

Quantum Mechanics(2017) - Lecture Notes  
Part-V General Principles of Quantum Theory

A Course of 10 Lectures to Be Given at IIT Bhubaneswar

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## §1 Structure of Classical Theories

### §1.1 Structure of physical theories

Classical theory of a physical system consists of components listed in Table (1) below.

Table 1: Components of a classical theory

SN	Components
1	States of the physical system; ‘Co-ordinates’
2	Dynamical Variables
3	Laws of Motion
4	Forces, Interactions

At first we shall briefly explain each item in the table and later discuss them by means of examples of different physical systems.

**Physical states:** By state of a physical system one means ways of specifying complete information about the system.

**Dynamical variables:** The dynamical variables of a classical system are functions of state of the system and can be computed when the state has been specified.

**Laws of motion:** Not only we are interested in knowing about a system at a given time, we also want to know how the system changes with time. In order to describe behaviour of a system under time evolution one needs to know the laws of motion. Several different forms of the laws of motion are available for mechanical systems.

- Newton’s laws
- Lagrangian equations of motion
- Hamilton’s equations
- Poisson bracket formalism

When applicable, all the above formalism are equivalent.

**Interactions:** A classical description is completed by specifying the forces of the interactions of the system. It should be remarked that while the laws of motion are general and are applicable to a wide variety of physical systems, the nature of forces or the explicit form of interactions differs from system to system. The interactions are specified by giving explicit expressions for forces acting on the bodies in the system.

**Classical Systems:** Some examples of classical systems of interest are

- System of point particles moving in a force field.
- One or more point particle moving on a surface of a sphere.
- Rigid body
- Vibrating string or a spring
- Electromagnetic waves
- Charged particles interacting with electromagnetic fields

**System of point particles** You are all familiar with the newtonian mechanics from your school days. A complete specification of state of a particle requires three position coordinates and three velocities. The dynamical variables are experimentally measurable quantities such as energy, momentum and angular momentum. They are functions of coordinates and velocities.

The equations of motion are given by the second law. For a system of point particles, the behaviour of each particle is governed by the equation of motion

$$m_\alpha \frac{d^2 \vec{r}_\alpha}{dt^2} = \vec{F}_\alpha \quad (1)$$

Note that the EOM are a set of second order differential equations in time. Therefore one needs to know the values of position and velocities at a time in order  $t_0$  to be able to predict the state of the system at a later time. One also needs to have information about all the forces acting on the particle. The Newton's laws require that the equations of motion be set up using the Cartesian coordinates to describe the particle. For a system consisting of several particles one needs to know all the forces, including the forces of constraint. In order to set up equations of motion in a non Cartesian system of coordinates one has to start from the Cartesian system and take into account of the constraints. In general finding solution may require a change variables from Cartesian coordinates to a new set of coordinates. Thus, for example, for a bead sliding on a sphere one should change from Cartesian coordinates to polar coordinates.

**Waves:** The state of a vibrating string is described completely by specifying the displacement and velocity of the string at each point. The vibrations are also governed by the Newton's Laws which can be used to derive the wave equation giving the propagation of waves in a medium.

**Charged particles and radiation** The systems consisting of charged particles interacting with electromagnetic fields are very important. These are governed by the Maxwell's equations and the Lorentz force equation. The state is described by specifying position and momenta of the charged particles and the electromagnetic fields, or the scalar and vector potentials, at all points in the space.

## §1.2 Formulations of classical theories

The Newtonian formulation has limitations which make it unsuitable for description of several physical systems. Many different formalisms exist which generalise the Newtonian formalism. We mention a few of these here which are useful for systems with a few degrees of freedom. Apart from Newtonian mechanics, other formulations of mechanics are

1. Lagrangian formulation
2. Hamiltonian and Poisson brackets
3. Hamilton Jacobi formulation

Each of the above formalism will be described briefly.

