolute value squared of which gave the relative probability density of finding the particle in any "location" in the configuration space of the generalised coordinates.

$$\therefore \rho(q_1, q_2, \dots) = \psi^*(q_1, q_2, \dots)\psi(q_1, q_2, \dots) = |\psi(q_1, q_2, \dots)|^2$$

To obtain the absolute probability density,the wave function (in most cases) is unit normalised according to

$$\iiint \cdots \int |\psi(q_1, \dots, q_f)|^2 dq_1 \dots dq_f = 1$$

In the general time-dependent case, $|\psi(q_1, \dots, q_f, t)|^2$ gives the probability density that the system is in the vicinity of $q_1, \dots, q_f$ at the time instant t and

$$\iiint \cdots \int |\psi(q_1, \dots, q_f, t)|^2 dq_1 \dots dq_f = 1$$

Let us now calculate

$$\iiint \cdots \int \rho(q_1, \dots, q_f, t) dq_1 \dots dq_f \equiv \iiint \cdots \int \psi^* \psi dq_1 \dots dq_f$$

and see under what condition it vanishes. The integration obviously has to be carried out over the entire domain of the variables. First of all we have

$$\frac{d}{dt} \iiint \cdots \int \rho(q_1, \dots, q_f, t) dq_1 \dots dq_f = \iiint \cdots \int \left(\psi^* \frac{\partial d\psi}{dt} + \frac{\partial d\psi^*}{dt} \psi \right) dq_1 \dots dq_f$$

From the time dependent Schrödinger equation, we have

$$H\left(-i\hbar \frac{d}{dq}, q\right)\psi - i\hbar \frac{\partial \psi}{\partial t} = 0$$

Using this, our equation now becomes,

$$\frac{1}{i\hbar}\iiint\cdots\int\left[\psi^* H\left(-i\hbar\frac{d}{dq},q\right)\psi-\left(H\left(-i\hbar\frac{d}{dq},q\right)\psi\right)^*\psi\right]dq_1\ldots dq_f$$

The necessary and sufficient condition for this expression to vanish i.e., for the conservation of total probability is,

$$\iiint\cdots\int\left[\psi^* H\left(-i\hbar\frac{d}{dq},q\right)\psi\right]dq_1\ldots dq_f=$$
$$\iiint\cdots\int\left[\left(H\left(-i\hbar\frac{d}{dq},q\right)\psi\right)^*\psi\right]dq_1\ldots dq_f$$

This condition has to be satisfied for all ψ's that satisfy the time dependent Schrödinger equation and boundary conditions. Now a linear operator A is called Hermitian when it satisfies

$$\iiint\cdots\int f^* A g dq_1 dq_2\cdots=\iiint\cdots\int (Af)^* g dq_1 dq_2\ldots$$

for any choice of the two functions f and g which satisfy the boundary conditions. Using this terminology, the necessary and sufficient condition for the conservation of probability is that the operator $H(-i\hbar(\partial/\partial q),q)$ hereafter called the Hamiltonian operator, is Hermitian. The Hermitian nature of the Hamiltonian operator of the dynamical systems necessarily follows from the fact that in matrix mechanics the physical quantities were all Hermitian matrices. Lets use the same symbol A for a Hermitian matrix and for its corresponding linear operator. Then, taking an orthonormal basis: $\chi_1(q),\chi_2(q),\ldots$, we say $f=\sum_n \eta_n\chi_n$ and $g=\sum_n \zeta_n\chi_n$. We define $A_{nn'}=\int\chi_n^* A\chi_{n'}dq$. Then, we have that

$$\begin{aligned}RHS&=\iiint\cdots\int f^* A g dq_1 dq_2\ldots\\&=\sum_n\sum_{n'}A^*_{n'n}\eta^*_n\zeta_{n'}\end{aligned}$$

$$\begin{aligned}LHS&=\iiint\cdots\int (Af)^* g dq_1 dq_2\ldots\\&=\sum_n\sum_{n'}\eta^*_n A_{nn'}\zeta_{n'}\end{aligned}$$

The Hermitian nature of the matrix A i.e., $A_{nn'}=A^*_{n'n}$, now assures the equality of both sides, namely the Hermitian nature of the operator A. When the operator A is not Hermitian, one can still find an operator $A^\dagger$ which satisfies

$$\iiint\cdots\int f^* A g dq_1 dq_2\cdots=\iiint\cdots\int (A^\dagger f)^* g dq_1 dq_2\ldots$$

The operator $A^\dagger$ is called the adjoint of A. In terms of this definition, a Hermitian operator is an operator which is the adjoint of itself. H being a self-adjoint linear operator, means that its corresponding matrix i.e., the Hamiltonian matrix H is Hermitian. Since this is guaranteed by definition, the total probability is conserved.

§3.2 The Bra-Ket notation of Dirac

Now that we have established a firm mathematical connection between vectors and functions, linear operators and matrices, self-adjoint operators and Hermitian matrices, we can simplify the notation as long as we define the quantities consistently.

- A vector is denoted by $|\rangle$, called a KET which is for example a column vector.
- A conjugate / dual of a vector is denoted by $\langle|$, called a BRA which is for example a row vector.
- Operators / matrices acting on kets is represented as $A|\psi\rangle$ which is understood as $\hat{A}\eta$ in matrix form or $A.f$ in the operator form
- A basis of function say $\{\chi_1, \chi_2, \dots\}$ is represented using kets as the basis denoted by $|\chi_1\rangle, |\chi_2\rangle, \dots$
- $A_{nn'} = \int \chi_n^* A \chi_{n'} dq$ is denoted as $\langle\chi_n| A |\chi_{n'}\rangle$. Moreover, we have from matrices that $A^\dagger = (A^T)^*$, hence $(A^\dagger)_{nn'} = A^*_{n'n}$ is denoted as $\langle\chi_n| A^\dagger |\chi_{n'}\rangle$ and $A^\dagger = A \implies \langle\chi_n| A^\dagger |\chi_{n'}\rangle = \langle\chi_n| A |\chi_{n'}\rangle$.
- A general state vector / wave function denoted by ψ is represented in basis ket expansion as $\psi = \sum_n c_n |\chi_n\rangle$.
- Using this notation, Schrodinger equation can then be written as,

$$H|\psi\rangle = i\hbar \frac{\partial \psi}{\partial t}$$

or $H|\chi_n\rangle = E|\chi_n\rangle$. Moreover, H being a linear operator, whenever $|\psi\rangle = \sum_n c_n |\chi_n\rangle$ holds, we have $H|\psi\rangle = \sum_n c_n H|\chi_n\rangle = \sum_n c_n E_n |\chi_n\rangle$

Moreover, if $|\psi(0)\rangle = \sum_n c_n(0)|\chi_n\rangle$ and $|\psi(t)\rangle = \sum_n c_n(t)|\chi_n\rangle$, then

$$i\hbar \frac{\partial \psi}{\partial t} = H|\chi(t)\rangle = \sum_n c_n E |\chi_n\rangle$$

$$i\hbar \sum_n \dot{c_n} |\chi_n\rangle = \sum_n c_n(t) E_n |\chi_n\rangle$$

Since $|\chi_n\rangle$'s are orthogonal and complete in the sense that any other function, $f(x)$ can be expressed as a linear combination of them, we have for all n

$$i\hbar \dot{c_n} = c_n(t) E_n \implies c_n(t) = c_n(0).e^{-iE_n t/\hbar}$$

$$\therefore |\psi(t)\rangle = \sum_n c_n(0).e^{-iE_n t/\hbar} |\chi_n\rangle$$

The set of all square-integrable functions $f(x)$, on a specified interval (a, b) such that $\int_a^b |f(x)|^2 dx < \infty$ constitutes a vector space which is referred to as the Hilbert Space. Technically, a Hilbert space is a complete inner product space, and the collection of square-integrable functions is only one example of a Hilbert space.

We define the inner product of two functions, $f(x)$ and $g(x)$, as follows :

$$\langle f \rangle g = \int_a^b f(x)^* g(x) dx$$

Notice in particular that $\langle g \rangle f = \langle f \rangle g^*$. Moreover, the inner product of $f(x)$ with itself

$$\langle f \rangle f = \int_a^b |f(x)|^2 dx$$

is real and non-negative; it's zero only when $f(x)$ is zero everywhere except at a few isolated points. A function is said to be normalized if its inner product with itself is 1; two functions are orthogonal if their inner product is 0; and a set of functions, $\{f(n)\}$, is orthonormal if they are normalized and mutually orthogonal: $\langle f_m \rangle f_n = \delta_{mn}$.

Finally, a set of functions is complete if any other function (in Hilbert space) can be expressed as a linear combination of them,

$$f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$$

If the functions $\{f_n(x)\}$ are orthonormal, the coefficients are given by Fourier's trick which is $c_n = \langle f_n \rangle f$.The expectation value of an observable $Q(x, p)$ can be expressed very neatly in inner-product notation

$$< Q > \; = \int \psi^* \hat{Q} \psi dx = \langle \psi \rangle \hat{Q} \psi$$

Now, the outcome of a measurement has got to be real, and so, a fortiori, is the average of many measurements $< Q > \; = \; < Q >^*$. However,the complex conjugate of an inner product reverses the order, so $\langle \psi \rangle \hat{Q} \psi = \langle \hat{Q} \psi \rangle \psi$ and this must hold true for any wave function ψ. This is the hermitian property

- If $|q_1, q_2, \ldots, q_f\rangle$ is a "basis ket" for coordinates $q_1, q_2, \ldots, q_f$, then the wave function $\psi(q_1, q_2, \ldots, q_f)$is denoted by $\langle q_1, q_2, \ldots, q_f \rangle \psi$.

$$\therefore \rho(q_1, q_2, \ldots, q_f) = |\psi(q_1, q_2, \ldots, q_f)|^2 = |\langle q_1, q_2, \ldots, q_f \rangle \psi|^2$$

Similarly for the time dependent case, we have

$$\rho(q_1, q_2, \ldots, q_f, t) = |\langle q_1, q_2, \ldots, q_f \rangle \psi(t)|^2$$

Extending this reasoning to a ket in a superposition of energy eigenkets, $|\psi\rangle = \sum_n c_n |\chi_n\rangle$ when $H|\chi_n\rangle = E|\chi_n\rangle$, the quantity $c_n \equiv \langle\chi_n\rangle\psi$ is interpreted such that $|c_n|^2 = |\langle\chi_n\rangle\psi|^2$ gives the relative probability that the system has energy E_n, assuming that not two $|\chi_n\rangle, |\chi_{n'}\rangle$ with $n \neq n'$ have equal energy E_n. This is called a non-degenerate spectrum of energy. When $|\psi\rangle$ is normalised to unity, $|c_n|^2$ is an absolute probability. Therefore, the system in such a superposition of energy eigenstates has an "extended" value of energy, and upon measuring the system's energy many many times, one gets an "average" or expectation value $\langle E\rangle$ given by $\langle E\rangle = \sum_n |c_n|^2 E_n$. This equation follows immediately upon interpreting $|c_n|^2$ as a probability and sure enough, this follows from the normalization of the wave function.

$$\begin{aligned} 1 = \langle\psi\rangle &= \langle\left(\sum_{n'} c_{n'}\chi_{n'}\right)\rangle\left(\sum_n c_n\chi_n\right) \\ &= \sum_{n'}\sum_n c^*_{n'}c_n\langle\chi_{n'}\rangle\chi_n = \sum_{n'}\sum_n c^*_{n'}c_n\delta_{n'n} \\ &= \sum_n c^*_n c_n = \sum_n |c_n|^2 \end{aligned}$$

$$\begin{aligned} \langle E\rangle &= \sum_n E_n c^*_n c_n = \sum_{n'}\sum_n c^*_{n'}c_n E_n\delta_{n'n} = \sum_{n'}\sum_n c^*_{n'}c_n E_n\langle\chi_{n'}\rangle\chi_n \\ &= \langle\left(\sum_{n'} c_{n'}\chi_{n'}\right)\rangle\left(\hat{H}\sum_n c_n\chi_n\right) = \langle\psi\rangle\hat{H}\psi \equiv \int \psi^*\hat{H}\psi dq \end{aligned}$$

We see that the moment we identify the quantity $|\psi|^2$ as a probability density, the entire statistical tool kit is out at our disposal. Moreover, the χ_n's are eigen functions or vectors of the time-independent Scrodinger equation $H|\chi_n\rangle = E|\chi_n\rangle$ in the non-degenerate situation. Following this we expressed a general state-ket $|\psi\rangle = \sum_n c_n|\chi_n\rangle$ which evolves as $|\psi(t)\rangle = \sum_n c_n(0).e^{-iE_nt/\hbar}|\chi_n\rangle = \sum_n c_n(t)|\chi_n\rangle$. Since $|c_n(t)|^2 = |c_n(0)|^2$, the probability of an isolated system being in the n-th energy eigen ket does not change with time.

§3.3 Refinement of the concept of the state of a system

We can now see how the Schrodinger wavefunction gives a more general and broader conception of a "state" of a quantum system. In the Bohr-Heisenberg picture, am atom was considered to exist in this or that stationary state, or an energy eigen-state, and made an instantaneous transition between stationary states. In the Schrodinger method, as a modified wave theory, superposition of "monochromatic waves" to form a general wave led to the possibility of describing a general state beyond a stationary state. Bohr's hypothesis of quantum jumps has to be understood as what happens to "real" systems which are not isolated. From this view point, Schrodinger's equation becomes the foundation equation for quantum mechanics like Newton's or Lagrange's or Hamilton's equation in classical mechanics, with the ability to describe systems starting from a free particle upwards. Many modern textbooks of quantum mechanics, therefore, call it a "postulate" of quantum mechanics- a rather overstated term.

§3.4 Physical quantities other than energy ?

Every dynamical quantity $\Omega(q, p)$ in classical physics becomes a linear operator $\hat{\Omega}(q, -i\hbar\partial/\partial(q))$. If Ω is real valued, then $\hat{\Omega}(q, -i\hbar\partial/\partial(q))$ is a self-adjoint operator/Hermitian matrix and its eigen functions ϕ_n are the solutions of $\hat{\Omega}(q, -i\hbar\partial/\partial(q))\phi_n = \omega_n\phi_n$ or $\Omega\,|\phi_n\rangle = \omega_n\,|\phi_n\rangle$. Any general state $|\psi\rangle$ can now be expanded as $|\psi\rangle = \sum_n a_n\,|\phi_n\rangle$. Then, $|a_n|^2 = |\langle\phi_n|\psi\rangle|^2$ is interpreted as the probability, when $\langle\psi\rangle$ is normalised to unity, that the system has the value ω_n for the quantity Ω. However, in general $|a_n|^2$ is not constant in time like in the special case when $\Omega = H$, where $|c_n|^2$ was constant for an expansion in Energy eigenkets. The expectation value of Ω in a state $|\psi\rangle$ is written, as mentioned before, as, $\langle\Omega\rangle = \sum_n |a_n|^2\omega_n = \langle\psi|\,\hat{\Omega}\,|\psi\rangle = \int \psi^*\Omega\psi dq$.

§3.5 Physical variables with continuous eigenvalues

Not all dynamical variables have discrete eigenvalues like ω_n, where $n = 1, 2, \ldots$. Let $\Omega\,|\phi_\omega\rangle = \omega\,|\phi_\omega\rangle$ whew ω is a continuous real number. Let $|\phi_\omega\rangle$ be the eigenfunction for eigenvalue ω, then a general state can be written as $|\psi\rangle = \int A(\omega)\,|\psi_\omega\rangle\,d\omega$ and $\langle\psi_{\omega'}\rangle\psi_\omega = \delta(\omega' - \omega)$. Then, $A(\omega') = \langle\phi_{\omega'}\rangle\psi$ and $|A(\omega')|^2 = |\langle\phi_{\omega'}\rangle\psi|^2$ is the probability density that Ω has a value ω'. The probability that Ω in a state ψ takes a value between ω and $\omega + d\omega$ is given as $\langle\psi|\,\Omega\,|\psi\rangle = \int |A(\omega)|^2\omega d\omega$.

In general Ω is a time varying quantity. We therefore have the following relation for the time evolution of its expectation value, by using the Schrödinger equation $i\hbar(\partial\psi/\partial t) = H\psi$ and $-i\hbar(\partial\psi^*/\partial t) = (H\psi)^* = \psi^*H^* = \psi^*H$.

$$\begin{aligned}
\frac{d}{dt}\langle\psi|\,\Omega\,|\psi\rangle &= \left\langle\frac{\partial\psi}{\partial t}\middle|\Omega\middle|\psi\right\rangle + \left\langle\psi\middle|\frac{\partial\Omega}{\partial t}\middle|\psi\right\rangle + \left\langle\psi\middle|\Omega\middle|\frac{\partial\psi}{\partial t}\right\rangle \\
&= -\frac{1}{i\hbar}\langle H\psi|\Omega|\psi\rangle + \frac{1}{i\hbar}\langle\psi|\Omega|H\psi\rangle + \left\langle\psi\middle|\frac{\partial\Omega}{\partial t}\middle|\psi\right\rangle \\
&= \frac{i}{\hbar}\langle\psi|[H,\Omega]|\psi\rangle + \left\langle\psi\middle|\frac{\partial\Omega}{\partial t}\middle|\psi\right\rangle \\
&= \frac{i}{\hbar}\langle[H,\Omega]\rangle + \left\langle\frac{\partial\Omega}{\partial t}\right\rangle \\
&= \frac{d\langle\Omega\rangle}{dt}
\end{aligned}$$

Notice that if the observable itself is time independent i.e., $\partial\Omega/\partial t$, then the equation reduces to

$$\left\langle\frac{\partial\Omega}{\partial t}\right\rangle \implies \frac{d\langle\Omega\rangle}{dt} = \frac{i}{\hbar}\langle[H,\Omega]\rangle$$

Then if the observable Ω commutes with the Hamiltonian, we have no evolution at all of the expectation value.

$$[H,\Omega] = 0 \implies \frac{d\langle\Omega\rangle}{dt} = 0$$

Introduction of the δ-Function

Resolution of the difficulty encountered in the Parceval relation for the case of continuous eigenvalues, gives the following orthonormal relation

$$\int \phi_v^*(x)[\phi(x)]_{v'-\frac{1}{2}\varepsilon}^{v'+\frac{1}{2}\varepsilon} dx = \begin{cases} 0 & \text{for } v < v' - \frac{1}{2}\varepsilon \text{ and } v > v' + \frac{1}{2}\varepsilon \\ 1 & \text{for } v' - \frac{1}{2}\varepsilon < v < v > v' + \frac{1}{2}\varepsilon \end{cases}$$

If we introduce a function $\Delta_\varepsilon(v)$ defined by

$$\Delta_\varepsilon(v) = \begin{cases} 0 & \text{for } v < -\frac{1}{2}\varepsilon \text{ and } v > \frac{1}{2}\varepsilon \\ \frac{1}{2}\varepsilon & \text{for } -\frac{1}{2}\varepsilon < v < +\frac{1}{2}\varepsilon \end{cases}$$

the orthonormal relation can then be rewritten as

$$\int \phi_v^*(x) \left(\frac{[\phi(x)]_{v'-\frac{1}{2}\varepsilon}^{v'+\frac{1}{2}\varepsilon}}{\varepsilon} \right) dx = \Delta_\varepsilon(v - v')$$

This equation holds true irrespective of the value of ε and in the limiting case if $\varepsilon \to 0$, the function $[\phi(x)]_{v'-\frac{1}{2}\varepsilon}^{v'+\frac{1}{2}\varepsilon}/\varepsilon$ becomes $\phi_{v'}(x)$. Hence, by introducing a new function $\delta(x)$ defined by,

$$\lim_{\varepsilon \to 0} \Delta_\varepsilon(x) = \delta(x)$$

the above relation can be written as

$$\int \phi_v^*(x)\phi_{v'}(x) = \delta(v - v')$$

Further, if Ω, H are commuting self-adjoint or Hermitian operators, then there always exist eigenf unctions that simultaneously satisfy eigenvalue equation with Ω, H i.e., $\Omega\phi = \omega\phi$ and $H\phi = E\phi$. Hence, $\phi_{\omega,E}$ is a state with definite Ω and E. Classically, we remember that if the Poisson bracket $[\Omega, H]_{P.B} = 0$, then Ω is a constant motion if $\partial\Omega/\partial t = 0$.