### Lagrangian form of classical dynamics

In the Lagrangian approach the state of a system is described by a set of generalized coordinates and velocities. The generalized coordinates are not restricted to be Cartesian. They are a set of independent variables  $q_k$  needed to specify the system completely. The knowledge of these variables  $q_k$ , called generalized coordinates, and their time derivatives allows us to compute all dynamical variables of the system. The dynamical laws or the equations of motion are given in terms of a single function of generalized coordinates and momenta,  $\mathcal{L}(q, \dot{q}, t)$ , called Lagrangian of the system. Knowing the Lagrangian, the equations of motion are given by

$$\frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{q}_k} \right) - \frac{\partial \mathcal{L}}{\partial q_k} = 0, \quad k = 1, 2, \dots \quad (2)$$

The Lagrangian formalism offers distinct advantages over the Newtonian formalism.

## Hamiltonian form of classical dynamics

In the Hamiltonian approach to the classical mechanics, the state of a system at time  $t$  is described by giving the values of generalised coordinates and momenta  $q_k, p_k, (k = 1, \dots, n)$  at that time. The canonical momentum  $p_k$  is defined as derivative of the Lagrangian of the system w.r.t. the generalised velocity  $\dot{q}_k$ :

$$p_k = \frac{\partial L}{\partial \dot{q}_k}. \quad (3)$$

The interaction is specified by giving Hamiltonian  $H(q, p)$  which determines the EOM. The EOM in the Hamiltonian approach take the form

$$\dot{q}_k = \frac{\partial H}{\partial p_k}, \quad \dot{p}_k = -\frac{\partial H}{\partial q_k}, \quad k = 1, \dots, n. \quad (4)$$

## Poisson bracket formalism

For two functions  $F(q, p), G(q, p)$  of canonical variables, the Poisson bracket  $[F, G]_{\text{PB}}$  is defined as

$$[F, G]_{\text{PB}} = \sum_k \left( \frac{\partial F}{\partial q_k} \frac{\partial G}{\partial p_k} - \frac{\partial F}{\partial p_k} \frac{\partial G}{\partial q_k} \right). \quad (5)$$

The Hamilton's equations, Eq.(5), written in terms of Poisson brackets assume the form

$$\dot{q}_k = [q_k, H]_{\text{PB}}, \quad \dot{p}_k = [p_k, H]_{\text{PB}}. \quad (6)$$

In general the time evolution of any dynamical variable is given by

$$\frac{dF}{dt} = [F, H]_{\text{PB}}. \quad (7)$$

The classical mechanics has been formulated in several different ways. We mention the Newtonian, the Lagrangian, the Hamiltonian and the Poisson bracket formulations. The Hamiltonian form of mechanics turns out to be the most convenient and suitable for making a transition to quantum mechanics; the Schrodinger and Heisenberg formulations of quantum mechanics requiring an understanding of the Hamiltonian and Poisson bracket formulations. Frequently it is asked if Lagrangian formulation has a role in the quantum theory ? The answer is in affirmative and the Lagrangian plays an essential role in the Feynman path integral approach to quantum mechanics.

### §1.3 Thermodynamics and statistical mechanics:

For systems consisting of a large number of particles, such as gases, the classical mechanics, in the form used for point particles, is not very useful. One needs to use statistical methods. While thermodynamics and statistical mechanics were successful in describing

the behaviour of a large number of systems very closely, there were some notable disagreements with experiments.

When it comes to the structure of thermodynamics and statistical mechanics, they too have the same structure that is outlined above for mechanics. Except that most of the time we talk about equilibrium situations. Therefore, we do not quite discuss time evolution. A discussion of time evolution of statistical systems falls under the non-equilibrium statistical mechanics and that is very hard subject.

## §2 Postulates of Quantum Mechanics

During the first three decades of the twentieth century when quantum theory was being developed several classical concepts had to be revised. A list of major changes that took places is as follows.

1. **Discontinuous nature of physical process** such as emission of radiation in Bohr model absorption of radiation in photoelectric effect.
2. **Quantization of physical observable quantities**, for example angular momentum and energy in Bohr model.

In quantum description, the dynamical variables are quantized, in general, they can take only some discrete values.

3. **Wave particle duality** was an important change in concepts that brought in major changes in the way we think of physical system. The fact that in quantum world both matter and radiation have dual nature had far reaching consequences. However, It must be remembered that the two natures are complimentary and do not manifest themselves in any single experiment ( Bohr complimentary principle).

In addition to the above mentioned changes, the quantum theory brought many new concepts and forced revision of several classical ideas. We recapitulate some important classical concepts which underwent a complete revision after the quantum revolution.

- The classical theories are deterministic, once initial state is specified the motion of the system is deterministic; out come of any measurement can be predicted.

The quantum theory is probabilistic; only probabilities of different possible outcomes of experiments can be predicted by the theory.

- In classical theory we associate a well defined trajectory with motion of particles. Waves are not localized and one cannot associate definite trajectories with waves. Properties of particles and waves are incompatible properties.

- In classical mechanics the states of a physical system are described by generalized coordinates and momenta. This changes completely in the quantum theory.
- In classical theories there is no restriction on simultaneous measurement of a pair of variables.

Unlike classical theories, a generalised coordinate and canonical conjugate momentum can not be measured to arbitrary accuracy simultaneously. In general two arbitrary dynamical variables cannot be measured simultaneously.

- The classical motion of particle is confined to regions where the total energy is greater than the potential energy. A particle cannot cross a region where the potential energy is higher than the kinetic energy.

A quantum particle can tunnel through a barrier, as is the case in alpha decay.

- In quantum world all particles and radiation have dual nature. However, The two natures are complimentary and do not manifest themselves in any single experiment. ( Bohr complementarity principle)
- In quantum description identical particles cannot be distinguished, they lose their identity.

Our understanding of classical concepts requires a major shift, or even a complete change. In addition many new concepts are brought in by the quantum theory.

In addition entire mathematical framework needed for description of quantum phenomena changes. While the mathematics prerequisite for classical mechanics for solution of problems is differential equations and partial differential equations, quantum mechanics brings in Hilbert spaces and probability theory in an essential way.

Also note that the kind of questions that are meaningful for a classical system, do not all remain valid questions in quantum mechanics. For example For a classical point particle we may ask for its position and momentum at different times but not for a quantum particle ( which is also a wave ). There are a whole host of new physically meaningful questions that are not asked in the classical physics.

At this stage you need to remember that above ideas from classical formulations will need a change. Why change is needed, what is the replacement , if any, and all such questions will be dealt with at a suitable stage later,

The transition from classical to quantum mechanics is conventionally made by following a route known as canonical quantization. This is the route we will follow. Later you might learn that there are several routes ( 10) to quantization.

You will understand all this more clearly as you move on and learn the subject. So, by the time we reach the end of this course, you will have understood basics of one of the



most common approach to quantum mechanics . Several revisits will be needed for you to gain better and fuller appreciation of the subject.

. Before closing, I leave you with a quote from the quantum mechanics book by Landau and Lifshitz [?] p3.

“Thus quantum mechanics occupies a very unusual place among physical theories; it contains classical mechanics as a limiting case, yet at the same time it requires this limiting case for its own formalism.”

Think about the statement Landau and Lifshitz make and about ‘intriguing’ relation between the classical and quantum theories.

## Why Begin With Postulates

### §2.1 Why begin with postulates

The inadequacy of classical theory and efforts to explain the observed physical phenomena led to a major revision of classical concepts and of the mathematical structure. Some of the earliest points of departure from the classical theory were (i) discrete nature of physical processes, as in Planck's hypothesis and (ii) *quantisation of dynamical variables*, for example, angular momentum in Bohr's theory.

The wave particle duality had far reaching consequences and has changed the way we understand and do physics. Here we will briefly highlight the important points that are best seen to emerge from implications of wave particle duality on thought experiments.

In a double slit interference experiment for electrons, because of the dual nature we would expect to see an interference pattern. However, when the intensity of the incident beam is reduced to single electron at a time, we are inclined to conclude that one would see a spot on the screen, and not an interference pattern. Still an interference pattern appears when the experiment is repeated with a large number of times. This can be understood only by associating a *probability amplitude* of electron reaching a point on the screen. It is accepted that the a prediction about exact location of the spot for in experiment with single electron is impossible and *indeterminacy* has entered in an essential way.

On similar lines, an analysis of the thought experiments on photon polarisation in the limit of low intensities involving single photon leads to the *indeterminacy* of polarisation state of a photon. This in turn introduces *indeterminacy* in outcomes of polarisation measurements. Again we are led to *probabilities* being associated with the out come of measurements of physical quantities. The indeterminacy is seen to arise due the *state of the photon being superposition of two different states of polarisation*.