Moreover, if $|\phi\rangle$ is an eigen vector of the operator Ω, then $\Omega|\phi\rangle = \omega|\phi\rangle$. We can then see that $\Omega^2|\phi\rangle = \omega^2|\phi\rangle$ or even in general $\Omega^n|\phi\rangle = \omega^n|\phi\rangle$. (If we apply the operator Ω to $\Omega|\phi\rangle = \omega|\phi\rangle$, we get $\Omega^2|\phi\rangle = \Omega\omega|\phi\rangle$. Since ω is an ordinary number and Ω is a linear operator, we can change the order of Ω and ω on *RHS* to read $\omega\Omega\phi$. $\therefore \Omega^2|\phi\rangle = \Omega\omega|\phi\rangle = \omega\Omega\phi = \omega^2\phi$. We pursue this argument further to prove for arbitrary n)

$$\therefore \left(\sum_i a_i \Omega^i \right) |\phi\rangle = \left(\sum_i a_i \omega^i \right) |\phi\rangle$$

Then we can conclude that the eigenstates of Ω are automatically the eigenstates of a polynomial or eventually a power (Taylor) series $F(\Omega)$ of Ω. If the value of Ω in an eigenstate is ω, the value of $F(\Omega)$ is definitely $F(\omega)$ i.e., $F(\Omega)|\phi\rangle = F(\omega)|\phi\rangle$. This property of $F(\Omega)$ can be used to give a

general definition of a function of an operator Ω, not necessarily a polynomial. Assuming, for simplicity, that Ω has only a discrete set of eigenvalues, we denote them by $\omega_1, \omega_2, \omega_3, \ldots$ and the corresponding normalized eigen functions by $\phi_1(q), \phi_2(q), \phi_3(q), \ldots$. Then we define a function $F(\Omega)$ of Ω by the requirement that $F(\Omega)$ has the same set of eigen functions $\phi_1(q), \phi_2(q), \phi_3(q), \ldots$ with eigenvalues $F(\omega_1), F(\omega_2), F(\omega_3), \ldots$. It is always possible to construct a linear operator having this property. To this end, we define the integral operator $\mathcal{G} = G_F(q, q')$ as follows,

$$G_F(q, q') = \sum_n F(\omega_n)\phi_n(q)\phi_n^*(q')$$

Then we can easily show by using the orthonormal relations among ϕ's that

$$\int G_F(q, q')\phi_n(q')dq = F(\omega_n)\phi_n(q)$$

§3.6 Unitary Transformation and general representation theory

Given an arbitrary state ket $|\psi\rangle$, we expand it in three ways, namely in terms of

- Energy eigenkets (discrete or continuous)
- Position eigenkets (continuous)
- Momentum eigenkets (continuous)

Example : If $|\psi(t)\rangle = \sum_n c_n(0).e^{-iE_nt/\hbar} |\phi_n\rangle$ or $|\psi\rangle = \sum_n c_n |\phi_n\rangle$

- $\langle\phi_n| |\psi\rangle$ is the energy representation of the ket where $H|\phi\rangle = E_n|\phi\rangle$
- $\langle q| |\phi\rangle$ is the position / coordinate representation of the KET and the "usual" wavefunction
- $\langle p| |\phi\rangle$ is the momentum representation or the momentum space wave function

In the "position representation", one can also express the superposition of energy eigenkets for example as $\langle q| |\phi\rangle = \sum_n c_n(0).e^{-iE_nt/\hbar} \langle q| |\phi_n\rangle$, etc. We saw earlier that any function $f(x)$ can be expended in terms of a basis functions $x_1, x_2, \ldots$ i.e., $f = \sum_i \eta_i\chi_i$. If f is a wave function corresponding to the state ket $|\psi\rangle$ then in the BRAKET notation this becomes $|\psi\rangle = \sum_i \eta_i |\chi_i\rangle$. In general, the $|\chi_i\rangle$ are eigen functions of some linear self-adjoint operator $\hat{\Omega}$ i.e., $\Omega|\chi_i\rangle = \omega_i|\chi_i\rangle$ or $\Omega(i\hbar(\partial/\partial q), q)\chi_i = \omega_i\chi_i$. Let the same $|\psi\rangle$ be given as $|\psi\rangle = \sum_i \xi_i |\phi_i\rangle$ where $|\phi_i\rangle$ are eigen functions of some other linear self-adjoint operator $\hat{\Phi}$ i.e., $\Phi|\phi_i\rangle = \varphi_i|\phi_i\rangle$ or $\Phi(i\hbar(\partial/\partial q), q)\phi_i = \varphi_i\phi_i$. Since $\{|\chi_i\rangle\}$ and $\{|\phi_i\rangle\}$ are eigen function of an eigen value equation and Ω and Φ are self-adjoint or Hermitian, the χ_i's and Φ_i's are orthonormal within each set i.e., $\langle\chi_i| |\chi_j\rangle = \delta_{ij}$ and

$\langle\phi_i|\,|\phi_j\rangle = \delta_{ij}$. Also, since they are complete sets, we also have $\sum_i |\chi_i\rangle\langle\chi_i| = \hat{\mathbb{I}}$ and $\sum_i |\phi_i\rangle\langle\phi_i| = \hat{\mathbb{I}}$.

$$\begin{aligned}
|\psi\rangle &= \sum_i \eta_i |\chi_i\rangle \\
&= \sum_i \eta_i \left(\sum_j |\phi_j\rangle\langle\phi_j|\right)|\chi_i\rangle \\
&= \sum_i \eta_i \sum_j |\phi_j\rangle\langle\phi_j|\,|\chi_i\rangle \\
&= \sum_j \left(\sum_i \langle\phi_j|\,|\chi_i\rangle\,\eta_i\right)|\phi_j\rangle \\
&= \sum_j \xi_j |\phi_j\rangle
\end{aligned}$$

Using the orthogonality of $|\phi_i\rangle$, we see that $\xi_j = \sum_i \langle\phi_j|\,|\chi_i\rangle\,\eta_i = \sum_i \mathcal{U}_{ji}\eta_i$. From the orthonormality of the respective eigen bases, we can show that the transformation matrix $\mathcal{U}_{ij}$ is unitary i.e., $\mathcal{U}^\dagger\mathcal{U} = \mathcal{U}\mathcal{U}^\dagger = \hat{\mathbf{I}}$. Therefore, a change of "representation" or basis is usually effected using a unitary transformation.

Every self-adjoint or Hermitian operator is guaranteed to have an orthogonal eigenbasis which is complete. In fact there is a whole class of matrices operators called Normal Matrices having this property i.e., $\mathcal{N}^\dagger\mathcal{N} = \mathcal{N}\mathcal{N}^\dagger$. Hermitian as well as anti-Hermitian ($A^\dagger = -A$) and unitary matrices are Normal matrices.

§3.7 The set of commuting variables of a system

Though in the context of this course we won't be encountering any 'degeneracy' of eigen- values, it is good to be informed that many physical systems have such degeneracies. By degeneracy we mean that two orthogonal eigenvectors of a physical variable have the same eigenvalue. In such a case, any linear combination of these eigenvectors will also have the same eigenvalue. How then would we choose the correct eigenbasis for this variable? It seems that an infinite number of linear combinations can be chosen. This is exactly the arbitrariness we are faced within the context of the Hamiltonian too. Then how do we resolve this arbitrariness; how do we chose the appropriate linear com- bination?

In practice, other dynamical variables that "commute" with the Hamiltonian help us resolve this. We know that two Hermitian matrices that commute with each other have simultaneous eigenvectors. If any such variable has a non-degenerate set of eigenvalues for the energy- degenerate eigenvectors, then we can use that to label the eigenkets and they become appropriate choice to expand an arbitrary state ket. In other words, the joint basis is no longer degenerate in both variables. In practice, we try to find the largest or maximal set of Hermitian matrices that commute with Hamiltonian and resolve the degeneracy of the energy eigenkets.

Example : In spherically symmetric systems with $1/r$ potential, total Energy (E) as well as total magnitude of Angular momentum (L^2) and anyone component of the Angular momentum (L_z) commute with each other.It is this full set - the maximally commuting set of variables or operators - that we use to label the degenerate energy eigenkets.

A question may arise as to whether is any theorem which states that one can always construct a matrix that commutes with the Hamiltonian and which is non- degenerate. A clever such attempt is to take a particular choice of eigen kets, label them as $i = 1$ through M and construct the matrix (diagonal matrix) of these labels. Then, this matrix

$$\begin{bmatrix} 1 & 0 & 0 & \dots \\ 0 & 2 & 0 & \dots \\ 0 & 0 & 3 & \dots \\ \vdots & \vdots & \vdots & M \end{bmatrix}$$

clearly commutes with the Hamiltonian matrix

$$\begin{bmatrix} E & 0 & 0 & \dots \\ 0 & E & 0 & \dots \\ 0 & 0 & E & \dots \\ \vdots & \vdots & \vdots & E \end{bmatrix}$$

in this subspace. However, the catch here is that this matrix of indices is for a particular choice of indexing the vectors and there are infinitely many such choices and that arbitrariness is what we need to address. Moreover, the matrix of indices has no physical meaning (dynamical). Therefore, we are not interested in a matrix that commutes, but a matrix corresponding to a dynamical variable that commutes with the Hamiltonian!

§3.8 Position and Momentum representations

Eigen functions of the position $\hat{q}$ operator

Let us consider a state represented, for instance, by $\psi(q) = C\delta(q - q^o)$ where C is a constant. In this state, the coordinate of the dynamical system has a definite value of q^o since, according to the definition of δ-function, its value is zero everywhere except at $q = q^o$. As can be seen from this example, there are certain states in which a certain dynamical quantity has a certain definite value. We call such states the eigenstate of this dynamical quantity. In other words, a dynamical quantity has a definite value in one of its eigenstates.

Quantum mechanics introduces the following basic assumption. Namely, *when the Schrodinger function of a dynamical system is the eigenfunction of the operator* Ω *belonging to the eigenvalue* ω*, the dynamical quantity* Ω *has the definite value* ω *in this state.*

The state in which the coordinate q has a definite value q^o is, according to our assumption, represented by the Schrodinger function satisfying

$$\hat{q}\phi_{q^o}(q) = q\phi_{q^o}(q) = q^o\phi_{q^o}(q)$$

In fact, its eigen function can be given as

$$\phi_{q^o}(q) = C\delta(q - q^o)$$

where C is a constant. In this case, the eigenvalue q^o is real. The eigen functions are not square integrable, but again they admit Dirac orthonormality.

$$\int \phi^*_{q^o}(q)\phi_{q^{o'}}(q)dq = |C|^2 \int \delta(q - q^o)\delta(q - q^{o'})dq = |C|^2\delta(q^o - q^{o'})$$

If we pick $C = 1$, then $\phi_{q^o}(q) = \delta(q - q^o)$ is normalised with respect to q^o because

$$\int \phi^*_{q^o}(q)\phi_{q^{o'}}(q)dq = \int \delta(q - q^o)\delta(q - q^{o'})dq = \delta(q^o - q^{o'})$$

In braket notation, we have if $q\,|q_o\rangle = q_o\,|q_o\rangle$, then $\langle q'|q|q_o\rangle = \langle q'|q_o|q_o\rangle = q_o\delta(q_o - q')$ which proves orthogonality and $\langle\phi_{q^o}\rangle\,\phi_{q^{o'}} = \delta(q^o - q^{o'})$. These eignefunctions are also complete because

$$f(x) = \int f(q^o)\phi_{q^o}(x)dq^o = \int f(q^o)\delta(x - q^o)dx$$

Eigen functions of the momentum $\hat{p}$ operator

Properties of the δ-Function

A straightforward property resulting from definition is

$$\delta(x) = \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases}$$

Moreover, since $\int \delta(x - x_o)dx = 1$ i.e., the function has an integral of 1 over its entire domain, hence it is also termed as distribution. Also for any function $f(x)$, $f(x) = \int f(x_o)\delta(x - x_o)dx$ or in other words, the delta function samples the function at any point. Besides, it also has the property,

$$\delta(ax) = \frac{1}{|a|}\delta(x)$$

In this case, the eigenvalue equation is with ψ_{p^0} as the eigen function and p^o as the eigenvalue,

$$-i\hbar\frac{\partial\psi_{p^o}(x)}{\partial x} = p^o\psi_{p^o}(x) \implies \frac{\partial\psi_{p^o}(x)}{\partial x} = \frac{ip^o}{\hbar}\psi_{p^o}(x)$$

The general solution in 1D is

$$\psi_{p^o}(x) = \psi_0 \exp \frac{ip^o x}{\hbar}$$

and for any generalised q is

$$\psi_{p^o}(q) = \text{constant} \times \exp \frac{ip^o q}{\hbar}$$

Since p^o is a continuous variable, we have for the orthogonality relation, where A is a constant

$$\int \psi^*_{p^o}(x)\psi_{p^{o'}}(x)dx = |A|^2 \int \exp \frac{i(p^{o'} - p^o)x}{\hbar} = |A|^2.2\pi\hbar.\delta(p^{o'} - p^o)$$

If we take A to be $1/\sqrt{h}$, then

$$\psi_{p^o}(x) = \frac{1}{\sqrt{h}} \exp \frac{ip_o x}{\hbar}$$

If $|p\rangle$ is a momentum eigenket, then $\psi_{p^o}(x) \equiv \langle x\rangle\, p$. Hence, we can say that $\langle x\rangle\, p = \exp ip_o x/\hbar/\sqrt{h}$. A general ket $|\psi\rangle$ expanded in momentum eigenkets looks like $|\psi\rangle = \int a_p\, |p\rangle\, dp$ because p is a continuous variable. In other words, $\psi(x) = \langle x\rangle\, \psi = \int a_p\, \langle x|\, |p\rangle\, dp = \int a_p \exp ip_o x/\hbar/\sqrt{h}dp$. For $|\psi\rangle$ to be a momentum eigen ket with definite momentum p^o i.e., $\psi(x) = \psi_{p^o}(x)$ then $a_p = \delta(p - p^o)$.

Note that $\psi_{p^o}(x)$ is not a normalised wave function or in other words $\int |\psi_{p^o}(x)|^2 \neq 1$ in fact its infinity. This suggests that this is not a really physical state occurring in nature. A physical state is never something that has an infinite spatial extent like the plane wave function. A more realistic scenario is that of a wave function that has a plane wavelike behaviour in a finite region of space. As an example, we have

$$\psi(x) = \frac{1}{\pi^{1/4}\delta^{1/2}} \exp -\frac{(x - x_o)^2}{2\delta^2} \exp \frac{ip_o x}{\hbar}$$

where the finiteness of extent is guaranteed by the gaussian prefactor and also $\psi(x)$ has been normalised to unity.

§3.9 Fluctuations/Uncertainty in physical quantities – Uncertainty Relation

Earlier we saw that the interpretation of the coefficient c_n in $|\psi\rangle = \sum_n c_n\, |x_n\rangle$ is that $|c_n|^2$ is the probability that energy has the value E_n for a non-degenerate spectrum. Naturally, this leads to the question -"If we measure the energy of the system several times, what is the spread of the energy values around the mean value?" In statistics, the variance, and standard deviation are measures of such a spread. Variance is computed as shown,

$$(\Delta\Omega)^2 = \langle(\Omega - \langle\Omega\rangle)^2\rangle = \langle\Omega^2\rangle - 2\langle\Omega\rangle\langle\Omega\rangle + \langle\langle\Omega\rangle^2\rangle = \langle\Omega^2\rangle - \langle\Omega\rangle^2$$

We use the standard gaussian integral,

$$\psi(x) = \frac{1}{\pi^{1/4}\delta^{1/2}} \exp -\frac{(x - x_o)^2}{2\delta^2} \exp \frac{ip_o x}{\hbar}$$

Exponential representation of the δ-Function

The Dirac delta function can be written in the form

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}dk$$

In order to evaluate the integral, we introduce a regularization factor, $e^{-k\epsilon}$, as follows

$$\begin{aligned}
\int_{-\infty}^{\infty} e^{ikx}dk &= \int_{-\infty}^{0} e^{ikx}dk + \int_{0}^{\infty} e^{ikx}dk \\
&= \int_{0}^{\infty} e^{-ikx}dk + \int_{0}^{\infty} e^{ikx}dk \\
&= \int_{0}^{\infty} (e^{ikx} + e^{-ikx})dk \\
&= \lim_{\epsilon\to 0^+}\int_{0}^{\infty} (e^{ikx} + e^{-ikx})e^{-k\epsilon}dk \\
&= \lim_{\epsilon\to 0^+}\int_{0}^{\infty} (e^{ik(x+i\epsilon)} + e^{-ik(x-i\epsilon)})dk \\
&= \lim_{\epsilon\to 0^+}\left[\frac{e^{ik(x+i\epsilon)}}{i(x+i\epsilon)} + \frac{e^{-ik(x-i\epsilon)}}{-i(x-i\epsilon)}\right]_0^{\infty} \\
&= \lim_{\epsilon\to 0^+}\left(0 + 0 - \frac{1}{i(x+i\epsilon)} - \frac{1}{-i(x-i\epsilon)}\right) \\
&= \lim_{\epsilon\to 0^+}\left(\frac{i}{x+i\epsilon} - \frac{i}{x-i\epsilon}\right) \\
&= \lim_{\epsilon\to 0^+}\frac{2\epsilon}{x^2+\epsilon^2} = \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases}
\end{aligned}$$

where we have used the fact that, for $\epsilon > 0$, $e^{-k\epsilon}$ goes to 0 as k goes to ∞. It remains to show that the final expression has the correct normalization. However,

$$\int_{-\infty}^{\infty}\frac{2\epsilon}{x^2+\epsilon^2}dx = 2\arctan\left(\frac{x}{\epsilon}\right)\Bigg|_{-\infty}^{\infty} = 2\pi$$

is independent of ϵ.

§3.9.i Uncertainty in x

We first calculate the uncertainty of the coordinate x. This wave packet has appreciable amplitude only in the region of width δ around x_0.

$$\langle x\rangle = \frac{1}{\pi^{1/2}\delta}\int x\exp\frac{(x-x_o)^2}{\delta^2}dx$$

which, after the change of integration variable by $x - x_o = x'$, becomes

$$\langle x\rangle = \frac{1}{\pi^{1/2}\delta}\left(x_o\int \exp -\frac{x'^2}{\delta^2}dx' + \cancel{\int x' \exp -\frac{x'^2}{\delta^2}dx'}\right)$$

The second term is obviously zero being of odd degree being present while the integral in the first term gives $\pi^{1/2}\delta$ from the standard gaussian integral.

$$\int_{\infty}^{\infty} \exp -\frac{x^2}{a^2}dx = \pi^{1/2}a$$

Hence, we obtain $\langle x\rangle = x_o$. This was expected from the shape of Gaussian. Now,

$$\begin{aligned}
\langle x^2\rangle &= \frac{1}{\pi^{1/2}\delta}\int x^2 \exp\frac{(x-x_o)^2}{\delta^2}dx \\
&= \frac{1}{\pi^{1/2}\delta}\left(x_o^2\int \exp -\frac{x'^2}{\delta^2}dx' + \int x'^2 \exp -\frac{x'^2}{\delta^2}dx'\right) \\
&= x_o^2 + \frac{1}{\pi^{1/2}\delta}\int x'^2 \exp -\frac{x'^2}{\delta^2}dx' \\
&= x_o^2 - \frac{1}{\pi^{1/2}\delta}\left(\frac{\partial}{\partial(1/\delta^2)}\int \exp -\frac{x'^2}{\delta^2}dx'\right) \\
&= x_o^2 + \frac{1}{\pi^{1/2}\delta}\left(\frac{1}{2}\pi^{1/2}\delta^3\right) \\
&= x_o^2 + \frac{1}{2}\delta^2
\end{aligned}$$

Therefore, for the fluctuations in x, we have

$$(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2 = \frac{1}{2}\delta^2$$

§3.9.ii Uncertainty in p

Working out in a similar way as above, we obtain $\langle p\rangle$

$$\begin{aligned}
&= -\frac{i\hbar}{\delta\pi^{1/2}}\int \exp -\frac{(x-x_o)^2}{2\delta^2}\exp -\frac{ip_o x}{\hbar}\times\frac{d}{dx}\left(\exp -\frac{(x-x_o)^2}{2\delta^2}\exp\frac{ip_o x}{\hbar}\right)dx \\
&= -\frac{i\hbar}{\delta\pi^{1/2}}\left(\frac{1}{\delta^2}\cancel{\int x' \exp -\frac{x'^2}{\delta^2}dx'} + \frac{i}{\hbar}p_o \exp -\frac{x'^2}{\delta^2}dx'\right) \\
&= -\frac{i\hbar}{\delta\pi^{1/2}}\cdot\frac{i}{\hbar}p_o.\pi^{1/2}\delta \\
&= p_o
\end{aligned}$$

Similarly, using the same manipulation as used above, we find that

$$\langle p^2\rangle = \frac{\hbar^2}{2\delta^2} + p_o^2$$

Therefore, for the fluctuations in p, we have

$$(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2 = \frac{\hbar^2}{2\delta^2}$$

Hence, we have

$$(\Delta x)^2 (\Delta p)^2 = \frac{\hbar^2}{4} \implies \Delta x . \Delta p = \frac{\hbar}{2}$$

where $\Delta x = \sqrt{(\Delta x)^2}$ and $\Delta p = \sqrt{(\Delta p)^2}$. This is the uncertainty relation which states that the uncertainty in x and the uncertainty in p are reciprocally related. When one decreases, the other increases.

§3.10 Consequences of the uncertainty relation

- Firstly, this is not a surprising result once one realises that $\psi(x) = \int a_p \exp ip_o x/\hbar / \sqrt{h} dp$ is just a fourier integral representation of $\psi(x)$ in the basis of $\exp ip_o x/\hbar / \sqrt{h}$. If $\psi(x)$ is a function in coordinate space, then a_p which is the fourier coefficient or fourier transformation of $\psi(x)$ is a function in the reciprocal momentum space. By the properties of Fourier transforms, a great spread in one space leads to a narrower spread in the reciprocal space, while keeping the product of the spreads constant. This is quite well know and the functions are displaying the same property.

- This uncertainty is in the wave function that describes the state of a quantum system. In other words, it is a property of the state and is not related to any experimental accuracy, as in limitations there in.

- Remember that in classical mechanics the phase space volume element for a single degree of freedom is $d\Omega = dp.dx$. The uncertainty relation creates a granularity to the phase space volume. And the size of the grain is roughly $\hbar$. If there are Nq's and Np's, we have $d\Omega = \prod_i dp_i dq_i \sim (\hbar)^N$ for this granulairty. In other words, the smallest phase space volume element for this system is of the size $\hbar^N$. However, classically, there is no such granularity. In the light of this, we can clearly see that the classical phase space volume,(or its continuity) is obtained in the limit $\hbar \to 0$. This is one clear instance where the quantum to classical description is obtained as a limit of $\hbar \to 0$. It is for this reason that when an expression or formula for a quantity features an $\hbar$ in it, its quantum origins are suspected more often than not! In fact $\hbar$ is a signature of quantumness of a phenomenon!

§3.11 Generalised uncertainty relation

We derived the uncertainty relation when ψ is of standard Gaussian integral form. We now derive it for a general wave packet case. For simplicity assume that $\langle q \rangle = 0$ and $\langle p \rangle = 0$. Then, $(\Delta q)^2 = \langle q^2 \rangle - \langle q \rangle^2 = \langle q^2 \rangle$ and $(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2 = \langle p^2 \rangle$. If $\langle q \rangle$, $\langle p \rangle \neq 0$, then we define

$q' = q - \langle q \rangle$ and $p' = p - \langle p \rangle$ to begin with noting that $\langle q' \rangle$, $\langle p' \rangle = 0$. We shall now calculate $\langle q^2 \rangle$, and $\langle p^2 \rangle$,

$$\langle q^2 \rangle = \int \psi^* q^2 \psi dq = \int (q\psi)^* q\psi dq = \int |q\psi|^2 dq$$

$$\langle p^2 \rangle = \int \psi^* p^2 \psi dq = \int (p\psi)^* p\psi dq = \int |p\psi|^2 dq$$

Here $p\psi = -i\hbar(\partial\psi/\partial q)$. We note that

$$\int |q\psi + i\alpha p\psi|^2 \geq 0 \, , \, \alpha \in \mathbb{R}$$

Accordingly we have,

$$\alpha^2 \int |p\psi|^2 dq + i\alpha \left(\int (q\psi)^* (p\psi) dq - \int (p\psi)^* (q\psi) dq \right) + \int |q\psi|^2 dq \geq 0$$

Noting that $\int (p\psi)^* (q\psi) dq = \int \psi^* pq\psi dq$, we have

$$\alpha^2 \int |p\psi|^2 dq + i\alpha \int \psi^* (qp - pq)\psi dq + \int |q\psi|^2 dq \geq 0$$

Using the previously shown relations, this becomes

$$\langle q^2 \rangle \geq i\alpha \langle qp - pq \rangle - \alpha^2 \langle p^2 \rangle$$

which as shown in assumption is

$$(\Delta q)^2 \geq i\alpha \langle qp - pq \rangle - \alpha^2 (\Delta p)^2$$

Now this relation should hold for any value of α. That is, for all values of a the values of the right-hand side can never exceed the left-hand side $(\Delta q)^2$ which is independent of α. Now the right-hand side becomes maximum at

$$\alpha = \frac{i\langle qp - pq \rangle}{2(\Delta p)^2}$$

the maximum value being

$$-\frac{1}{4} \left(\frac{\langle qp - pq \rangle^2}{(\Delta p)^2} \right)$$

According to the argument mentioned above, this value cannot exceed $(\Delta q)^2$. Thus the following inequality must hold,

$$(\Delta q)^2 \geq -\frac{1}{4} \left(\frac{\langle qp - pq \rangle^2}{(\Delta p)^2} \right) \implies (\Delta q)^2 (\Delta p)^2 \geq -\frac{1}{4} \langle qp - pq \rangle^2$$

In the meantime, the canonical commutation relation gives $\langle qp - pq \rangle = i\hbar$. Hence,

$$(\Delta q)^2 (\Delta p)^2 \geq \frac{1}{4} \left(\frac{h}{2\pi} \right)^2 \implies (\Delta q)(\Delta p) \geq \frac{1}{2} \left(\frac{h}{2\pi} \right)$$

Hence, we have in general for canonically conjugate variables,

$$(\Delta A)(\Delta B) \geq -\frac{i|\langle AB - BA\rangle|}{2}$$

Note that this above general formulation assumes that the expectation value $\langle AB - BA\rangle$ is well defined in a given state. What this means is that the action of both AB and BA on a state $|\psi\rangle$ keeps the ket within the Hilbert space. This may sometimes be violated as shown below.

Example : Consider a particle wave function on a ring. The angular momentum p_ϕ and the angle variable ϕ are a canonical pair. If we consider a particle with a well-defined momentum on this ring, such that $\Delta p_\phi = 0$, we see that the uncertainty in the angular coordinate is always $\Delta\phi \leq 2\pi$ and therefore finite. So the uncertainty relation as written above cannot be true for this system. This is a common problem when a canonical variable is defined only on a finite domain, something typical of angle variables. What is the origin of this discrepancy?

To begin with, all the wave functions ψ on the ring have to satisfy the below two conditions :

$$\psi(\phi) = \psi(\phi + 2\pi)\ ,\ \frac{d\psi}{d\phi} = \frac{d\psi(\phi + 2\pi)}{d\phi}$$

Hence, ψ single-valued, periodic in ϕ and has continuous derivatives. We may then take $\hat{q} = \hat{\phi}$, $\hat{p} = \hat{p_\phi} = -i\hbar(\partial/\partial\phi)$. We notice that $p\,|\psi\rangle$ is periodic in ϕ similar to ψ and hence belongs to the Hilbert space i.e., $|\chi(\phi)\rangle = p\,|\psi(\phi)\rangle$ and $|\chi(\phi + 2\pi)\rangle = |\chi(\phi)\rangle$. However, on the other hand, $\hat{\phi}\psi = \phi\psi$ is not periodic and therefore does not belong to the Hilbert space of smooth, single-valued, periodic functions of ϕ. For this system, the uncertainty relation is $\Delta\phi.\Delta\psi \geq 0$.

4 Time evolution of quantum systems

§4.1 The different “pictures" of quantum mechanical formalism

§4.1.i Heisenberg Picture

Historically, Heisenberg's picture/approach came first. According to this approach, which has a close analogy with classical particle mechanics, dynamical variables like $\hat{q}$, $\hat{p}$, $\hat{\Omega}(q,p)$ etc evolve according to the following relation where $\hat{H}$ is the Hamiltonian of the system.

$$i\hbar\frac{d\hat{\Omega}}{dt} = i\hbar\frac{\partial\hat{\Omega}}{\partial t} + [\hat{\Omega},\hat{H}]$$

Since these operators/matrices act on state vectors, it is implicitly assumed in this approach that the state kets do not evolve in time. At any given instant of time t, for a ket ψ,

$$\langle\hat{\Omega}(t)\rangle = \langle\psi|\hat{\Omega}(t)|\psi\rangle \implies i\hbar\frac{d\langle\hat{\Omega}(t)\rangle}{dt} = i\hbar\left\langle\frac{\partial\hat{\Omega}(t)}{\partial t}\right\rangle + \langle[\hat{\Omega},\hat{H}]\rangle$$

For operators that don't explicitly depend on time, we have the Heisenberg equation of motion given by

$$i\hbar\frac{d\hat{\Omega}}{dt} = [\hat{\Omega},\hat{H}]$$

Therefore, operators evolve while state kets don't in the Heisenberg picture. However, since the operators evolve in time, their eigen-kets, which as basis kets for expanding a general state ket ψ, evolve in time. Hence, $\hat{\Omega}(t)\,|\phi_n(t)\rangle = \omega_n\,|\phi_n(t)\rangle$.

§4.1.ii Schrödinger picture

In this approach, state kets $|\psi(t)\rangle$ evolve according to the Schrodinger equation as

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = H\,|\psi(t)\rangle$$

Implicitly, we assume the operators $\hat{\Omega}(q,p)$ do not evolve in time. However, since $|\psi(t)\rangle$ evolve, hence $\langle\hat{\Omega}(t)\rangle$ given by $\langle\psi|\hat{\Omega}(t)|\psi\rangle$ evolves as

$$i\hbar\frac{d}{dt}\left(\langle\psi(t)|\hat{\Omega}|\psi(t)\rangle\right) = \langle\psi(t)|[\hat{\Omega},\hat{H}](t)|\psi(t)\rangle$$

Since, $\hat{\Omega}$ doesn't evolve, its eigen basis kets don't as well i.e., $\hat{\Omega}\,|\phi_n\rangle = \omega_n\,|\phi_n\rangle$ and if $|\psi(0)\rangle = \sum_n c_n(0)\,|\phi_n\rangle$ then $|\psi(t)\rangle = \sum_n c_n(t)\,|\phi_n\rangle$.

§4.1.iii Relation between the Heisenberg and Schrödinger pictures

To obtain the relation, let $|\psi\rangle_H$ be a Heisenberg-picture state ket and $|\psi\rangle_S$ be a Schrodinger-picture state ket. For a system Hamiltonian $\hat{H}$, we have

$$i\hbar\frac{\partial|\psi\rangle}{\partial t} = \hat{H}\,|\psi(t)\rangle$$

Since we know that $\langle\Omega(t)\rangle$ is same in both the pictures and ${}_H\langle\psi|\,|\psi\rangle_H = {}_S\langle\psi|\,|\psi\rangle_S = 1$, we expect $|\psi\rangle_H = \mathcal{U}_H\,|\psi\rangle_S$ where $\mathcal{U}_H$ is a unitary transformation. Also we want $|\psi\rangle_H$ to not explicitly depend on time, hence

$$\frac{\partial|\psi\rangle_H}{\partial t} = 0 \implies \frac{\partial}{\partial t}[\mathcal{U}_H\,|\psi\rangle_S] = 0$$

$$\implies \frac{\partial\mathcal{U}_H}{\partial t}\,|\psi\rangle_S + \mathcal{U}_H\frac{\partial|\psi\rangle_S}{\partial t} = \frac{\partial\mathcal{U}_H}{\partial t}\,|\psi\rangle_S + \frac{\mathcal{U}_{\mathcal{H}}H}{i\hbar}\,|\psi\rangle_S = 0$$

Since $\mathcal{U}_H$ is a unitary transformation, we have $\mathcal{U}_H^\dagger\mathcal{U}_H = 1$, hence

$$\therefore (i\hbar\mathcal{U}_H^\dagger\dot{\mathcal{U}}_H + H)\,|\psi\rangle_S = 0$$

Since this must be true for every ket $|\psi\rangle_S$, we need $i\hbar\mathcal{U}_H^\dagger\dot{\mathcal{U}}_H + H = 0$ or $\mathcal{U}_H^\dagger\dot{\mathcal{U}}_H = (i/\hbar)H$. This differential equation has a solution $\hat{\mathcal{U}}_H(t) = \exp(i/\hbar)Ht$. Hence, we have

$$|\psi\rangle_H = \mathcal{U}_H(t)\,|\psi(t)\rangle_S = \exp\frac{iHt}{\hbar}\,|\psi(t)\rangle_S$$

When H is independent of time, we can integrate the Schrödinger equation to get $|\psi(t)\rangle_S = \exp -(i/\hbar)\hat{H}t\,|\psi(0)\rangle_S$. We can therefore identify the Heisenberg picture ket to be just the initial Schrödinger ket and that is naturally a static object i.e., $|\psi\rangle_H = |\psi(0)\rangle_S$.

Since it is the expectation values that have a correspondence with measurements, both pictures should be able to describe the systems equivalently. However, one or the other is more appropriate for describing the system dynamics. In most atomic systems, we talk in terms of wave function and therefore Schrödinger approach seems more natural. However, in field theory, where there is no concept of a wave function, we almost always use the Heisenberg equation of motion. You will see this being the case later on, when we discuss the EM field along a 1-D transmission line. There we will not write the time-evolution of any wave function, but will talk exclusively in terms of the time evaluations of the field operators.

§4.1.iv Interaction picture

Many a time we have a Hamiltonian $\hat{H}$ of the form $H_o + V(t)$ where H_o is a time-independent Hamiltonian that depicts several uncoupled systems and $V(t)$ denotes a time-dependent interaction energy between them. In such situations, we use a different picture called the Interaction picture. In this picture, we isolate the effect of the time-dependent interaction term on the evolution of the system. Let us start with the Schrodinger picture to begin with,

$$i\hbar\frac{\partial|\psi\rangle_S}{\partial t} = H\,|\psi\rangle_S = H_o\,|\psi_S\rangle + V(t)\,|\psi\rangle_S$$

Similar to the Heisenberg picture, we want

$$|\psi(t)\rangle_I = \mathcal{U}_I(t)\,|\psi(t)\rangle_S \implies |\psi(t)\rangle_S = \mathcal{U}_I^\dagger\,|\psi(t)\rangle_I$$

where the subscript I denotes interaction and the time evolution of $|\psi\rangle_I$ is almost entirely governed by $V(t)$. Hence, we have

$$H_o\mathcal{U}_I^\dagger\,|\psi(t)\rangle_I + V\mathcal{U}_I^\dagger\,|\psi(t)\rangle_I = i\hbar\frac{\partial}{\partial t}\left[\mathcal{U}_I^\dagger\,|\psi(t)\rangle_I\right]$$

$$\implies H_o\mathcal{U}_I^\dagger\,|\psi\rangle_I + V\mathcal{U}_I^\dagger\,|\psi\rangle_I = i\hbar\frac{\partial\mathcal{U}_I^\dagger}{\partial t}\,|\psi\rangle_I + i\hbar\mathcal{U}_I^\dagger\frac{\partial|\psi\rangle_I}{\partial t}$$

$$\therefore i\hbar\frac{\partial|\psi\rangle_I}{\partial t} = \left[\mathcal{U}_I.(H_o+V)\mathcal{U}_I^\dagger - i\hbar\mathcal{U}_I\dot{\mathcal{U}}_I^\dagger\right]|\psi\rangle_I$$

Therefore, in general, consider a transformation of one ket into another using a time-dependent unitary transformation $\mathcal{U}(t)$, such that $|\psi\rangle_I = \mathcal{U}_I(t)\,|\psi(t)\rangle_S$. If the original ket satisfies

$$i\hbar\frac{\partial|\psi\rangle_S}{\partial t} = H\,|\psi\rangle_S$$

then the transformed Hamiltonian $\tilde{H}$ which satisfies

$$i\hbar\frac{\partial|\psi\rangle_I}{\partial t} = \tilde{H}\,|\psi\rangle_I$$

is given by

$$\tilde{H} = \mathcal{U}_I H\mathcal{U}_I^\dagger - i\hbar\mathcal{U}_I\dot{\mathcal{U}}_I^\dagger$$

If we now make a particular choice of $\mathcal{U}(t)$ such that the transformed Hamiltonian is almost entirely $V(t)$, that is we choose $\mathcal{U}_I H_o\mathcal{U}_I^\dagger - i\hbar\mathcal{U}_I\dot{\mathcal{U}}_I^\dagger = 0$, which has the solution $\mathcal{U}_I = \exp(i/\hbar)H_o t$ then we get

$$i\hbar\frac{\partial|\psi\rangle_I}{\partial t} = \left[\mathcal{U}_I V\mathcal{U}_I^\dagger\right]|\psi\rangle_I$$

$$\therefore |\psi\rangle_I = \mathcal{U}_I(t)\,|\psi(t)\rangle_S = \exp\frac{iH_o t}{\hbar}\,|\psi(t)\rangle_S$$

$$\implies i\hbar\frac{\partial|\psi\rangle_I}{\partial t} = V_1(t)\,|\psi\rangle_I \;,\; V_I(t) = \left[\mathcal{U}_I V\mathcal{U}_I^\dagger\right]$$

In summary, from a mathematical point of view, the different pictures we just discussed are nothing but a few unitary transformations acting on all states of a system. They are exactly analogous to rotating the set of coordinate axes. If a point in coordinate space is analogous to a state, its coordinates depend on the set of axes chosen. In the same way, the same state can be described in all the different pictures connected mutually via unitary transformations. Since it is the "same physical state" being described, the measured values of any variable should comes out the same.

$$\therefore \langle\Omega(t)\rangle = {}_S\langle\psi(t)|\Omega|\psi(t)\rangle_S = {}_H\langle\psi(t)|\Omega|\psi(t)\rangle_H = {}_I\langle\psi(t)|\Omega|\psi(t)\rangle_I$$

The Interaction picture is particularly useful in situations where we deal with an external agent interacting with or driving an otherwise isolated system. Such a system typically has a total Hamiltonian of the form $H = H_o + V(t)$. We will see that the process of measurement necessarily involves such an interaction between a probe and the system to be measured

§4.2 Time evolution of a system in general - Dyson series

Let $H = H_o + V(t)$. When $V(t) = 0$, H_O is just a time-independent Hamiltonian and we have $H_o |\phi_n\rangle = E_n |\phi_n\rangle$. Any ket $|\psi(0)\rangle_S = \sum_n c_n |\phi_n\rangle$ evolves as $|\psi(t)\rangle_S = \sum_n c_n \exp -(i/\hbar)E_n t |\phi_n\rangle$. When $H = H_o + V$ for $V \neq 0$, we start by going into the interaction picture.

$$|\psi(t)\rangle_I = \mathcal{U}_I(t) |\psi(t)\rangle_S = \exp \frac{iH_o t}{\hbar} |\psi(t)\rangle_S$$

$$i\hbar \frac{\partial |\psi(t)\rangle_I}{\partial t} = \left[\mathcal{U}_I V \mathcal{U}_I^\dagger\right] |\psi\rangle_I = V_I(t) |\psi\rangle_I$$

Since time evolution of a ket is a unitary operator i.e., $\langle\psi(t)\rangle = \langle\psi(0)\rangle = 1$, we have $|\psi(t)\rangle_I = \mathcal{U}(t,0) |\psi(0)\rangle_I$ where $|\psi(0)\rangle_I$ is any initial interaction ket. Since the state has all the information about the system at time t, the state of the system at the time $t + dt$ depends only on the state at time t and on the evolution operator $\mathcal{U}(t, t + dt)$ (that thus depends only on the times t and $t + dt$, not on any previous times, otherwise it would bring extra information to the system). Hence, we have as an operator equation

$$i\hbar \frac{\partial \mathcal{U}(t,0)}{\partial t} = V_I(t)\mathcal{U}(t,0)$$

with initial condition $\mathcal{U}_I(t,t) = \mathbf{1}$, the identity operator. When V_I is time dependent and $V_I(t)$ does not commute at different time, it is no longer possible to find a simple explicit expression for $U_I(t)$. Indeed we could be tempted to write $U_I(t) = \exp -\int_0^t V_I(t')dt'$. However, in general

$$e^A e^B \neq e^{A+B} \text{ if } [A, B] \neq 0$$

Moreover, we can see that for $0 = t_0 < t_1 < t$, we have

$$\mathcal{U}(t, t_0) = \mathcal{U}(t, t_1)\mathcal{U}(t_1, t_0)$$

The given differential equation is however equivalent to the following integral equation,

$$\mathcal{U}_I(t,0) = \mathbf{1} + \left(-\frac{i}{\hbar}\right) \int_0^t V_I(t')\mathcal{U}_I(t',0)dt'$$

We keep iterating this to obtain t

$$\mathcal{U}_I(t,t_0) = \mathbf{1} + \left(-\frac{i}{\hbar}\right) \int_0^t V_I(t')dt' + \left(-\frac{i}{\hbar}\right)^2 \int_0^t \int_0^{t'} V_I(t')V_I(t'')dt'dt''$$
$$+ \left(-\frac{i}{\hbar}\right)^3 \int_0^t \int_0^{t'} \int_0^{t'''} V_I(t')V_I(t'')V_I(t''')dt'dt''dt''' + \dots$$

In general, we can write this for a time evolution between t_0 and t as,

$$\mathcal{U}_I(t,0) = \mathbf{1} + \left(-\frac{i}{\hbar}\right) \int_{t_0}^t V_I(t')dt' + \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^t \int_{t_0}^{t'} V_I(t')V_I(t'')dt'dt'' + \dots$$

$$+ \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^t \int_{t_0}^{t'} \cdots \int_{t_0}^{t''''\dots(n-1)\text{ times}} V_I(t')V_I(t'')\dots V_I(t'''\dots n\text{ times})dt'dt''\dots dt'''\dots n\text{ times} + \dots \infty$$

This series is called **Dyson series**.