This theory of itself does not

It has to be emphasised that the suggestion here is that indeterminacy is of a fundamental nature and not due to some limitation of the quantum theory or of the measuring apparatus.

An analysis of Heisenberg microscope thought experiments to *measure position and momentum of particles simultaneously* leads to the Heisenberg uncertainty principle. It asserts that the position and momentum of a particle cannot be measured simultaneously. This is forced due to the observed dual nature of electrons and photons.

Thus we are naturally led to ask the following, and many more, questions.

- If we have to incorporate the *superposition principle of quantum states*, how are the states and dynamical variables to be described in quantum theory?
- If some dynamical variables are *quantised*, how are we to compute the allowed values of dynamical variables?
- Acceptance of *indeterminacy* leads us to ask what is the scheme to compute the probabilities of different possible outcomes of an experiment?
- The *uncertainty principle* is an outcome of Heisenberg microscope thought experiment and a consequence of wave particle duality. This analysis gives us no clue about which other pairs of dynamical variables cannot be measured simultaneously. In fact we do not have a precise mathematical formulation of the uncertainty principle; it is not clear “How is the uncertainty in a dynamical variable even defined precisely?”

The answers to these, and many more, questions, will be obtained by an application of the postulates of quantum mechanics. Learning the postulates also allows us maintain a clear understanding of what is assumed and what is derived.

There are several different ways of formulating quantisation applying to physical systems. The postulates will in general appear different in different scheme. Remember that the postulates, to be described below, give us one of several possible schemes, of ‘doing’ quantum mechanics.

**Learn from Masters:** *We strongly recommend that the reader should go through a few pages of a terse but an illuminating discussion of superposition principle, indeterminacy, simultaneous measurement, and related issues from the very first section of the first chapter of Landau Lifshitz. A ‘teaser’ from of this part of the book, reproduced below, should serve as an inducement for going to the original book.*

This circumstance shows that, in quantum mechanics, there is no such concept as . . . .

A complete description of the state . . . in classical mechanics . . . In quantum mechanics such a description is impossible. . . .

A very important consequence follows . . . . Where as a classical description. . . with complete accuracy, . . . quantum mechanics evidently cannot do this. . . . Hence quantum mechanics cannot . . . completely definite predictions. . . .

All measuring process in . . . may be divided into two classes. . . .

We shall often find that by no means . . . can be measured simultaneously. We shall now formulate the meaning of a *complete description* of a state in quantum mechanics. . . .

In quantum mechanics we shall understand by the states of a quantum system . . . .

Landau Lifshitz

## §2.2 Postulates of Quantum Mechanics

1. **States of physical system** *The state of a quantum mechanical system is represented by a vector in a complex vector space with inner product (Hilbert Space).*

The null vector does not represent any state. Two non-null vectors represent the same state if and only if they are linearly dependent. Thus  $|\psi_1\rangle$  and  $|\psi_2\rangle$  represent the same state if there exists a complex number  $c$  such that

$$|\psi_2\rangle = c|\psi_1\rangle \quad (8)$$

A vector that represents state of physical system will be called state vector. The quantum mechanical states represented by vectors in Hilbert space are called pure states. There are other possible states which are called mixed states. These are represented by a density matrix  $\rho$ . The density matrix is an operator having properties that it is hermitian and that its eigenvalues are between 0 and 1. A density matrix  $\rho$  corresponds to a pure state if and only if  $\rho^2 = \rho$ .

2. **Dynamical Variables** *The dynamical variables of a physical system are represented by linear operators in the vector space.*

A linear operator representing a dynamical variable must have real eigenvalues and their eigenvectors must form a complete set. These properties are satisfied by self adjoint operators (hermitian operators). So we demand that the dynamical variables be represented by self adjoint operators in Hilbert space. An operator representing a dynamical variable will also be called an observable.

3. **Measurement postulate and probabilities** *If the system is in a state  $|\psi\rangle$ , a measurement of dynamical variable  $A$  will give one of its eigenvalues  $\alpha_k$  with probability equal to  $|\langle u_k|\psi\rangle|^2$ , where  $|u_k\rangle$  is the eigenvector of  $\hat{A}$  corresponding to eigenvalue  $\alpha_k$ .*  
<sup>1</sup>

A result of any measurement of a dynamical variable is one of the eigenvalues of the corresponding operator. Conversely, every eigenvalue of an observable representing a dynamical variable is a possible result of a measurement of the dynamical variable.