§4.3 Energy time uncertainty relations

The uncertainty relation between position and momentum of a particle is given by $\Delta x \Delta p \geq \hbar/2$. We have a similar-looking uncertainty principle between ΔE and Δt where $\Delta E \Delta t \simeq h$. However it is important to note that this is of a very different nature and origin compared to the position-momentum uncertainty. Consider a ket $|\psi\rangle$ written as an expansion in energy eigenkets $|\phi_n\rangle$ when $H|\phi_n\rangle = E_n|\phi_n\rangle$. Hence, $|\psi(0)\rangle = \sum_n c_n |\phi_n\rangle$. From Schrodinger's equation, we have that the time-evolved ket is $|\psi(t)\rangle = \sum_n c_n \exp -(i/\hbar)Ht\,|\phi_n\rangle$. The time evolution operator, $\exp -(i/\hbar)Ht$ in terms of $|\phi_n\rangle\langle\phi_n|$, is (using $\langle\phi_{n'}\rangle\phi_n = \delta_{nn'}$)

$$\exp\frac{-iHt}{\hbar} = \sum_n \sum_{n'} |\phi_{n'}\rangle\langle\phi_{n'}| \exp\frac{-iHt}{\hbar} |\phi_n\rangle\langle\phi_n| = \sum_n |\phi_n\rangle \exp\frac{-iE_n t}{\hbar}\langle\phi_n|$$

The time-evolution operator written in this form enables us to solve any initial-value problem once the expansion of the initial ket in terms of $\{|\phi_n\rangle\}$ is known. Hence, for $|\psi(0)\rangle = \sum_n c_n|\phi_n\rangle = \sum_n |\phi_n\rangle\langle\phi_n\rangle\psi(0)$, we have

$$|\psi(t)\rangle = \exp\frac{-iHt}{\hbar}|\psi(0)\rangle = \sum_n |\phi_n\rangle\langle\phi_n\rangle\psi(0)\exp\frac{-iE_n t}{\hbar} = \sum_n c_n \exp\frac{-iE_n t}{\hbar}|\phi_n\rangle$$

The overlap of $|\psi(t)\rangle$ with $|\psi(0)\rangle$ is called the **Correlation amplitude** denoted as $C(t) = \langle\psi(0)|\,|\psi(t)\rangle$.

$$C(t) = \left(\sum_n c_n^* \langle\phi_n|\right)\left[\sum_{n'} c_{n'} \exp\frac{-iE_{n'}t}{\hbar}|\phi_{n'}\rangle\right] = \sum_n |c_n|^2 \exp\frac{-iE_n t}{\hbar}$$

As we sum over many terms with oscillating time dependence of different frequencies, a strong cancellation is possible for moderately large values of t. We expect the correlation amplitude that starts with unity at $t = 0$ to decrease in magnitude with time. To estimate $C(t)$ in a more concrete manner, let us suppose that the state ket can be regarded as a superposition of so many energy eigenkets with similar energies that we can regard them as exhibiting essentially a quasi-continuous spectrum. It is then legitimate to replace the sum by the integral

$$\sum_n \to \int \rho(E)dE\ ,\ c_n \to g(E)|_{E\simeq E_n}$$

where $\rho(E)$ characterizes the density of energy eigenstates. Then, we have

$$C(t) = \int |g(E)|^2 \rho(E) \exp\frac{-iEt}{\hbar} dE$$

subject to the normalization condition

$$\int |g(E)|^2 \rho(E) dE = 1$$

In a realistic physical situation $|g(E)|^2\rho(E)$ may be peaked around $E = E_0$ with width ΔE. Hence, rewriting $C(t)$ as

$$C(t) = \exp\frac{-iE_0 t}{\hbar}\int |g(E)|^2\rho(E)\exp\frac{-i(E-E_0)t}{\hbar}dE$$

we see that as t becomes large, the integrand oscillates very rapidly unless the energy interval $|E - E_0|$ is small compared with $\hbar/t$. If the interval for which $|E - E_0| \simeq \hbar/t$ holds is much narrower than ΔE, the width of $|g(E)|^2\rho(E)$, we get essentially no contribution to $C(t)$ because of strong cancellations since the relative phase difference between the term at E_0 and $E + E_0$ becomes nearly π. The characteristic time at which the modulus of the correlation amplitude starts becoming appreciably different from 1 is given by

$$t \simeq \frac{\hbar}{\Delta E}$$

This t is also typically the time scale over which a transition happens. Therefore, if the ket is a superposition of a broad range of energy eigenkets, or if its energy is very uncertain, then the time interval for which the ket will remain, or its lifetime is roughly given by the inverse of the uncertainty in energy. To summarize, as a result of time evolution the state ket of a physical system ceases to retain its original form after a time interval of order $\hbar/\Delta E$. In the literature this point is often said to illustrate the energy-time uncertainty relation

$$\Delta E \Delta t \simeq h$$

III

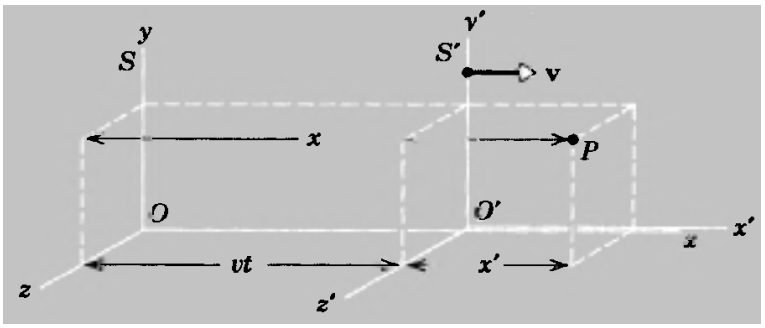
Relativity

5 Experimental Background

Lets begin the discussion by considering a physical event i.e., one which happens independently of the reference frame which me might use to describe it. We define an inertial system as a frame of reference in which the law of inertia - Newton's first law - holds. An un-accelerated system is one in which when the body is acted on by zero net external force it will move with a constant velocity. Frames accelerating with respect to such a frame are not inertial. Equations of motion remain invariant if one changes to a frame of reference which moves at a uniform velocity with respect to other inertial frames. The special theory of relativity deals with only description of events by observers in inertial reference frames.

§5.1 Galilean Transformation

Consider now an inertial reference frame S and another inertial frame S' which moves at a constant velocity v with respect to S. For convenience, we choose the three sets of axes to be parallel and allow relative motion to be along the common x, x' axis. We can easily generalise to arbitrary orientations and relative velocity of the frames later, but the physical principles involved are not affected by the particular simple choice we make at present. Note that also we can just as well consider S to be moving at velocity $-v$ with respect to S'.



Let an event occur at point P whose space and time coordinate we measure in each inertial frame. An observer attached to S specifies the location and time of occurrence of this event by ascribing space coordinates x, y, z and time coordinate t to it. An observer attached to S' specifies the same event by space-time coordinates x', y', z' and t'. Lets now see the relationship between the measurements x, y, z, t and x', y', z', t'. The length-measuring instruments used by the inertial observers have been compared and calibrated against one other and the clocks have been synchronised and calibrated against one other. The classical procedure is to assume that the time and length intervals are absolute, i.e., they are same for all inertial observers of the same events.

For simplicity, let us say that the clocks of each observer read zero at the instant that the

origins O and O' of the frames S and S', which are in relative motion coincide. Then the Galilean coordinate transformations which relate x, y, z, t to x', y', z', t' are given as,

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

It is assumed that time can be defined independently of the reference frame, which is expresses in the transformation equations by absence of a transformation for t. We can make this assumption of the universal nature of time explicit by adding to the Galilean transformations, the equation

$$t' = t$$

It follows at once that time time interval between the occurrence of two events, say P and Q is same for each observer i.e.,

$$t_{P'} - t_{Q'} = t_P - t_Q$$

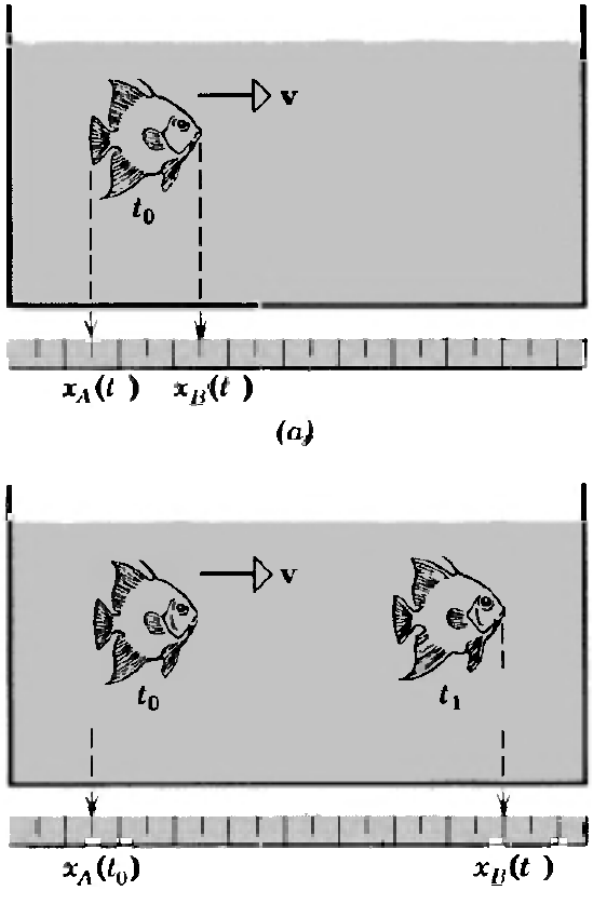
and the distance or space interval between two points, say A and B measured at a given instant, is same for each observer i.e.,

$$x_B{}' - x_A{}' = x_B - x_A$$

Lets look at it more carefully. Say A and B are the endpoints of a rod, for example which are at rest in the S-frame. Then the primed observer for whom the rod is moving with velocity $-v$, will measure the end-point locations $x_A{}'$ and $x_B{}'$, whereas the unprimed observer locates them at x_A and x_B. Using the Galilean transformation equations, however, we find that $x_B{}' = x_B - vt_B$ and $x_A{}' = x_A - vt$ so that $x_B{}' - x_A{}' = x_B - x_A - v(t_B - t_A)$. Since the two endpoints are measured at the same instant, $t_A = t_B$ and we obtain $x_B{}' - x_A{}' = x_B - x_A$, as found above. This assumption - that measurements are made at the same instant - is crucial in our definition of the length of a rod. Surely, we should not measure the locations of the end-points at different times to get the length of a moving rod. It would be like measuring the location of the tail of a swimming fish at one instant and of its head at another instant in order to determine its length.

Hence, we obtain the following equations,

$$\begin{aligned} |x'_B - x'_A| &= |x_B - x_A| \\ |y'_B - y'_A| &= |y_B - y_A| \\ |z'_B - z'_A| &= |z_B - z_A| \\ \therefore \sqrt{\Delta x'^2 + \Delta y'^2 + \Delta z'^2} &= \sqrt{\Delta x^2 + \Delta y^2 + \Delta z^2} \\ \Delta t' &= \Delta t \end{aligned}$$



§5.2 Newtonian Relativity

Lets now see how the measurements of different inertial observers compare with regard to the velocities and accelerations of objects. The velocity transformation follows at once. Starting from $x' = x - vt$, differentiating it with respect to t gives

$$\frac{dx'}{dt} = \frac{dx}{dt} - v$$

However, since $t' = t$, the operation d/dt is identical to d/dt' so that we have

$$\frac{dx'}{dt} = \frac{dx'}{dt'}$$
$$\therefore \frac{dx'}{dt'} = \frac{dx}{dt} - v$$

Similarly, we have

$$\frac{dy'}{dt'} = \frac{dy}{dt}, \frac{dz'}{dt'} = \frac{dz}{dt}$$

However, $dx'/dt' = u'_x$ is x-component of the velocity measured in S' and $dx/dt = u_x$ is the x-component of the velocity measured in S and so on, so we have simply the classical velocity addition theorem .

$$u'_x = u_x - v$$
$$u'_y = u_y$$
$$u'_z = u_z$$

In the more general case, when the relative velocity of the frame has components along all three axes, we obtain $\vec{u}' = \vec{u} - \vec{v}$. To obtain the acceleration transformation, we merely differentiate the velocity relations. Proceeding as before, we obtain

$$\begin{aligned} \frac{d}{dt'}(u'_x) &= \frac{d}{dt}(u_x - v) \\ \implies \frac{du'_x}{dt'} &= \frac{du_x}{dt} \quad \because \ (v \text{ is a constant }) \\ \frac{du'_y}{dt'} &= \frac{du_y}{dt} \\ \frac{du'_z}{dt'} &= \frac{du_z}{dt} \end{aligned}$$

That is $a'_x = a_x, a'_y = a_y$ and $a'_z = a_z$. In other words, $\vec{a}' = \vec{a}$. Here, since we are only talking about he relative velocity of one frame with respect to another and not the absolute velocity of a frame, it sometimes called Newtonian Relativity.

§5.3 Wave Equation

Consider the following wave equation,

$$\frac{\partial^2 f}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 f}{\partial t^2} = 0$$

We find from the Galilean transformation $x' = x - vt$ that,

$$\frac{\partial x'}{\partial x} = 1 \, , \, \frac{\partial x'}{\partial t} = -v \, , \, \frac{\partial t'}{\partial t} = \frac{\partial y'}{\partial y} = \frac{\partial z'}{\partial z} = 1$$

and

$$\frac{\partial x'}{\partial y} = \frac{\partial x'}{\partial z} = \frac{\partial y'}{\partial x} = \frac{\partial t'}{\partial x} = \cdots = 0$$

From chain rule and using the above results we have,

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial x'}\frac{\partial x'}{\partial x} + \frac{\partial f}{\partial y'}\frac{\partial y'}{\partial x} + \frac{\partial f}{\partial z'}\frac{\partial z'}{\partial x} + \frac{\partial f}{\partial t'}\frac{\partial t'}{\partial x} = \frac{\partial f}{\partial x'}$$

$$\implies \frac{\partial^2 f}{\partial x^2} = \frac{\partial^2 f}{\partial x'^2}$$

Moreover,

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial x'}\frac{\partial x'}{\partial t} + \frac{\partial f}{\partial y'}\frac{\partial y'}{\partial t} + \frac{\partial f}{\partial z'}\frac{\partial z'}{\partial t} + \frac{\partial f}{\partial t'}\frac{\partial t'}{\partial t} = -v\frac{\partial f}{\partial x'} + \frac{\partial f}{\partial t'}$$

$$\implies \frac{\partial^2 f}{\partial t^2} = \left(-v\frac{\partial}{\partial x'} + \frac{\partial}{\partial t'}\right)\left(-v\frac{\partial}{\partial x'} + \frac{\partial}{\partial t'}\right)f = \frac{\partial^2 f}{\partial t'^2} - 2v\frac{\partial^2 f}{\partial x'\partial t'} + v^2\frac{\partial^2 f}{\partial x'^2}$$

Substituting these expressions in the wave equation gives

$$\frac{\partial^2 f}{\partial x'^2} - \frac{1}{c^2}\frac{\partial^2 f}{\partial t'^2} + \frac{1}{c^2}\left(2v\frac{\partial^2 f}{\partial x'\partial t'} - v^2\frac{\partial^2 f}{\partial x'^2}\right) = 0$$

These shows that the wave equation is not invariant under Galilean transformation for the left hand side of the equation has changed.

§5.4 Electromagnetism

We shall now see that the electromagnetic situation is different from the mechanical one, as far as the Galilean transformations are concerned. Consider a pulse of light (i.e., an electromagnetic pulse) traveling to the right with respect to the medium through which it is propagated at a speed c. Consider S as an inertial in which an observer measures the speed of light to be exactly $c = (1/\sqrt{\epsilon_o\mu_o}) = 2.997925 \times 10^8$ m/sec. In a frame S' moving at a constant speed v with respect to this ether frame, an observer would measure a different speed for the light pulse, ranging from $c + v$ to $c - v$ depending on the direction of relative motion, according to the Galilean velocity transformation.

Hence, the speed of light is certainly not invariant under a Galilean transformation. If these transformations really do apply to optical or electromagnetic phenomena, then there is one inertial system, and only one, in which the measured speed of light is exactly c. We would then have a physical way of identifying an absolute (or rest) frame and of determining by optical experiments carried out in some other frame what the relative velocity of that frame is with respect to the absolute one.

A more formal way of saying this is as follows. Maxwell's equations of electromagnetism, from which we deduce the electromagnetic wave equation for example, contain the constant $c = (1/\sqrt{\epsilon_o\mu_o})$ which is identified as the velocity of propagation of a plane wave in vacuum. However, such a velocity cannot be the same for observers in different inertial frames, according to the Galilean transformations, so that electromagnetic effects will probably not be the same for different inertial observers. In fact, Maxwell's equations are not preserved in form by the Galilean transformations, although Newton's laws are. In going from frame S to frame S', the form of the wave equation, for example, changes as shown in the previous section. However, if we accept both the Galilean transformations and Maxwell's equations as basically correct, then it automatically follows that there exists a unique privileged frame of reference in which Maxwell's equations are valid and in which light is propagated at a speed $c = (1/\sqrt{\epsilon_o\mu_o})$.

The situation then seems to be as follows. The fact that the Galilean relativity principle does apply to the Newtonian laws of mechanics but not to Maxwell's laws of electromagnetism requires us to choose the correct consequences from amongst the following possibilities.

1. A relativity principle exists for mechanics, but not for electrodynamics; in electrodynamics there is a preferred inertial frame. Should this alternative be correct, the Galilean transformations would apply and we would be able to locate the ether frame experimentally.

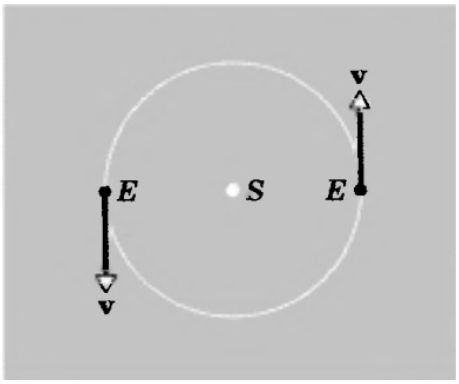
2. A relativity principle exists both for mechanics and for electrodynamics, but the laws of electrodynamics as given by Maxwell are not correct. If this alternative were correct, we ought to be able to perform experiments that show deviations from Maxwell's electrodynamics and reformulate the electromagnetic laws. The Galilean transformations would apply here also.

3. A relativity principle exists both for mechanics and for electrodynamics, but the laws of mechanics as given by Newton are not correct. If this alternative is the correct one, we should be able to perform experiments which show deviations from Newtonian mechanics and reformulate the mechanical laws. In that event, the correct transformation laws would not be the Galilean ones (for they are inconsistent with the invariance of Maxwell's equations) but some other ones which are consistent with classical electromagnetism and the new mechanics.