As an example, let  $|u_1\rangle, |u_2\rangle, \dots, |u_n\rangle$  represent the eigenvectors of an observable  $\hat{A}$ . If the state vector of a physical system,  $|u_i\rangle$ , is an eigenvector of an operator  $\hat{A}$  representing a dynamical variable  $A$ , a measurement of the dynamical variable gives value  $\alpha$  with probability 1. Here  $\alpha$  is the eigenvalue of  $\hat{A}$  corresponding the eigenvector  $|u_i\rangle$ . Conversely, if the measurement of  $A$  gives the value  $\alpha$  with probability 1, the state of system will be represented by a vector which will be eigenvector of the operator  $\hat{A}$  corresponding to the eigenvalue  $\alpha$ .

In general state vector  $|\psi\rangle$  will not be an eigenvector of the given dynamical variable. In such a case a measurement of the variable  $A$  will results in values  $\alpha_1, \alpha_2, \dots, \alpha_n$  with probabilities  $c_1|\alpha_1\rangle, c_2|\alpha_2\rangle, \dots, c_n|\alpha_n\rangle$  where  $c_1, c_2, \dots, c_n$  are the coefficients in the expansion of the state vector  $|\psi\rangle$

$$|\psi\rangle = \sum_k c_k |u_k\rangle \quad (9)$$

in terms of eigenvectors of  $\hat{A}$ .

Here  $|\psi\rangle$  and  $|u_k\rangle$  are assumed to be normalized.

$$\langle\psi|\psi\rangle = 1; \quad \langle u_k|u_k\rangle = 1, k = 1, 2, \dots \quad (10)$$

4. **Commutation relations** *The operators corresponding to the generalized coordinates and momenta  $\{q_k, p_k\}$  of a classical system satisfy*

$$\hat{q}_i \hat{q}_j - \hat{q}_j \hat{q}_i = 0 \quad (11)$$

$$\hat{p}_i \hat{p}_j - \hat{p}_j \hat{p}_i = 0 \quad (12)$$

$$\hat{q}_i \hat{p}_j - \hat{p}_j \hat{q}_i = i\hbar \delta_{ij} \quad (13)$$

*The above relations are called canonical commutation relations.*

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<sup>1</sup>Requires modification when eigenvalues of  $A$  are degenerate.

5. Equation of motion *The time development of a system is governed by the Schrodinger equation*

$$i\hbar \frac{d}{dt}|\psi t\rangle = \hat{H}|\psi t\rangle \quad (14)$$

where  $|\psi t\rangle$  is the state vector of the system at time  $t$  and  $\hat{H}$  is the operator representing the Hamiltonian of the system.

6. Symmetrization postulate for identical particles *For a system of identical particles, the state of the system remains unchanged under exchange of a pair of particles, it should be either symmetric or antisymmetric under an exchange of all the variables of the two identical particles.*<sup>2</sup>

## §3 Superposition Principle

### §3.1 Photon polarization experiment

Certain crystals, for example tourmaline, have a preferred axis, call it *passing axis*. When a light beam is incident on a such a crystal, it which allows light vibrations parallel to its optic axis to pass and absorbs all the vibrations which are perpendicular to the passing axis. By rotating the crystal, we can get a beam which is polarised along different directions.

Now consider unpolarised light incident on a tourmaline crystal. The vibrations of the beam coming out of the crystal will be along the preferred axis of the tourmaline crystal. Let this beam be allowed to pass through a similar second crystal. Let the second crystal be placed with its passing axis parallel to that of the first crystal. All the light coming out of the first one will have vibrations parallel to the passing axis of the second crystal and will be fully transmitted through the second crystal too.

Next, if the first crystal is rotated by  $\pi/2$ , no light will pass through the second crystal. In case the angle of rotation of the first crystal is  $\alpha \neq \pi/2$ , the light from the first crystal will be obliquely polarised and a fraction  $\cos^2 \alpha$  of the incident intensity will be transmitted.

Next, we consider the same arrangement with the passing axes of the two crystals at a certain angle. Let the intensity of the incident beam so low that at any time only one photon passes through the apparatus. It is obvious that when the two axes are parallel, the photon will be transmitted through the apparatus and that it will be absorbed, when the two axes are perpendicular.

What do we expect when the photon incident on the second crystal with its passing axis making an angle  $\alpha \neq 0, \pi/2$  with the passing axis of first crystal.

From what is known in wave theory, one cannot conclude anything about the outcome of this experiment. Certainly, we cannot say that a part of photon is transmitted and a

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<sup>2</sup>T&C apply

part is absorbed; because the photon is indivisible! However, when we wait for a long time, we will find that a fraction  $\cos^2\alpha$ , of the total number photons incident on the second crystal, will pass through. Therefore, all that can be said about the single photon is that sometimes it will pass through the second crystal and sometimes it will get absorbed. What can we say about the states of photon in the three cases of parallel, perpendicular and oblique polarisation? In order to explain the outcome of the experiment for a large number of photons, it must be admitted that the photon in oblique polarisation is partly in the state with parallel polarisation and partly in the state with perpendicular polarisation. Obviously, every polarisation state of photon must then be regarded as a superposition of states of polarisation along two perpendicular directions.

*This superposition of states comes with indeterminacy that no prediction is possible about the outcome of an experiment involving a single photon, only the outcome of experiment repeated several times can be predicted.*

For a single photon with oblique polarisation, one is forced to assign a probability of getting transmitted or absorbed. One arrives at similar conclusions by analysis of other thought experiments involving electrons. For an electron a Stern Gerlach set up acts exactly like a tourmaline crystal for the photons. .

Here is what Dirac has to say about non classical nature of superposition principle

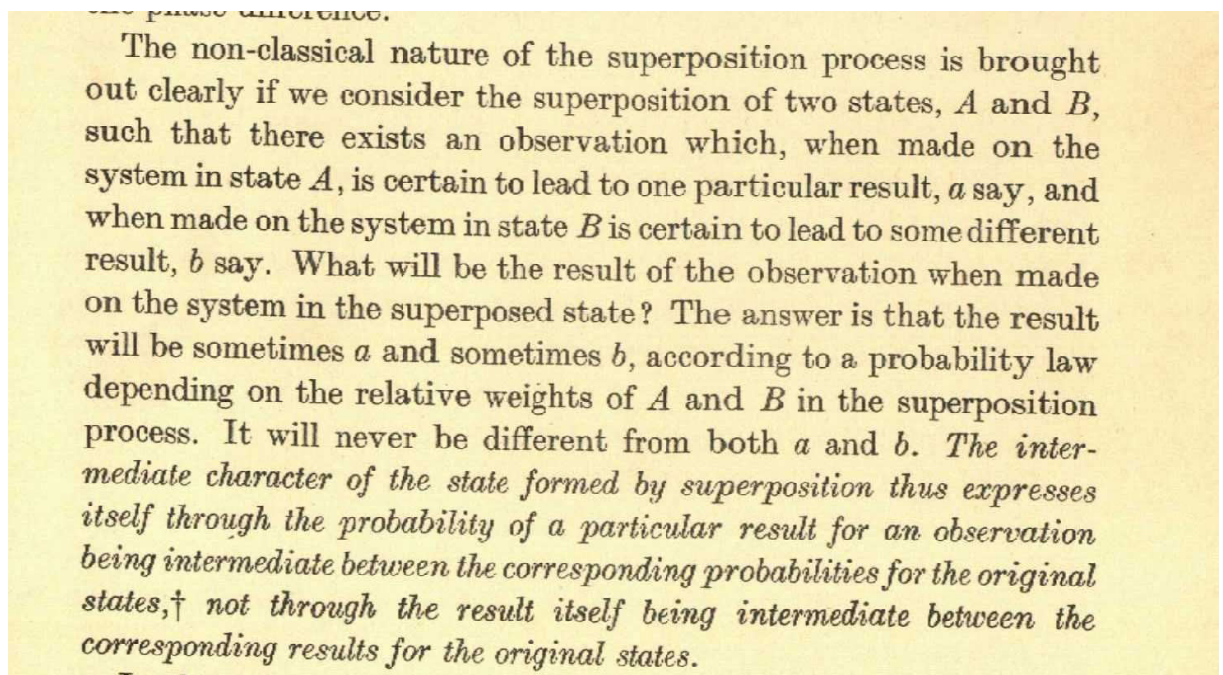


Fig. 1 Dirac-Page 13

Dirac summarises discussion of photon polarisation experiment by saying that super-



position leads to indeterminacy in quantum case and hence it is different from that in classical Physics.