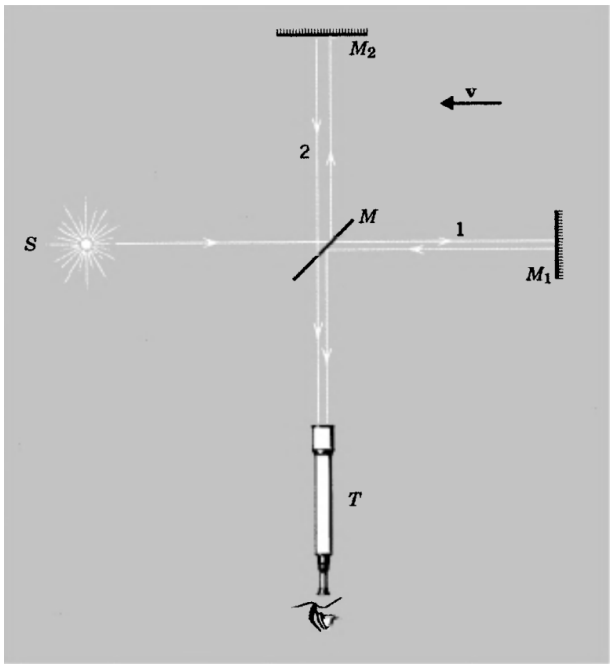
Intuitively, we know that Newtonian mechanics breaks down at high speeds so we should not be surprised to learn that alternative 3, leading to Einsteinian relativity, is the correct one. In the following sections, we shall look at the experimental bases for rejecting alternatives 1 and 2, as a fruitful prelude to finding the new relativity principle and transformation laws of alternative 3.

§5.5 The Michelson-Morley Experiment

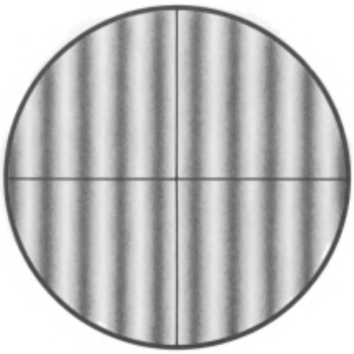
The obvious experiment would be one in which we can measure the speed of light in a variety of inertial systems, noting whether the measured speed is different in different systems, and if so, noting especially whether there is evidence for a single unique system - the "ether" frame - in which the speed of light is c, the value predicted from electromagnetic theory. Let us now describe the Michelson-Morley experiment. The Michelson interferometer is fixed on the earth. If we imagine the "ether" to be fixed with respect to the sun, then the earth (and interferometer) moves through the ether at a speed of 30 km/sec, in different directions in different season as shown below in the figure.



For the moment, neglect the earth's spinning motion. The beam of light (plane waves, or parallel rays) from the laboratory source S (fixed with respect to the instrument) is split by the partially silvered mirror M into two coherent beams, beam 1 being transmitted through M and beam 2 being reflected off of M. Beam 1 is reflected back to M by mirror M_1 and beam 2 by mirror M_2 in the manner shown below.



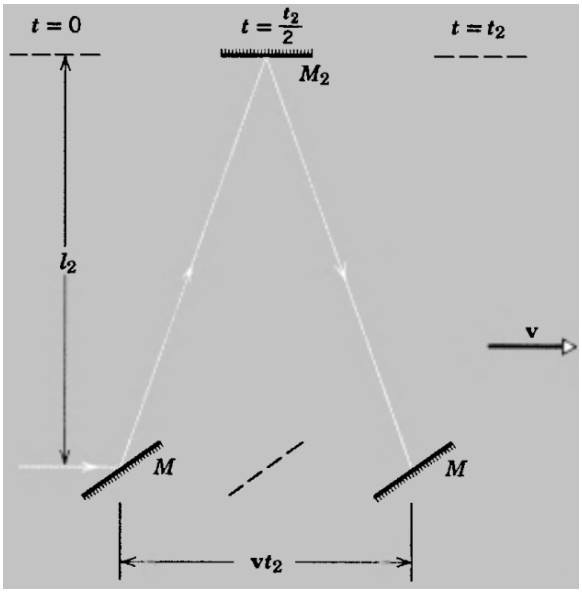
Then the returning beam 1 is partially reflected and the returning beam 2 is partially transmitted back by M to a telescope at where they interfere. The interference is constructive or destructive depending on the phase difference of the beams. The partially silvered mirror surface M is inclined at 45^o to the beam directions. If M_I and M_2 are very nearly (but not quite) at right angles, we shall observe a fringe system in the telescope as shown, consisting of nearly parallel lines.



Let us compute the phase difference between the beams 1 and 2. This difference can arise from two causes, the different path lengths traveled, l_1 and l_2, and the different speeds of travel with respect to the instrument because of the "ether wind" v. The second cause, for the moment, is the crucial one. The different speeds are much like the different cross-stream and up-and-down-stream speeds with respect to shore of a swimmer in a moving stream. The time for beam 1 to travel from M to M_1 and back is

$$t_1 = \frac{l_1}{c-v} + \frac{l_1}{c+v} = l_1\left(\frac{2c}{c^2-v^2}\right) = \frac{2l_1}{c}\left(\frac{1}{1-v^2/c^2}\right)$$

for the light, whose speed is c in the ether, has an upstream speed of $c - v$ with respect to the apparatus and a downstream speed of $c + v$. The path of beam 2, traveling from M to M_2 and back, is a cross-stream path through the ether, as shown below, enabling



the beam to return to the (advancing) mirror M. In the above figure, v is the velocity of the interferometer with respect to the ether. The transmit time is given by

$$2\left[l_2^2 + \left(\frac{vt_2}{2}\right)^2\right]^{1/2} = ct_2$$

This can be alternatively stated as,

$$t_2 = \frac{2l_2}{\sqrt{c^2 - v^2}} = \frac{2l_2}{c} \frac{1}{\sqrt{1 - v^2/c^2}}$$

The calculation of t_2 is made in the ether frame, that of t_1 in the frame of the apparatus. Since time is an absolute in classical physics, this is perfectly acceptable classically. The difference in transit times is

$$\Delta t = t_2 - t_1 = \frac{2}{c}\left[\frac{l_2}{\sqrt{1 - v^2/c^2}} - \frac{l_1}{1 - v^2/c^2}\right]$$

Suppose that the instrument is rotated through 90 degrees, thereby making l_1 the cross-stream length and l_2 the downstream length. If the corresponding times are now designated by primes, the same analysis as above gives the transit-time difference as

$$\Delta t' = t_2' - t_1' = \frac{2}{c}\left[\frac{l_2}{1 - v^2/c^2} - \frac{l_1}{\sqrt{1 - v^2/c^2}}\right]$$

Hence, the rotation changes the differences by

$$\Delta t' - \Delta t' = \frac{2}{c}\left[\frac{l_2 + l_1}{1 - v^2/c^2} - \frac{l_2 + l_1}{\sqrt{1 - v^2/c^2}}\right]$$

Using the binomial expansion and dropping terms higher than the second-order, we find

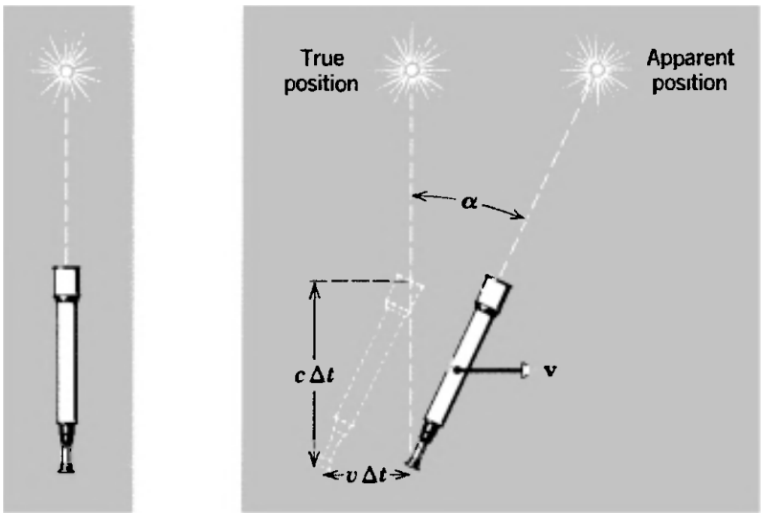
$$\Delta t' - \Delta t' = \frac{2}{c}(l_1 + l_2)\left[1 + \frac{v^2}{c^2} - 1 - \frac{1}{2}\frac{v^2}{c^2}\right] = \left(\frac{l_1 + l_2}{c}\right)\frac{v^2}{c^2}$$

Therefore, the rotation should cause a shift in the fringe pattern, since it changes the phase relationship between beams 1 and 2. If the optical path difference between the beams changes by one wavelength, for example, there will be a shift of one fringe across the cross- hairs of the viewing telescope. Observations were made day and night (as the earth spins about its axis) and during all seasons of the year (as the earth rotates about the sun), but the expected fringe shift was not observed. Indeed, the experimental conclusion was that there was no fringe shift at all. One way to interpret the null result of the Michelson-Morley experiment is to conclude simply that the measured speed of light is the same, that is, c, for all directions in every inertial system. Since this was such a blow to the ether hypothesis, several ideas were proposed to explain the null effect and retain the notion of ether.

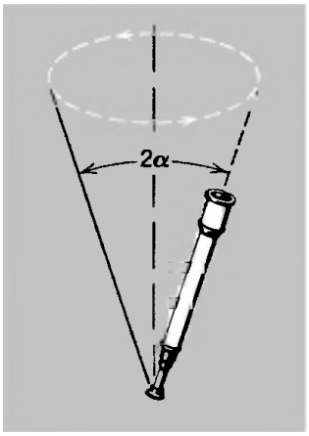
One such advanced idea was the ether-drag hypothesis. This hypothesis assumed that the ether frame was attached to all bodies of finite mass, that is, dragged along with such bodies. The assumption of such a local ether would automatically give a null result in the Michelson-Morley experiment. Its attraction lay in the fact that it did not require modification of classical mechanics or electromagnetism. However, there were two well-established effects which contradicted the ether-drag hypothesis one of which was stellar aberration which we shall consider now.

The aberration of light was first reported by Bradley in 1727. He observed that (with respect to astronomical coordinates fixed with respect to the earth) the stars appear to move in circles, the angular diameter of these circular orbits being about 41 seconds of arc. This can be understood as follows. Imagine that a star is directly overhead so that a telescope would have to be pointed straight up to see it if the earth were at rest in the ether. That is, the rays of light coming from the star would proceed straight down the telescope tube. Now, imagine that the earth is moving to the right through the ether with a speed v. In order for the rays to pass down the telescope tube without hitting its sides—that is, in order to see the star—we would have to tilt the telescope as shown below. The light proceeds straight down in the ether (as before) but, during the time Δt that the light travels the vertical distance $l = c\Delta t$ from the objective lens to the eyepiece, the telescope has moved a distance $v\Delta t$ to the right. The eyepiece, at the time the ray leaves the telescope, is on the same vertical line as the objective lens was at the time the ray entered the telescope. From the point of view of the telescope, the ray travels along the axis from objective lens to eyepiece. The angle of tilt of the telescope, α is given by

$$\tan\alpha = \frac{v\Delta t}{c\Delta t} = \frac{v}{c}$$



It was known that the earth goes around the sun at a speed of about 30 km/sec, so that with $c = 3 \times 10^5$ km/sec, we obtain an angle $\alpha = 20.5$ sec of arc. The earth's motion is nearly circular so that the direction of aberration reverses every six months, the telescope axis tracing out a cone of aberration during the year. The angular diameter of the cone, or of the observed circular path of the star, would then be $2\alpha = 41$ sec of arc, in excellent agreement with the observations. For stars not directly overhead, the analysis, although more involved, is similar and identical in principle.



The important thing we conclude from this agreement is that the ether is not dragged around with the earth. If it were, the ether would be at rest with respect to the earth, the telescope would not have to be tilted, and there would be no aberration at all. That is, the ether would be moving (with the earth) to the right with speed v, so there would be no need to correct for the earth's motion through the ether; the light ray would be swept along with the ether just as a wind carries a sound wave with it. Hence, if there is an ether, it is not dragged along by the earth but, instead, the earth moves freely through it. Therefore, we cannot explain the Michelson-Morley result by means of an ether-drag hypothesis.

6 Relativistic Kinematics

§6.1 Law of constancy of speed of light

Einstein proposed that speed of light is constant, regardless of the frame of reference due to the no time gap / fringe shift result of Michelson Morley experiment. Thus, if we denote by $f(v_1, v_2)$ - the velocity of v_1 with respect to v_2, then we need it to satisfy the following two properties, namely

(*i*) $f(v_1, v_2) = -f(v_2, v_1)$

(*ii*) $f(c, v) = c$

We know that classically $f(v_1, v_2) = v_1 - v_2$. However, this clearly fails the second property. Thus, we assume that $f(v_1, v_2) = g(v_1, v_2)(v_1 - v_2)$. We require $g(v_1, v_2) \to 1$ for small v_1/c and v_2/c along with $f(c, v) = c \implies c = g(c, v)(c - v)$.

$$g(c, v) = \frac{c}{c - v} = \frac{1}{1 - v/c} = g\left(\frac{v}{c}\right)$$

Moreover, since $f(c, -v) = c$, we also have that

$$g(c, -v) = \frac{1}{1 + v/c} = g\left(\frac{-v}{c}\right)$$

Hence, we can assume that

$$g(v_1, v_2) = g\left(\frac{v_1.v_2}{c^2}\right)$$

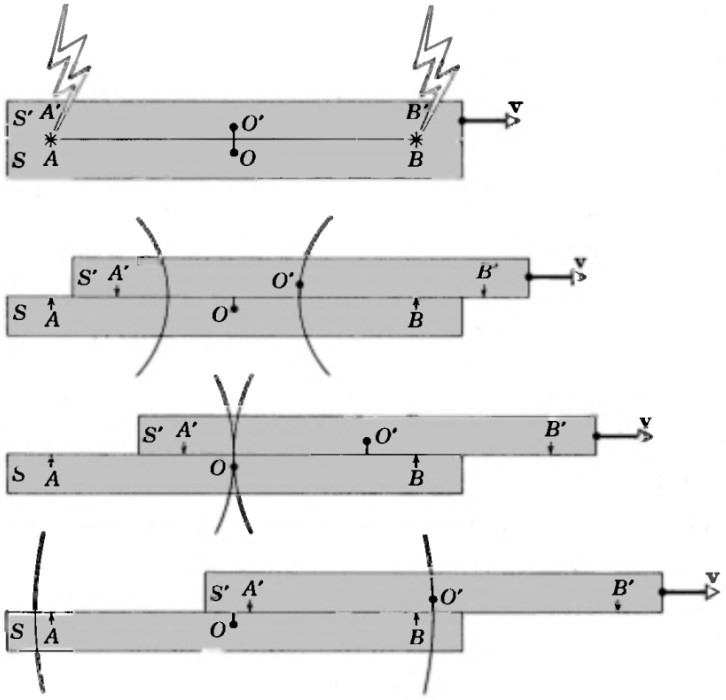
§6.2 The Relativity of Simultaneity

Events occurring at two different places in a frame for which we know the procedure for synchronizing clocks (To synchronize clocks, let the people be standing in a line at intervals of L length. At $t = 0$. observer 1 throws a light pulse towards the other observers. Observer 2 receives the signal when $t = L/c$ for observer 1. Observer 2 hence sets his clock to L/c when he receives the pulse. Observer 3 receives the pulse at $2L/c$ and sets his clock accordingly. This was we can synchronize the clocks. However, this can only be done when observers are in the same frame. Clocks cannot be synced across frames) must be called simultaneous when the clocks at the respective places record the same time for them. Suppose that one inertial observer does find that two separated events are simultaneous. Will these same events be measured as simultaneous by an observer on another inertial frame which is moving with speed v with respect to the first? (Remember, each observer uses an identical procedure to synchronize the clocks in his reference frame.) If not, simultaneity is not independent of the frame of reference used to describe events. Instead of being absolute, simultaneity would be a relative concept. Indeed, this is exactly what

we find to be true, in direct contradiction to the classical assumption.

To understand this, let us consider an example. Let there be two inertial reference frames S' and S having a relative velocity. Each frame has its own meter sticks and synchronized clocks. The observers note that two lightning bolts strike each, hitting and leaving permanent marks in the frames. Assume that afterwards, by measurements, each inertial observer finds that he was located exactly at the midpoint of the marks which were left on his reference frame. In the above figure (a) shows that these marks are left at A, B on the S-frame and at A' and B' on the S' frame, the observers being at O and O'. Since each observer knows he was at the midpoint of the mark left by these events, he will conclude that they were simultaneous if the light signals from them arrive simultaneously at his clock. If, on the other hand, one signal arrives before the other, he will conclude that one event preceded the other. Since each observer has a synchronized set of clocks, he can conclude either that the clocks at the marks read the same time when the marks were made (simultaneous case) or that they read different times (non-simultaneous case).

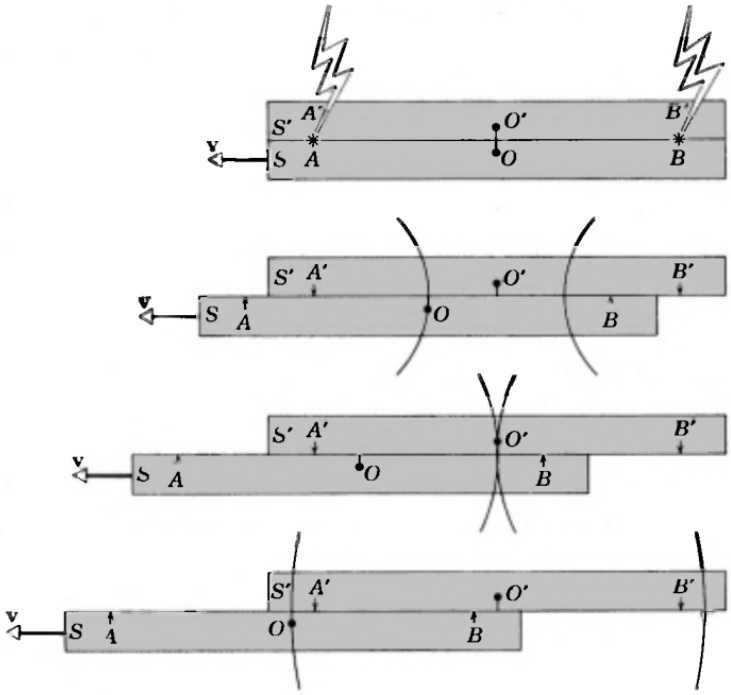
The below figure represents the point of view of the S-frame with the S'-frame moving to the right. A light wave leaves A, A' and B, B' in (a). Successive drawings correspond to the assumption that event AA' and event BB' are simultaneous in the S-frame. In (b) one wavefront reaches O'. In (c) both wave fronts reach O In (d) the other wavefront reaches O'.



Many different possibilities exist in principle as to what the measurements might show. Let us suppose, for the sake of argument, that the S-observer finds that the lightning bolts struck simultaneously. Will the S'-observer also find these events to be simultaneous ? In figures (b) to (d), we take the point of view of the S-observer and see the S'-frame moving, to the right. At the

instant the lightning struck at A and A', these two points coincide, and at the instant the lightning struck at B and B' those two points coincide. The S-observer found these two events to occur at the same instant, so that at that instant O and O' must coincide also for him. However, the light signals from the events take a finite time to reach O and during this time O' travels to the right as shown in figures (b) to (d). Hence, the signal from event BB' arrives at O'(Fig. b) before it gets to O (Fig. c), whereas the signal from event AA' arrives at O (Fig. c) before it gets to O' (Fig. d). Consistent with our starting assumption, the S-observer finds the events to be simultaneous (both signals arrive at O at the same instant). The S'-observer, however, finds that event BB' precedes event AA' in time; they are not simultaneous to him. Therefore, two separated events which are simultaneous with respect to one frame of reference are not necessarily simultaneous with respect to another frame.

Now we could have supposed, just as well, that the lightning bolts struck so that the S'-observer found them to be simultaneous. In that case the light signals reach O' simultaneously, rather than O. We show this in the below figure where now we take the point of view of S'. The S-frame moves to the left relative to the S'-observer. But, in this case, the signals do not reach O simultaneously ; the signal from event AA' reaches O before that from event BB'. Here the S'-observer finds the events to be simultaneous but the S-observer finds that event AA' precedes event BB'.



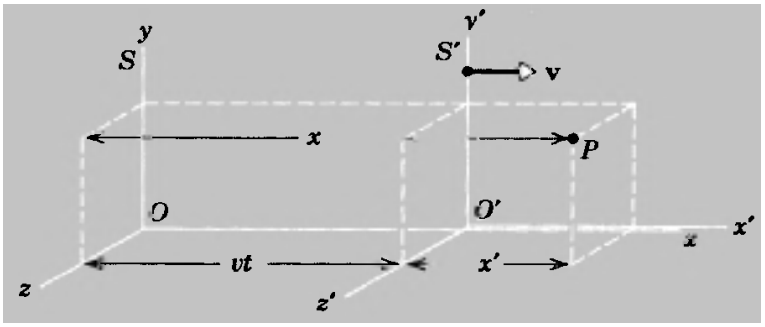
Hence, neither frame is preferred and the situation is perfectly reciprocal. Simultaneity is genuinely a relative concept, not an absolute one. Indeed, the two figures become indistinguishable if you turn one of them upside down. Neither observer can assert absolutely that he is at rest. Instead, each observer correctly states only that the other one is moving relative to him and

that the signals travel with finite speed c relative to him. It should be clear that if we had an infinitely fast signal, then simultaneity would be an absolute concept; for the frames would not move at all relative to one another in the (zero) time it would take the signal to reach the observers.

Note that in these arguments, we have shown that if one observer finds the events to be simultaneous, then the other one will find them not to be simultaneous Of course, it could also happen that neither observer finds the events to be simultaneous but then they would disagree either on the time order of the events or on the time interval elapsing between the events, or both.

§6.3 Derivation of Lorentz Transformation Equations

We have seen that the Galilean transformation equations must be replace with new ones consistent with the experiment. Here, we shall derive these new equations using the facts we have established. For this, we observe an event in one inertial frame S and characterize its location and time by specifying the coordinates x, y, z, t of the event. In a second-inertial frame S', the same event is recorded as the space-time coordinates x', y', z', t'. We now seek the functional relationships $x' = x'(x, y, z, t)$, $y' = y'(x, y, z, t)$, $z' = z'(x, y, z, t)$ and $t' = t'(x, y, z, t)$. That is, we want equations which relate one observer's space-time coordinates of an event with the other observer's space-time coordinate for the same event. We simplify the algebra by choosing the relative velocity of the S and S' frames to be along the common $x - x'$ axis and by keeping the corresponding planes parallel. This does not impose any fundamental restrictions on our results for space is isotropic - that is, has the same properties in all directions. At the instant, the origins O and O' coincide, we let the clocks there read $t = 0$ and $t' = 0$, respectively.



We shall use the fundamental postulates of relativity theory and in addition the homogeneity assumption (which can be paraphrased by saying that all points in space and time are equivalent) which means, for example, that the results of a measurement of length or time interval of a specific event should not depend on where or when the interval happens in our reference frame. As we shall explain subsequently, this assumption requires that transformation equations must be linear i.e., they involve only the first power in the variables. Hence, the most general form the

equations can take is

$$x' = a_{11}x + a_{12}y + a_{13}z + a_{14}t$$
$$y' = a_{21}x + a_{22}y + a_{23}z + a_{24}t$$
$$z' = a_{31}x + a_{32}y + a_{33}z + a_{34}t$$
$$t' = a_{41}x + a_{42}y + a_{43}z + a_{44}t$$

Here, the sub scripted coefficients are constants that we must determine to obtain the exact the transformation equations. Note that we have not excluded the possible dependence of space and time coordinates upon one another. If the equations were not linear, we would violate the homogeneity assumption. For examples, suppose that x' depended on the square of x as $x' = a_{11}x^2$. Then the distance between two points in the primed frame would be related to the location of these points in the unprimed frame by $x'_2 - x'_1 = a_{11}(x_2^2 - x_1^2)$. Suppose now that a rod of unit length in S had its end points at $x_2 = 2$ and $x_1 = 1$. then $x'_2 - x'_1 = 3a_{11}$. If instead the same rod happened to be located at $x_2 = 5$ and $x_1 = 4$, then we would obtain $x'_2 - x'_1 = 9a_{11}$. That is the measured length of the rod would depend on where it is in space. Likewise, we can reject any dependence on t that is not linear, for the time interval of an event should not depend on the numerical settings of the hands of the observer's clock. The relationships must then be linear in order to not give the choice of origin of our space-time coordinates (or some other point) a physical preference over all other points.

Now regarding these sixteen coefficients, it is expected that their value depends on the relative velocity v of the two inertial frames. For example if $v = 0$, then the two frames would coincide at all times and we expect $a_{11} = a_{22} = a_{33} = a_{44} = 1$, all other coefficients being zero. More generally, if v is small compared to c, the coefficients should lead to the (classical) Galilean transformation equations. We seek to find the coefficients for any value of v, that is as functions of v.

How then do we determine the values of these sixteen coefficients ? Basically, we use the postulates of relativity, namely (1) The Principle of Relativity - that no preferred inertial system exists, the laws of physics being the same in all inertial systems and (2) The Principle of the Constancy of the Speed of Light - that the speed of light in free space has the same value c in all inertial systems. Let us proceed.

The x-axis coincides continuously with the x'-axis. This will be so only if for $y = 0, z = 0$ (which characterizes points on the x-axis) it always follows that $y' = 0, z' = 0$ (which characterizes points on the x'-axis). Hence, the transformation formulas for y and z must be of the form $y' = a_{22}y + a_{23}z$ and $z' = a_{32}y + a_{33}z$. That is, the coefficients a_{21}, a_{24}, a_{31} and a_{34} must be zero. Likewise, the $x - y$ plane (which is characterized by $z = 0$) should transform over to the $x' - y'$ plane (which is characterized by $z' = 0$); similarly, for the $x - z$ and $x' - z'$ planes, $y = 0$ should give $y' = 0$. Hence, it follows that a_{23} and a_{32} are zero so that $y' = a_{22}y$ and $z' = a_{33}z$.

These remaining constant coefficients, a_{22} and a_{33}, can be evaluated using the relativity postulate. We illustrate for a_{22}. Suppose that we have a rod lying along the y-axis, measured by S to be of unit length. According to the S' observer, the rod's length will be a_{22}, (i.e., $y' = a_{22} \times 1$).

Now, suppose that the very same rod is brought to rest along the y' axis of the S'-frame. The primed observer must measure the same length (unity) for this rod when it is at rest in his frame as the unprimed observer measures when the rod is at rest with respect to him ; other- wise there would be an asymmetry in the frames. In this case, however, the S-observer would measure the rod's length to be $1/a_{22}$ (i.e., $y = (1/a_{22})y' = (1/a_{22}) \times 1$). Now, because of the reciprocal nature of these length measurements, the first postulate requires that these measurements be identical, for otherwise the frames would not be equivalent physically. Hence, we must have $a_{22} = l/a_{22}$ or $a_{22} = l$. The argument is identical in determining that $a_{33} = 1$ Therefore, our two middle transformation equations become $y' = y$ and $z = z'$. There remain transformation equations for x' and t', namely

$$x' = a_{11}x + a_{12}y + a_{13}z + a_{14}t$$

$$t' = a_{41}x + a_{42}y + a_{43}z + a_{44}t$$

Lets first look at the t' equation. For reasons of symmetry, we assume that t' does not depend on y and z. Otherwise, clocks placed symmetrically in the $y - z$ plane (such as at $+y, -y$ or$+z, -z$) about the x-axis would appear to disagree as observed from S', which would contradict the isotropy of space. Hence, $a_{42} = a_{43} = 0$. As for the x'-equation, we know that a point having $x' = 0$ appears to move in the direction of the positive x-axis with speed v, so that the statement $x' = 0$ must be identical to the statement $x = vt$. Therefore, we expect $x' = a_{11}(x - vt)$ to be the correct transformation equation. (That is, $x = vt$ always gives $x' = 0$ in this equation.) Hence, $x' = a_{11}x - a_{11}vt = a_{11}x + a_{14}t$. This gives us $a_{14} = -a_{11}$, and our four equations have now been reduced to

$$x' = a_{11}(x - vt)$$
$$y' = y$$
$$z' = z$$
$$t' = a_{41}x + a_{44}t$$

There remains the task of determining the three coefficients a_{11}, a_{41}, and a_{44}. To do this, we use the principle of the constancy of the velocity of light. Let us assume that at the time $t = 0$ a spherical electromagnetic wave leaves the origin of S, which coincides with the origin of S' at that moment. The wave propagates with a speed c in all directions in each inertial frame. Its progress, then, is described by the equation of sphere whose radius expands with time at a rate c in terms of either the primed or unprimed set of coordinates. That is,

$$x^2 + y^2 + z^2 = c^2t^2$$
$$\text{or } x'^2 + y'^2 + z'^2 = c^2t'^2$$

Rewriting the latter equation, with the help of transformation equations, we see that

$$a_{11}^2(x - vt)^2 + y^2 + z^2 = c^2(a_{41}x + a_{44}t)^2$$

$$\implies (a_{11}^2 - c^2a_{41}^2)x^2 + y^2 + z^2 - 2(va_{11}^2 + c^2a_{41}a_{44})xt = (c^2a_{44}^2 - v2a_{11}^2)t^2$$

Now, since this expression and $x^2 + y^2 + z^2 = c^2t^2$ represent the same thing, for them to agree we need that,

$$\begin{aligned} c^2a_{44}^2 - v^2a_{11}^2 &= c^2 \\ a_{11}^2 - c^2a_{41}^2 &= 1 \\ va_{11}^2 + c^2a_{41}a_{44} &= 0 \end{aligned}$$

Here we have three equations in three unknowns, whose solution, we can verify by substitution into the three equations above, is

$$\begin{aligned} a_{44} &= 1/\sqrt{1 - v^2/c^2} \\ a_{11} &= 1/\sqrt{1 - v^2/c^2} \\ a_{41} &= -(v/c^2)/\sqrt{1 - v^2/c^2} \end{aligned}$$

Substitution finally yields the new sought after transformation equations namely,

$$\begin{aligned} x' &= \frac{x - vt}{\sqrt{1 - v^2/c^2}} \\ y' &= y \\ z' &= z \\ t' &= \frac{t - (v/c^2)x}{\sqrt{1 - v^2/c^2}} \end{aligned}$$

These are the so called Lorentz transformation equations. We see that if we were to exchange our frames of reference in other words, consider the given space-time coordinates of the event to be those observed in S' rather than in S, the only change allowed by the relativity principle is the physical one of a change in relative velocity from v to $-v$. That is, from S' the S-frame moves to the left whereas from S the S'-frame moves to the right. When we solve the above equations for x, y, z and t in terms of the primed coordinates, we obtain

$$\begin{aligned} x &= \frac{x' + vt'}{\sqrt{1 - v^2/c^2}} \\ y &= y' \\ z &= z' \\ t &= \frac{t' + (v/c^2)x}{\sqrt{1 - v^2/c^2}} \end{aligned}$$

which are identical in form with the earlier equations except that, as required, v changes to $-v$. We also see that that for speeds small compared to c, that is, for $v/c << 1$, the Lorentz equations reduce to (approximately) the correct Galilean transformation equations. This is the case, for when $v/c << 1$, the equations become

$$\begin{aligned} x' &= x - vt \\ y' &= y \\ z' &= z \\ t' &= t \end{aligned}$$

In the time equation, $t' = (t - vx/c^2)/\sqrt{1 - v^2/c^2}$, consider the motion of the origin O', for example given by $x = vt$, then we have $t' = (t - v^2t/c^2)/\sqrt{1 - v^2/c^2} =$

§6.4 Consequences of Lorentz Transformation

First consequence is this : ***A body's length is measured to be greatest when it is at rest relative to the observer. When it moves with a velocity*** v ***relative to the observer its measured length is contracted in the direction of its motion by the factor*** $\sqrt{1 - v^2/c^2}$***, whereas its dimensions perpendicular to the direction of motion are unaffected.*** To prove the italicized statement, imagine a rod lying at rest along the x'-axis of the S'-frame. Its end points are measured to be at x'_2 and x'_1, so that its rest length is $x'_2 - x'_1$. What is the rod's length as measured by the S-frame observer for whom the rod moves with the relative speed v ? For convenience, we shall let $v/c = \beta$. From the first Lorentz equation we have

$$x'_2 = \frac{x_2 - vt_2}{\sqrt{1-\beta^2}} \, , \, x'_1 = \frac{x_1 - vt_1}{\sqrt{1-\beta^2}} \implies x'_2 - x'_1 = \frac{(x_2 - x_1) - v(t_2 - t_1)}{\sqrt{1-\beta^2}}$$

Now the length of the rod in the S-frame is simply the distance between the end points, x_2 and x_1, of the moving rod measured at the same instant in that frame. Hence, with $t_2 = t_l$, we obtain

$$x'_2 - x'_1 = \frac{x_2 - x_1}{\sqrt{1-\beta^2}} \implies x_2 - x_1 = (x'_2 - x'_1)\sqrt{1-\beta^2}$$

so that the measured length of the moving rod, $x_2^- x_1$, is contracted by the factory $\sqrt{1-\beta^2}$ from its rest length, $x'_2 - x'_1$. As for the dimensions of the rod along y and z, perpendicular to the relative motion, it follows at once from the transformation equations $y' = y$ and $z' = z$ that these are measured to be the same by both observers. A second consequence is this : ***A clock is measured to go at its fastest rate when it is at rest relative to the observer. When it moves with a velocity*** v ***relative to the observer, its rate is measured to have slowed down by a factor*** $\sqrt{1 - v^2/c^2}$**.** To prove these italicized statements, consider a clock to be at rest at the position x' in the S'-frame. It may simplify matters to picture the hand of this clock going around and to let unit time be the time it takes the hand of the clock to go around once. Hence, the events we observe (the two successive coincidences of the hand of the clock with a given marker on the face of the clock) span the time interval t' to $t' + 1$ in the primed coordinates. The S-frame observer records these events as occurring at times

$$t_1 = \frac{t' + (v/c^2)x'}{\sqrt{1 - v^2/c^2}} \, , \, t_2 = \frac{(t' + 1) + (v/c^2)x'}{\sqrt{1 - v^2/c^2}}$$

The clock in the S'-frame is at a fixed position x', but the time t_1 and t_2 are read from two different clocks in the S-frame, namely the stationary S-clock that happens to be coincident with the moving clock at the beginning of the interval, and the stationary S-clock coincident with the moving clock at the end of the interval. These clocks are synchronized, however, so that the time interval they record for the event is simply

$$t_2 - t_1 = \frac{1}{\sqrt{1-\beta^2}}$$

Clearly, if, instead of unit time, the S'-clock recorded a time interval $t'_2 - t'_1$, the S-clock would have recorded the corresponding interval

$$t_2 - t_1 = \frac{t'_2 - t'_1}{\sqrt{1-\beta^2}}$$

Hence, unit time measured on the S'-clock is recorded as a longer time on the S-clocks. From the point of view of observer S, the moving S'-clock appears slowed down, that is, it appears to run at a rate which is slow by the factor $\sqrt{1-\beta^2}$. This result applies to all S'-clocks observed from S, for the location x' in our proof was arbitrary. It is common in relativity to speak of the frame in which the observed body is at rest as the ***proper frame***. The length of a rod in such a frame is then called the proper length. Likewise, the proper time interval is the time interval recorded by a clock attached to the observed body. The proper time interval can be thought of equivalently as the time interval between two events occurring at the same place in the S'-frame or the time interval measured by a single clock at one place. A non-proper (or improper) time interval would be a time interval measured by two different clocks at two different places.

A third consequence of the Lorentz transformation equations is this : ***Although clocks in a moving frame all appear to go at the same slow rate when observed from a stationary frame with respect to which the clocks move, the moving clocks appear to differ from one another in their readings by a phase constant which depends on their location, that is, they appear to be unsynchronized.*** This becomes evident at once from the transformation equation

$$t = \frac{t' + (v/c^2)x}{\sqrt{1 - v^2/c^2}}$$

For consider an instant of time in the S-frame, that is, a given value of t. Then, to satisfy this equation, $t' + (v/c^2)x'$ must have a definite fixed value. This means the greater is x' (i.e., the farther away an S'-clock is stationed on the x'-axis) the smaller is t' (i.e., the further behind in time its reading appears to be). Hence, the moving clocks appear to be out of phase, or synchronization, with one another. We shall see that this is just another manifestation of the fact that two events that occur simultaneously in the S-frame are not, in general, measured to be simultaneous in the S'-frame, and vice versa. ***All the results of this section are reciprocal. That is, no matter which frame we take as the proper frame, the observer in the other frame measures a contracted length and dilated (expanded) time interval and finds the moving clocks to be out of synchronization.*** This led to the development of several paradoxes such as the Twin Paradox.

As an aside, we shall see that ***length contraction is a necessary consequence of time dilation***. Imagine, for example, that two different inertial observers, one sitting on a train moving through a station with uniform velocity v and the other at rest in the station, want to measure the length of the station's platform. The ground observer measures the length to be L and claims that the passenger covered this distance in a time L/v. This time, Δt, is a non-proper time, for the events observed (passenger passes back end of platform, passenger passes front end of platform) occur at two different places in the ground (S) frame and are timed by two different clocks. The

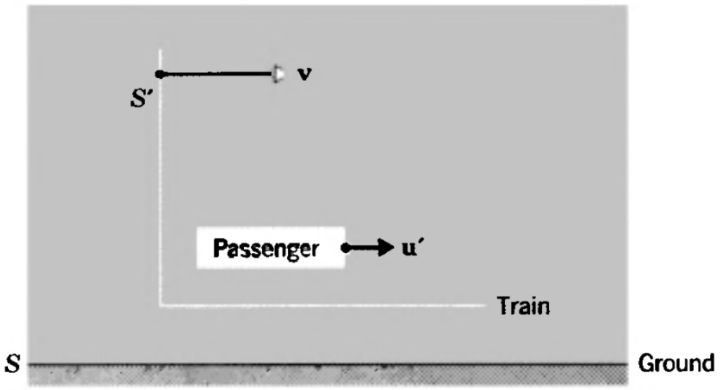
passenger, however, observes the platform approach and recede and finds the two events to occur at the same place in his (S') frame. That is, his clock (wrist watch, say) is located at each event as it occurs. He measures a proper-time interval $\Delta t'$, which, as we have just seen, is related to Δt by $\Delta t' = \Delta t\sqrt{1 - v^2/c^2}$. However, $\Delta t = L/v$ so that $\Delta t' = L\sqrt{1 - v^2/c^2}/v$. The passenger claims that the platform moves with the same speed v relative to him so that he would measure the distance from back to front of the platform at $v\Delta t'$. Hence, the length of the platform to him is $L' = v\Delta t' = L\sqrt{1 - v^2/c^2}$. This is the length-contraction result, namely, that a body of rest length L is measured to have a length $L\sqrt{1 - v^2/c^2}$ parallel to the relative motion in a frame in which the body moves with speed v.

§6.5 The Relativistic Addition of Velocities

In classical physics, if we have a train moving with a velocity $\vec{v}$ with respect to ground and a passenger on the train moves with a velocity $\vec{u'}$ with respect to the train, then the passenger's velocity relative to the ground $\vec{u}$ is just the vector sum of the two velocities, that is, $u = \vec{u'} + v$. This is simply the classical, or Galilean, velocity addition theorem. How do velocities add in special relativity theory?

Consider, for the moment, the special case wherein all velocities are along the common $x - x'$ direction of two inertial frames S and S'. Let S be the ground frame and S' the frame of the train, whose speed relative to the ground is v. The passenger's speed in the S'-frame is u', and his position on the train as time goes on can be described by $x' = u't'$. What is the speed of the passenger observed from the ground? Using the Lorentz transformation equations, we have

$$x' = \frac{x - vt}{\sqrt{1 - v^2/c^2}} = u't' \ , \ t' = \frac{t - (v/c^2)x}{\sqrt{1 - v^2/c^2}}$$



Combining these yields,

$$x - vt = u'\left(t - \frac{v}{c^2}x\right) \implies x = \left(\frac{u' + v}{1 + u'v/c^2}\right)t$$

If we call the passenger's speed relative to ground u, then his ground location as time goes on is given by $x = ut$. Comparing this with the last equation, we obtain

$$u = \frac{u' + v}{1 + u'v/c^2}$$

This is the relativistic, or Einstein velocity addition theorem. If u' and v are very small compared to c, the the formula reduces to the classical result, $u = u' + v$, for then the second term in the denominator is negligible compared to one. On the other hand, if $u' = c$, it always follows that $u = c$ no matter what the value of v. Of course, $u' = c$ means that our "passenger" is a light pulse and we know that an assumption used to derive the transformation formulas was exactly this result; that is, that all observers measure the same speed c for light. Formally, we get, with $u' = c$

$$u = \frac{u' + v}{1 + u'v/c^2} = \frac{c + v}{c(c + v)}c^2 = c$$

Hence, any velocity (less than c) relativistically added to c gives a resultant c. In this sense, c plays the same role in relativity that an infinite velocity plays in the classical case. Thus far, we have considered only the transformation of velocities parallel to the direction of relative motion of the two frames of reference (the $x^{-}x'$ direction). To signify this, we should put x subscripts on u and u', obtaining

$$u_x = \frac{u'_x + v}{1 + u'_x(v/c^2)}$$

For velocities that are perpendicular to the direction of relative motion, the result is more involved. Initially, we saw that experiment forced us to the conclusion that the Galilean transformations had to be replaced and the basic laws of mechanics, which were consistent with those transformations, needed to be modified. Then, we obtained the new transformation equations, the Lorentz transformations, and examined their implications for kinematical phenomena. Now we must consider dynamic phenomena and find how to modify the laws of classical mechanics so that the new mechanics is consistent with relativity.