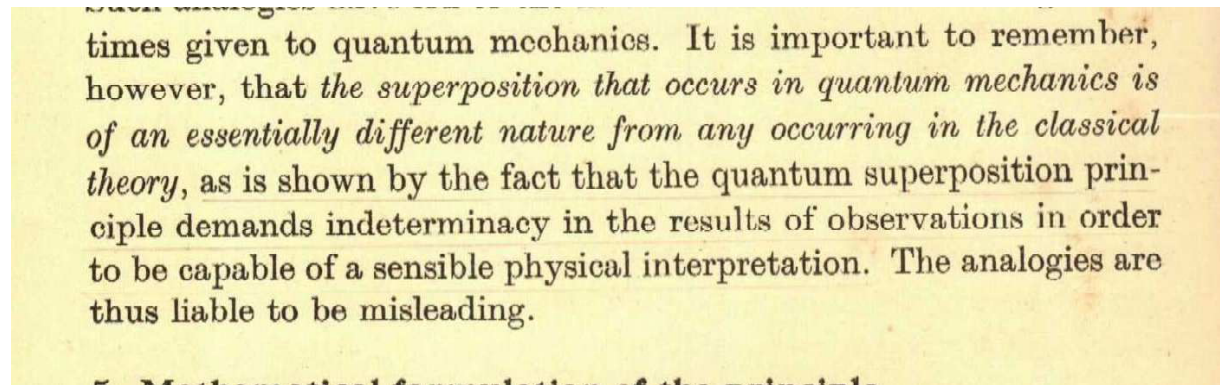


Fig. 2 Dirac-Page13

### §3.2 Double slit experiment with electrons

Before starting to read this thought experiment, it is a good idea to revise<sup>3</sup> thought experiments with bullets, and remember what would happen for the classical particles.

Let us first consider a double slit experiment can be done with one of the two slits can be kept open for half the time. The second slit is kept open for remaining half the time and the experiment is repeated. *In this one will not get the interference pattern as in the case when both the slits are kept open.* What is observed is just the combined distribution for two single slits. One would see the same pattern even if the experiment is done with very very low intensity beams, sending one electron at a time. In this case the behaviour of electrons is no different from bullets.

In a double slit interference experiment for electrons we would expect to see an interference pattern as is the case for any wave. However, when the intensity of the incident beam is reduced and we seek the result of the experiment performed with a single electron, we are inclined to conclude that one would see a spot on the screen, and not an interference pattern, due to indivisibility of the particle nature. Still an interference pattern appears when the experiment is repeated with a large number of times.

The double slit experiment shows that the quantum dual behaviour of electron is different from what is expected of classical particles such as bullets. It is also different from what is expected of waves in the classical theory.

When both the slits are kept open, it makes no difference what the beam intensity is. The interference experiment is done sending one electron at one time or having an

<sup>3</sup>A K Kapoor, QM-01:Classical Theories Revisited §1.3

intense beam. In a manner similar to the photon polarisation experiment. *the results can be understood only by considering the 'translational' state of the electron as superposition of two states corresponding to electron passing through one of the two slits.*

Within the accepted interpretations of quantum mechanics, this is explained by associating a probability amplitude of electron reaching a point on the screen and accepting that a prediction about the exact location of the spot in experiment with single electron is impossible and indeterminacy has entered in an essential way. It has to emphasised that the suggestion here is that indeterminacy is of fundamental nature of physical systems. It is neither due to limitation of the quantum theory nor due to a limitation of a measuring device.

We strongly recommend the reader to go through the relevant section so the books by Dirac[?] and Feynman [?].