Basically, classical Newtonian mechanics is inconsistent with relativity because its laws are invariant under a Galilean transformation and not under a Lorentz transformation. This formal result is plausible, as well, from other considerations. For example, in Newtonian mechanics a force can accelerate a particle to indefinite speeds, whereas in relativity the limiting speed is c. Another difficulty with classical mechanics is that it permits action-at-a-distance forces while requiring action and reaction forces to be equal. Such equality of action and reaction has no meaning in relativity except for contact forces, because the simultaneity of separated events is relative.

Example : *In classical mechanics, we may say that two bodies on a frictionless surface connected by a light stretched spring arc subject to equal but opposite forces at the same instant. In relativity, where simultaneity of separated events is a relative concept, "the same instant" differs from one inertial observer to another. Unless the action and reaction are contact forces (so that the interacting particles are not separated) we cannot give meaning to them independent of the*

frame of reference used.

In seeking a new law of motion that is consistent with relativity, we therefore exclude "action-at-a-distance" forces. However, we can include collision phenomena (contact forces), for example, which doesn't involve the action-at-a-distance concept. In either case, when we obtain a law of motion that is invariant under a Lorentz transformation, we must also insure that it reduces to the Newtonian form as $v/c \to 0$ since, in the domain where $v/c << 1$, Newton's laws are consistent with experiment. Thus, the relativistic law of motion will be a generalization of the classical one.

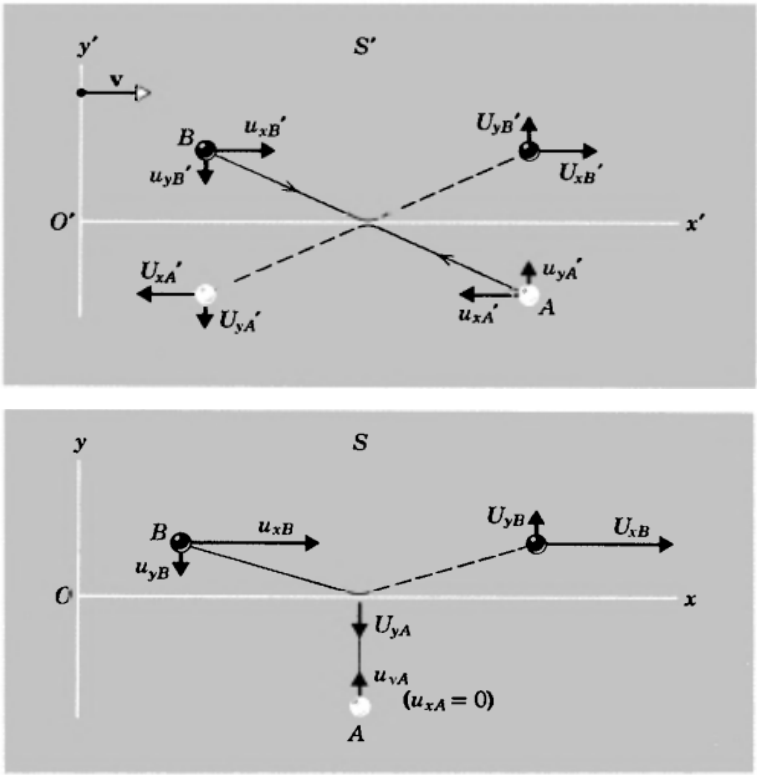
We shall proceed by studying collisions first. Here we assume that the interaction between particles takes place only during an infinitesimally short time interval in which the particles have negligible separation (i.e.,the range of forces is short compared to the dimensions of the system). During the collision the particles are accelerated, but before and after the interaction there is no acceleration. The laws of conservation of momentum and energy are valid classically during this interaction. If we require that these conservation laws also be valid relativistically (i.e.,invariant under a Lorentz transformation) and hence that they be general laws of physics, we must modify them from the classical form in such a way that they also reduce to the classical form as $v/c \to 0$. In this way, we shall obtain the relativistic law of motion.

7 Relativistic Dynamics

§7.1 The Need to Redefine Momentum

The first thing we wish to show is that if we want to find a quantity like momentum (for which there is a conservation law in classical physics) that is also subject to a conservation law in relativity, then we cannot use the same expression for momentum as the classical one. We must, instead, redefine momentum in order that a law of conservation of momentum in collisions be invariant under a Lorentz transformation.

Let us first analyze an elastic collision between two identical bodies as seen by different inertial observers, S and S', according to Newtonian mechanics. We choose the collision (as shown in figure below) to be highly symmetrical in S' : the bodies, say A and B, have initial velocities that are equal in magnitude but opposite in direction, the total momentum being zero. That is, $\mathbf{u}_{yA}{}' = -\mathbf{u}_{yB}{}'$ and $\mathbf{u}_{xA}{}' = -\mathbf{u}_{xB}{}'$. Since the collision is elastic, the final velocities have the same magnitude as the initial velocities, the total momentum after collision remaining zero. We have $\mathbf{u}_{yA}{}' = -\mathbf{U}_{yA}{}' = \mathbf{U}_{yB}{}' = -\mathbf{u}_{yB}{}'$ and $\mathbf{u}_{xA}{}' = \mathbf{U}_{xA}{}' = \mathbf{U}_{xB}{}' = -\mathbf{u}_{xB}{}'$. That is, observer S' notes that the y'-components of velocity for the bodies simply reverse their signs during the collision, the x'-components remaining unchanged.



reverse their signs during the collision, the x'-components remaining unchanged.

As seen by observer S, the reference frame S' is moving to the right with a speed v. We deliberately choose

$$\mathbf{v} = \mathbf{u}_{xB}{}' = -\mathbf{u}_{xA}{}'$$

so that the body A has no x-component of motion in frame S (see Fig. 3-1b). The y-components of velocity should be unaffected by the transformation, according to Newtonian mechanics, and momentum should still be conserved in the collision as viewed by S. That is, $\mathbf{u}_{yA} = \mathbf{u}_{yA}{}'$, $\mathbf{u}_{yB} = \mathbf{u}_{yB}{}', \mathbf{u}_{yA} = -\mathbf{U}_{yA}$ and $\mathbf{u}_{yB} = -\mathbf{U}_{yB}$. The momentum lost by body $A, 2mu_{yA}$, equals that gained by body $B, 2mu_{yB}$, so that in magnitude

$$2mu_{yA} = 2mu_{yB}$$

and, because the bodies have identical mass m, we conclude that

$$u_{yA} = u_{yB}$$

These are the Newtonian results. Now, let us see whether these results are consistent with the Lorentz transformations. They are not, for they contradict the relativistic velocity transformations. If we use the velocity transformation equations we find that relativity requires, for body B,

$$u_{yB}{}' = \frac{u_{yB}\sqrt{1-\beta^2}}{1 - u_{xB}v/c^2}$$

whereas for body A, for which $u_{xA} = 0$,

$$u_{yA}{}' = u_{yA}\sqrt{1-\beta^2}$$

Hence, the y-components of velocity are affected by the relativistic transformations. For one thing, they do not have the same values in one frame as in the other, but, more important, if they are equal to one another in magnitude in one frame, they are not necessarily equal to one another in the other frame. In fact, assuming as before that $u_{yB} = u_{yA}$, we find by combining and rearranging the above equations, that

$$u_{yA} = \frac{u_{yB}}{1 - u_{xB}v/c^2}$$

in contradiction to Newton's result. Hence, changes in the y-component velocities have different magnitudes in one frame than in the other during the collision. The result is that, if we compute momentum according to the classical formulas $\mathbf{p} = m\mathbf{u}$ and $\mathbf{p}' = m\mathbf{u}'$ then when momentum is conserved in a collision in one frame it is not conserved in the other frame.

This result contradicts the basic postulate of special relativity that the laws of physics are the same in all inertial systems. If the conservation of momentum in collisions is to be a law of physics, then the classical definition of momentum cannot be correct in general. We notice that the disagreement between the two equations becomes trivial when $u_{xB} << c$ and $v << c$, so that

it is at high speeds that the Newtonian formulation of the momentum conservation law breaks down. We need a generalization of the definition of momentum, therefore, that reduces to the classical result at low speeds.

In the next section, we shall show that it is possible to preserve the form of the classical definition of the momentum of a particle, $\mathbf{p} = m\mathbf{u}$, where $\mathbf{p}$ is the momentum, m the mass, and $\mathbf{u}$ the velocity of a particle, and also to preserve the classical law of the conservation of momentum of a system of interacting particles, providing that we modify the classical concept of mass. We need to let the mass of a particle be a function of its speed u, that is, $m = m_0/\sqrt{1 - u^2/c^2}$ where m_0 is the classical mass and m is the relativistic mass of the particle. Clearly, as u/c tends to zero, m tends to m_0. The relativistic momentum then becomes $\mathbf{p} = m\mathbf{u} = m_0\mathbf{u}/\sqrt{1-\beta^2}$ and reduces to the classical expression $\mathbf{p} = m_0\mathbf{u}$ as $\beta \to 0$. Let us now deduce these results.

§7.2 Relativistic Momentum

In the equation based on momentum conservation, we assumed that the mass m was the same for each body, and, in this way, we were led to the (incorrect) result that the y-component velocities had equal magnitude. True, the bodies were identical when placed side by side at rest. However, since the measured length of a rod and the measured rate of a clock are affected by the motion of the rod or the clock relative to the observer, it may be that the measured mass of a body also depends on its motion with respect to the observer. In that case the form of the Newtonian momentum still could be correct so that, for example, we could rewrite the earlier equation as

$$2m_A u_{yA} = 2m_B u_{yB}$$

The masses are now labelled as m_A and m_B, however, to suggest that they may have different values. Bodies A and B travel at different speeds in the S-frame and, if we accept the relativistic result for the speeds, we obtain

$$m_B = m_A \frac{u_{yA}}{u_{yB}} = \frac{m_A}{1 - u_{xB}v/c^2}$$

Hence, the relativistic masses, m_A and m_B, are not equal if the relativistic conservation of momentum law is to have the same form as the Newtonian law. It remains to find how the relativistic mass must vary with the speed. We can simplify the equation by eliminating v. Recall that $v = u_{xB}'$ and that u_{xB}' is related to u_{xB} by the Lorentz velocity transformation

$$u_{xB}(= v) = \frac{u_{xB} - v}{1 - u_{xB}v/c^2}$$

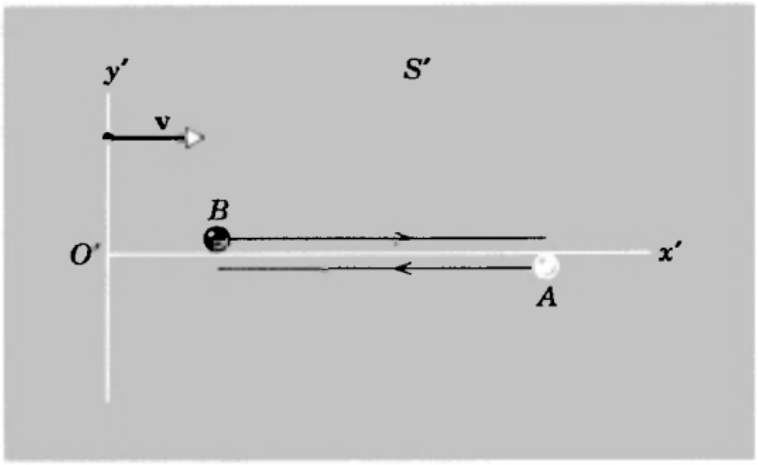
Solving for v, we get

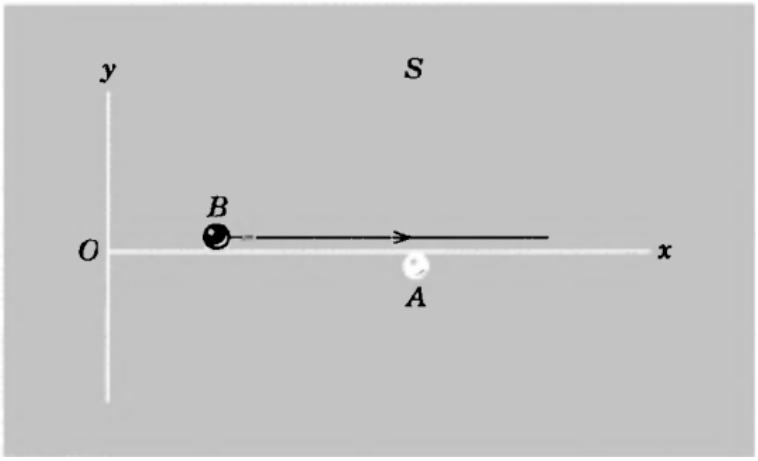
$$v = \frac{c^2}{u_{xB}}(1 - \sqrt{1 - (u_{xB}/c^2)})$$

Substituting this expression for v in m_A, we get

$$m_A = \frac{m_B}{\sqrt{1 - (u_{xB}/c^2)}}$$

We can find how the relativistic mass of either particle varies with the speed in a simple manner by considering a special case of the collision in which the $y - y'$ velocity components are made to approach zero. Then, the particles' speeds will be identical to the magnitude of their respective x-component velocities. This is illustrated in the below figures. Observer S' simply sees two bodies moving past each other making a grazing collision; observer S sees body A at rest and body B moving past it, at a speed u_{xB}, again making a grazing collision. Our derived equation must apply to this grazing collision as well because we put no restriction on $u_y{}'$ while deriving it.





Since body A is at rest in S its mass m_A must be the ordinary Newtonian mass which we now call the rest mass and denote by m_0. This is the same as the mass of body B when body B is at rest, the two bodies being identical. However, in S, body B is moving with a speed u_{xB}, which we can simply call u; its mass m_B, which we can call the relativistic mass and denote by m, will not be m_0. From our equation, we obtain

$$m = \frac{m_0}{\sqrt{1 - u^2/c^2}}$$

which tells us how the relativistic mass m of a body moving at a speed u varies with u. We see at once that when $u = 0$ the body then being at rest, we obtain $m = m_0$, the rest mass. More generally, as $u/c \to 0$, we find $m \to m_0$, which is the Newtonian limit of the more general expression for the relativistic mass m.

Hence, if we want to preserve the form of the classical momentum conservation law while requiring that the law be relativistically invariant, we must define the mass of a moving body by the above equation. That is, momentum still has the form $m\mathbf{u}$, but mass is defined as $m = m_0/\sqrt{1 - u^2/c^2}$. Note that u is the speed of the body relative to S, which we can regard as the laboratory frame, and that u has no connection necessarily with changing reference frames. By accepting this as our definition of the mass of a moving body, we implicitly assume that the mass of a body does not depend on its acceleration relative to the reference frame, although it does depend on its speed. Mass remains a scalar quantity in the sense that its value is independent of the direction of the velocity of the body. The rest mass m_0 is often called the proper mass, for it is the mass of the body measured, like proper length and proper time, in the inertial frame in which the body is at rest.

We have presented above a derivation of an expression for relativistic momentum which obviously centers around a very special case. For example, the velocity of the particle (B) is parallel to the relative $S - S'$ velocity and the derivation depended only upon invoking conservation of momentum in the y-direction. Such a derivation enables us to make an educated guess as to what the general result may be. We have avoided rather involved general derivations which, however, lead to exactly the same results. When the general case is done, u becomes the absolute value of the velocity of the particle; that is, $u^2 = u_x^2 + u_y^2 + u_z^2$.

To complete our particular deduction, we need to carry our argument two steps further. First, using the expression for momentum which we have tentatively derived, we can demonstrate explicitly that if the momentum of a system of interacting particles is conserved in one inertial frame S, then (using the Lorentz transformation) it is conserved in any other inertial frame S'. In fact, it turns out that this form of a momentum is the only one that does have this property. Second, this momentum conservation law is an experimental fact; that is, experiment proves this relativistic law to be true. Not only have we found a definition of momentum that conserves this quantity in the theory, but the theory is in harmony with physical experiment.

Hence, to conclude, in order to make the conservation of momentum in collisions a law that is experimentally valid in all reference frames, we must define momentum, not as $m_0\mathbf{u}$, but as

$$\mathbf{p} = \frac{m_0\mathbf{u}}{\sqrt{1 - u^2/c^2}}$$

Note that the magnitude u of the total velocity appears in the denominator when the equation is written in component form.

§7.3 The Relativistic Force Law and the Dynamics of a Single Particle

Newton's second law must now be generalised to

$$\mathbf{F} = \frac{d}{dt}(\mathbf{p}) = \frac{d}{dt}\left(\frac{m_0\mathbf{u}}{\sqrt{1-u^2/c^2}}\right)$$

in relativistic mechanics. When the law is written in this form we can immediately deduce the law of the conservation of relativistic momentum from it; when $\mathbf{F}$ is zero, $\mathrm{p} = m_0\mathbf{u}/\sqrt{1-u^2/c^2}$ must be a constant. In the absence of external forces, the momentum is conserved. Furthermore, when $\mathbf{F}$ as defined above is not zero, we can easily derive the result that if, for a system of interacting particles, the total relativistic momentum changes by an amount $\Delta\mathbf{P}$, then this change is equal to the total impulse $\int \mathbf{F}dt$ given to the system. Hence, the force defined by the above equation has the general properties we seek. Notice that this new form of the law, is not equivalent to writing $F = ma = (m_0/\sqrt{1-u^2/c^2})(d\mathbf{u}/dt)$, in which we simply multiply the acceleration by the relativistic mass.

In Newtonian mechanics we defined the kinetic energy, K, of a particle to be equal to the work done by an external force in increasing the speed of the particle from zero to some value u. That is,

$$K = \int_{u=0}^{u=u} \mathbf{F}.d\mathbf{l}$$

where $\mathbf{F}\cdot d\mathbf{l}$ is the work done by the force $\mathbf{F}$ in displacing the particle through $d\mathbf{l}$ For simplicity, we can limit the motion to one dimension, say $x$the three-dimensional case being an easy extension. Then, classically,

$$K = \int_{u=0}^{u=u} F dx = \int m_0\left(\frac{du}{dt}\right)dx = \int m_0 du\frac{dx}{dt} = m_0\int_0^u u du = \frac{1}{2}m_0u^2.$$

Here we write the particle mass as m_0 to emphasize that, in Newtonian mechanics, we do not regard the mass as varying with the speed, and we take the force to bc $m_0a = m_0(du/dt)$.

In relativistic mechanics, it proves useful to use a corresponding definition for kinetic energy in which, however, we use the relativistic equation of motion, rather than the Newtonian one. Then, relativistically,

$$K = \int_{u=0}^{u=u} F dx = \int \frac{d}{dt}(mu)\,dx = \int d(mu)\frac{dx}{dt}$$
$$= \int (m\,du + u\,dm)\,u = \int_{y=0}^{u=u} (mu\,du + u^2\,dm)$$

in which both m and u are variables. These quantities are related, furthermore, as $,m = m_0/\sqrt{1-u^2/c^2}$, which we can rewrite as

$$m^2c^2 - m^2u^2 = {m_0}^2c^2.$$

Taking differentials in this equation yields

$$2mc^2dm - m^2 2u\,du - u^2 2m\,dm = 0$$

which, on division by $2m$, can be written also as

$$mudu + u^2dm = c^2dm$$

The left side of this equation is exactly the integrand obtained above. Hence, we can write the relativistic expression for the kinetic energy of a particle as

$$K = \int_{u=0}^{u=u} c^2\,dm = e^2 \int_{m=m_0}^{m=m} dm\ = mc^2 - m_0c^2$$

Substituting the expression for mass, we obtain

$$K = m_0c^2\left[\frac{1}{\sqrt{1-u^2/c^2}} - 1\right]$$

The relativistic expression for K must reduce to the classical result, $1/2m_0u^2$, when $u/c << 1$. Let us check this from, the binomial theorem expansion in (u/c),

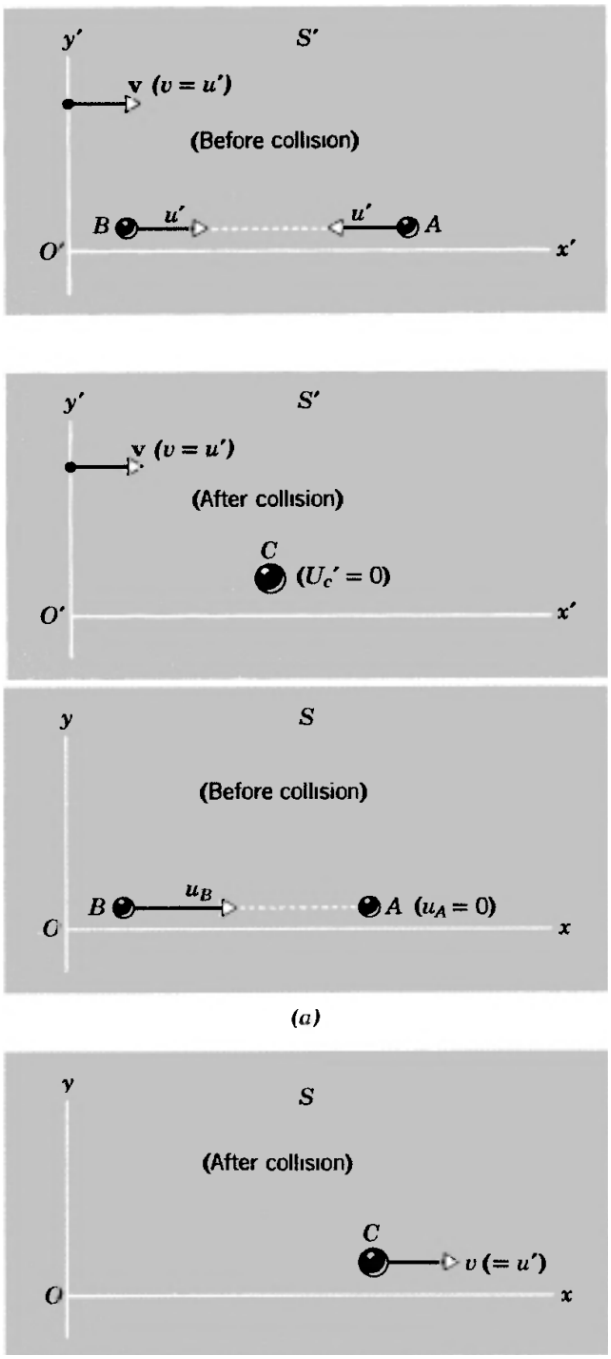
$$\begin{aligned} K &= m_0c^2[(1/\sqrt{1-u^2/c^2}) - 1] \\ &= m_0c^2\left[\left(1-\frac{u^2}{c^2}\right)^{-1/2} - 1\right] \\ &= m_0c^2\left[1 + \frac{1}{2}\left(\frac{u}{c}\right)^2 + \frac{3}{8}\left(\frac{u}{c}\right)^4 + \ldots - 1\right] \\ &= \frac{1}{2}m_0u^2, \end{aligned}$$

in which we take only the first two terms in the expansion as significant when $u/c << 1$, thereby confirming the Newtonian limit of the relativistic result. Also, if we take $mc^2 = E$, where E is called the total energy of the particle, have

$$E = mc^2 = \frac{m_0c^2}{\sqrt{1-u^2/c^2}}$$

§7.4 The Equivalence of Mass and Energy

In the first section, we examined an elastic collision, that is, a collision in which the kinetic energy of the bodies remained constant. Now let us consider an inelastic collision. In particular, consider two identical bodies of rest mass m_0, each with kinetic energy K as seen by a particular observer S', which collide and stick together forming a single body of rest mass M_0. The situation before and after the collision in the S'-frame is shown in the below figure : here, before collision, bodies A and B each have a speed u', with velocities oppositely directed and along the x'-axis; the combined body C, formed by the collision, is at rest in S', as required by conservation of momentum. In another reference frame S, moving with respect to S' with a speed $v(= u')$ to the left along the common $x - x'$ axis, the combined body C will have a velocity of magnitude u



directed to the right along x. Body A will be stationary before collision in this frame and body B will have a speed u_B The situation in the S-frame is also shown. The velocity u_B in the S-frame can be obtained from the relativistic velocity transformation equation, as

$$u_B = \frac{u' + v}{1 + u'v/c^2} = \frac{u' + u'}{1 + u'^2/c^2} = 2u'/(1 + u'^2/c^2)$$

The relativistic mass of B in the S-frame can be verified to be

$$m_B = \frac{m_0}{\sqrt{1 - u_B^2/c^2}} = \frac{m_0(1 + u'^2/c^2)}{(1 - u'^2/c^2)}$$

In S, the combined mass C travels at a speed $v(= u')$ after collision, since it was stationary in S'. Hence, applying conservation of relativistic momentum in the x-direction in this frame (the y-component of momentum is automatically conserved), we have

$$\text{(before)} = \text{(after)}$$

$$\frac{m_0}{\sqrt{1 - u_B^2/c^2}} u_B + 0 = \frac{M_0}{\sqrt{1 - v^2/c^2}} v.$$

With $v = u'$ and u_B as given above, this becomes

$$\frac{m_0(1 + u'^2/c^2)}{(1 - u'^2/c^2)} \cdot \frac{2u'}{(1 + u'^2/c^2)} = \frac{M_0 u'}{\sqrt{1 - u'^2/c^2}}$$

$$\implies M_0 = \frac{2m_0}{\sqrt{1 - u'^2/c^2}}$$

The rest mass of the combined body is not the sum of the rest masses of the original bodies ($2m_0$) but is greater by an amount

$$M_0 - 2m_0 = 2m_0 \left(\frac{1}{\sqrt{1 - u'^2/c^2}} - 1 \right)$$

Before the collision, the bodies had kinetic energy in S' equal to

$$K_A + K_B = 2K = 2m_0 c^2 \left(\frac{1}{\sqrt{1 - u'^2/c^2}} - 1 \right)$$

but all the kinetic energy disappeared on collision. In its place, after the collision, there appears some form of internal energy, such as heat energy or excitation energy. We now see that this extra internal energy results in the rest mass (inertia) of the combined body being greater than the total rest mass (inertia) of the two separate bodies. Thus, rest mass is equivalent to energy (rest-mass energy) and must be included in applying the conservation of energy principle. This result follows from the Lorentz transformation and the conservation of momentum principle which were used in arriving at it.

From the above equations, we see that $K_A + K_B = (M_0 - 2m_0)c^2$, which shows directly, in this case, that the energy associated with the increase in rest mass after the collision, $\Delta m_0 c^2$, equals the kinetic energy present before the collision. We can say, then, that although in an inelastic collision kinetic energy alone is not conserved, total energy is conserved. The total energy includes rest-mass energy plus kinetic energy. Furthermore, the conservation of total

energy is equivalent to the conservation of relativistic mass. We shall prove this shortly. Let us look at a rather interesting formulation now.

$$\overrightarrow{\mathrm{P}} = \frac{m_0 \overrightarrow{u}}{\sqrt{1 - u^2/c^2}}$$

$$P^2 = \frac{m_0^2 u^2}{1 - u^2/c^2} \quad \Longrightarrow \quad P^2 \left(1 - \frac{u^2}{c^2}\right) = m_0^2 u^2$$

$$\therefore u^2 \left(m_0^2 + \frac{p^2}{c^2}\right) = P^2 \quad \Longrightarrow u^2 = \frac{p^2}{m_0^2 + p^2/c^2}$$

Now,

$$\begin{aligned} E^2 &= \frac{m_0^2 c^4}{1 - u^2/c^2} = \frac{m_0^2 c^4}{1 - \left(\dfrac{p^2}{m_0^2 + p^2/c^2}\right)\dfrac{1}{c^2}} \\ &= \frac{\left(m_0^2 + p^2/c^2\right) c^2 \cdot m_0^2 c^4}{m_0^2 c^2 + p^2 - p^2} \\ &= \frac{\left(m_0^2 + p^2/c^2\right) \cdot m_0^2 c^6}{m_0^2 c^2} \\ &= p^2 c^2 + m_0^2 c^4 \end{aligned}$$

The energy $m_0 c^2$ when $p = 0$ is termed as rest mass energy. This is the energy associated with the mere existence of the particle. In non-relativistic physics, this term is termed 0. However, nuclear fission and other nuclear processes have amply confirmed the reality of mass energy.

As promised, we now show that, in both frames S and S', the total energy is conserved in the completely inelastic collision above. Consider first the S'-frame. Before the collision the total energy is

$$2\left(m_0 c^2 + K\right) = 2m_0 c^2 / \sqrt{1 - u'^2/c^2}$$

After the collision the total energy is

$$M_0 c^2 = \left(\frac{2m_0}{\sqrt{1 - u'^2/c^2}}\right) c^2 = 2m_0 c^2 / \sqrt{1 - u'^2/c^2}$$

Hence, the total energy is conserved in the collision in frame S'. Now consider the S-frame. Before the collision, the total energy is

$$\begin{aligned} m_0 c^2 + \left(m_0 c^2 + K_B\right) &= 2m_0 c^2 + m_0 c^2 \left[\frac{1}{\sqrt{1 - u_B^2/c^2}} - 1\right] \\ &= 2m_0 c^2 + m_0 c^2 \left[\frac{2u'^2/c^2}{1 - u'^2/c^2}\right] = \frac{2m_0 c^2}{(1 - u'^2/c^2)} \end{aligned}$$

After the collision, the total energy is

$$M_0c^2 + K_c = \frac{2m_0}{\sqrt{1-u'^2/c^2}}c^2 + \frac{2m_0}{\sqrt{1-u'^2/c^2}}c^2\left[\frac{1}{\sqrt{1-v^2/c^2}} - 1\right].$$

which, with $v = u'$, becomes

$$\frac{2m_0}{\sqrt{1-u'^2/c^2}}c^2 + \frac{2m_0}{\sqrt{1-u'^2/c^2}}c^2\left[\frac{1}{\sqrt{1-u'^2/c^2}} - 1\right] = \frac{2m_0c^2}{(1-u'2/c^2)}.$$

Hence, the total energy is conserved in the collision in frame S. Now we show that the relativistic mass is also conserved in each frame. Consider first the S'-frame. Before the collision the relativistic mass is

$$\frac{m_0}{\sqrt{1-u'^2/c^2}} + \frac{m_0}{\sqrt{1-u'^2/c^2}} = \frac{2m_0}{\sqrt{1-u'^2/c^2}}.$$

After the collision the relativistic mass is the same as the rest mass, for $U_c{}' = 0$; that is,

$$M_0/\sqrt{1-U_c{}'^2/c^2} = \left(\frac{2m_0}{1-u'^2/c^2}\right)/\sqrt{1-0} = \frac{2m_0}{\sqrt{1-u'^2/c^2}}$$

Hence, the relativistic mass is conserved in the collision in frame S'. Now consider the S-frame. Before the collision the relativistic mass is

$$m_0 + \frac{m_0}{\sqrt{1-u_B^2/c^2}} = m_0 + m_0\frac{\left(1+u'^2/c^2\right)}{(1-u'^2/c^2)} = \frac{2m_0}{(1-u'^2/c^2)}$$

After the collision the relativistic mass is

$$M_0/\sqrt{1-v^2/c^2} = \left(\frac{2m_0}{\sqrt{1-u'^2/c^2}}\right)/\sqrt{1-u'^2/c^2} = \frac{2m_0}{(1-u'^2/c^2)}.$$

Hence, the relativistic mass is conserved in the collision in frame S. We have seen that the conservation of total energy is equivalent to the conservation of (relativistic) mass. That is, the invariance of energy implies the invariance of (relativistic) mass. Mass and energy are equivalent; they form a single invariant that we can call mass-energy. Simply by multiplying the mass equations above by the universal constant c^2, we obtain numerically the corresponding energy equations. The relation $E = mc^2$ expresses the fact that mass-energy can be expressed in energy units (E) or equivalently in mass units ($m = E/c^2$).

§7.5 Alternate definitions of Relativistic quantities

We defined $\vec{P}$ as $m_0\vec{u}/\sqrt{1-u^2/c^2}$ where $\vec{u} = d\vec{x}/dt$. An equivalent definition is $\vec{p} = m_0\vec{U}$ where $\vec{U} = d\vec{r}/d\tau$ and $d\tau = (\sqrt{1-u^2/c^2})dt$. $d\tau$ was earlier called as proper time. Consider a frame S with respect to which a particle is moving with velocity $\vec{u}$. The time dt elapsed in S, by time dilation is $d\tau/\sqrt{1-u^2/c^2}$ where $d\tau$ is the time elapsed in the frame of the particle - the proper

frame of the particle - hence, the name proper time. (Note that we have visited this topic earlier as well). $d\tau$ is by definition, invariant under Lorentz transformation ! (Think about this) i.e., in other words for every object moving with $u < c$ relative to any frame S, one can define a frame co-moving with the particle i.e., its proper frame. In terms of proper time, we now have an alternate set of definitions for Kinematics and Dynamics quantities.

$$\begin{aligned}
\mathbf{U} &= \frac{d\mathbf{r}}{d\tau} \rightarrow \text{Relativistic Velocity} \\
\mathbf{P} &= m_0 \cdot U \rightarrow \text{Relativistic Momentum} \\
\mathbf{F} &= \frac{d\mathbf{P}}{d\tau} \rightarrow \text{Relativistic Force} \\
\mathbf{a} &= \frac{d\mathbf{U}}{d\tau} \rightarrow \text{Relativistic Acceleration}
\end{aligned}$$

§7.6 Transformations of Momentum, Energy , Mass and Force

Until now, we investigated the dynamics of a single particle using the relativistic equation of motion that was found to be in agreement with experiment for the motion of high-speed charged particles. There we introduced the relativistic mass and the total energy, including the rest-mass energy. However, all the formulas that we used were applicable in one reference frame, which we called the laboratory frame. Often, as when analyzing nuclear reactions, it is useful to be able to transform these relations to other inertial reference frames, like the center-of-mass frame. Therefore, we present here the relations that connect the values of the momentum, energy, mass, and force in one frame S to the corresponding values of these quantities in another frame S', which moves with uniform velocity $\mathbf{v}$ with respect to S along the common $x - x'$ axes. We shall thereby gain some new insights into relativity. We begin with a relation between the velocity of $\vec{u}$ ($|u|^2 = u_x^2 u_y^2 + u_z^2$) of a particle in S and its velocity $\vec{u'}$ ($|u'|^2 = u_x'^2 + u_y'^2 + u_z'^2$) in S', then

$$u'_x = \frac{u_x - v}{1 - u_x(v/c^2)} \quad u'_y = \frac{u_y\sqrt{1 - v^2/c^2}}{1 - u_x(v/c^2)} \quad u'_z = \frac{u_z\sqrt{1 - v^2/c^2}}{1 - u_x(v/c^2)}$$

Consider,

$$\begin{aligned}
c^2 - u'^2 &= c^2 - u_x'^2 - u_y'^2 - u_z'^2 \\
&= c^2 - \left(\frac{u_x - v}{1 - u_x(v/c^2)}\right)^2 - \left(\frac{u_y\sqrt{1 - v^2/c^2}}{1 - u_x(v/c^2)}\right)^2 - \left(\frac{u_z\sqrt{1 - v^2/c^2}}{1 - u_x(v/c^2)}\right)^2 \\
&= c^2 - \left[\frac{u_x^2 + v^2 - 2u_x v + u_y^2\left(1 - v^2/c^2\right) + u_z^2\left(1 - v^2/c^2\right)^2}{(1 - u_x(v/c^2)^2)}\right] \\
&= \frac{\left(1 - u_x(v/c^2)\right)^2 c^2 - \left[u^2 - u_y^2(v^2/c^2) - u_z^2(v^2/c^2) + v^2 - 2u_x v\right]}{\left(1 - u_x(v/c^2)\right)^2}
\end{aligned}$$

$$= \frac{c^2 + u_x^2(v^2/c^2) - \cancel{2u_xv} - u^2 + u_y^2(v^2/c^2) + u_z^2(v^2/c^2) + \cancel{2u_xv}}{(1 - u_x(v/c^2))^2}$$
$$= \frac{c^2 + u^2(v^2/c^2) - u^2 - v^2}{(1 - u_x(v/c^2))^2}$$

We thus have that the following useful identity,

$$c^2 - u'^2 = \frac{c^2 - u^2 - v^2\left(1 - u^2/c^2\right)}{(1 - u_x(v/c^2))^2}$$
$$= \frac{c^2\left(1 - u^2/c^2\right) - v^2\left(1 - u^2/c^2\right)}{(1 - u_x(v/c^2))^2}$$
$$\therefore 1 - \frac{u'^2}{c^2} = \frac{(1 - u^2/c^2)(1 - v^2/c^2)}{(1 - u_x(v/c^2))^2}$$
$$\implies \frac{1}{\sqrt{1 - u'^2/c^2}} = \frac{1 - u_x(v/c^2)}{\sqrt{1 - u^2/c^2}\sqrt{1 - v^2/c^2}}$$

We now can easily obtain the transformations for the components of momentum and for the energy. In frame S we have (by definition)

$$p_x = \frac{m_0u_x}{\sqrt{1 - u^2/c^2}}, \qquad p_y = \frac{m_0u_y}{\sqrt{1 - u^2/c^2}},$$
$$p_z = \frac{m_0u_z}{\sqrt{1 - u^2/c^2}}, \qquad E = \frac{m_0c^2}{\sqrt{1 - u^2/c^2}}$$

In frame S' the corresponding quantities are (by definition)

$$p_{x'} = \frac{m_0u_{x'}}{\sqrt{1 - u'^2/c^2}}, \qquad p_{y'} = \frac{m_0u_{y'}}{\sqrt{1 - u'^2/c^2}},$$
$$p_{z'} = \frac{m_0u_{z'}}{\sqrt{1 - u'^2/c^2}}, \qquad E = \frac{m_0c^2}{\sqrt{1 - u'^2/c^2}}.$$

Using the identity proved and the transformation equations for the velocity components, we can easily verify that the relations between these quantities are

$$p_x = \frac{1}{\sqrt{1 - v^2/c^2}}\left(p_{x'} + \frac{E'v}{c^2}\right)$$
$$p_y = p_y',$$
$$p_z = p_z',$$
$$E = \frac{1}{\sqrt{1 - v^2/c^2}}(E' + vp_x')$$

The inverse relations, obtained by sending v to $-v$ and interchanging primed and unprimed quantities, are

$$\begin{aligned} p_{x'} &= \frac{1}{\sqrt{1-v^2/c^2}}\left(p_x - \frac{Ev}{c^2}\right) \\ p_{y'} &= p_y, \\ p_{z'} &= p_z, \\ E' &= \frac{1}{\sqrt{1-v^2/c^2}}(E - vp_x). \end{aligned}$$

If these results are compared to the original Lorentz transformations involving x, y, z, t and x', y', z', t', we find a striking analogy. The quantities p_x, p_y, p_z and E/c^2 transform exactly as the space-time coordinates x, y, z and t of a particle transform. This is an excellent way to remember the transformations. For example,

$$\begin{aligned} x' &= \frac{x - vt}{\sqrt{1-v^2/c^2}} \\ p_{x'} &= \frac{p_x - v(E/c^2)}{\sqrt{1-v^2/c^2}}. \\ t' &= \frac{t - (v/c^2)x}{\sqrt{1-v^2/c^2}} \\ \frac{E'}{c^2} &= \frac{(E/c^2) - (v/c^2)p_x}{\sqrt{1-v^2/c^2}} \end{aligned}$$

Any four quantities A_0, A_1, A_2 and A_3 such that

$$\begin{aligned} \text{time component} \rightarrow \quad & A_0' = \gamma(A_0 - \beta A_1) \\ \text{3-vector} \rightarrow & \begin{cases} A_1' = \gamma(A_1 - \beta A_0) \\ A_2' = A_2 \\ A_3' = A_3 \end{cases} \end{aligned}$$

are said to form a four vector. Hence, momentum and energy form one 4-vector where momentum behave like the " space " co-ordinate and energy is like the " time" co-ordinate. Four momentum conservation now subsumes both 3-momentum conservation and total energy conservation. One can show that $U \equiv dX/d\tau$ where $X \equiv (ct, \vec{x})$, $a = dU/d\tau$, $P = m_0 U$ and $F = dP/d\tau$ are all 4-vectors. In electrodynamics, $(c\rho_0, \vec{j})$ form a 4-vector i.e., charge and current density. Similarly, $(\Phi/c, \vec{A})$ which are electromagnetic scalar and vector potentials.