However, one may still ask whether the quantum theory is complete in its present form and if the unusual features appear due to the restrictions on the domain of application such as nonrelativistic situations. We shall not dwell upon these and other similar questions here, as a meaningful discussion is beyond the scope of these lecture notes.

## Food for your thought

In classical mechanics the state of physical system are described by specifying simultaneous values of coordinates and momenta.

An analysis of thought several experiments to measure position and momentum of particles leads to the Heisenberg uncertainty principle which asserts that the position and momentum of a particle cannot be measured simultaneously. This happens due to an uncontrollable disturbance, usually in momentum (position), when a measurement of position (momentum) is made. *We are then naturally led to ask how are the states and dynamical variables are to described in quantum theory?*

Early developments suggested that in general dynamical variables are quantised. *We must then face several questions how do we compute the allowed values of dynamical variables which may be quantised? What is the method to compute the probabilities of different possible outcomes of an experiment?*

The polarisation and interference thought experiments involving the photon and electrons leads to the superposition principle of *quantum states*. *In what way can the superposition principle be formulated mathematically.*

Since the thought experiments suggest that only probabilities of outcomes of experiments involving single electron or a single photon can be predicted. *How does one compute the probabilities?*

The answers to all such questions can, in principle, be obtained by appealing to the postulates of quantum mechanics.



Flagged for revision

We end this short introduction with quotes from Feynman:

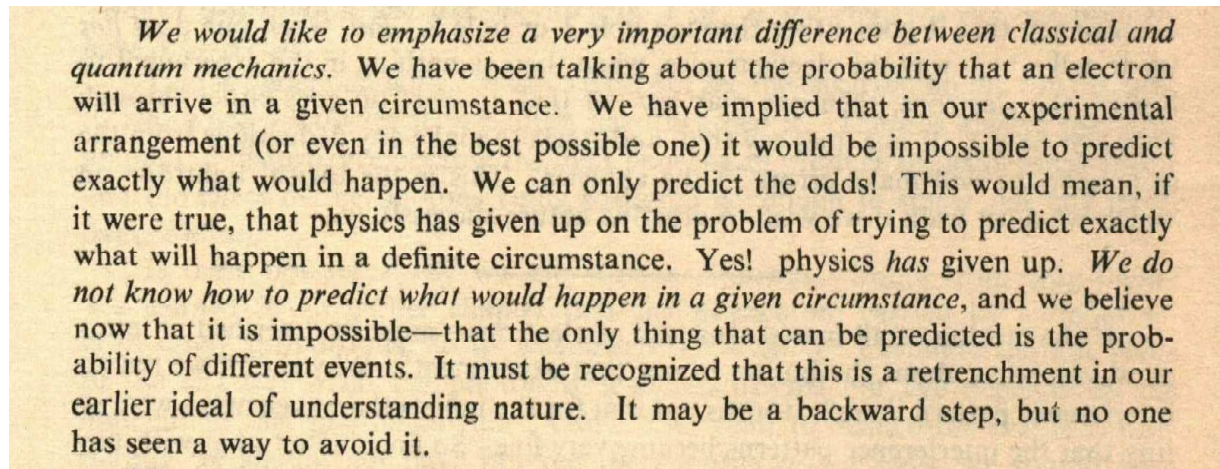


Fig. 3 Feynman-§1-10

The double slit experiment, that Feynman said has never been done, has actually been performed. A detailed information about the double slit experiment with low intensity beams can be found in the article Peter Rodgers in September (2001) issue of Physics World.

## Notes and References

It is strongly recommended that the reader should go through the following sections of the books by Dirac and Feynman.

- *The polarization of photons*, Dirac [?], §2
- *Interference of photons*, Dirac [?]. §3
- *Superposition and Indeterminacy*, Dirac [?] §4  
In this section compelling reasons for superposition of quantum states are given.
- *An experiment with electrons*, Feynman [?], §1-4
- *The interference of electron waves*, Feynman [?] §1-5.
- *Watching the electrons*, Feynman [?] §1-6
- *First principle of quantum mechanics*, Feynman [?]: §1-7. Feynman presents a short summary of conclusions of the thought experiments.

## §4 Probability and Average Value

### §4.1 The Third Postulate

The third postulate has several parts. In this section we use the notation  $A$  to denote a dynamical variable,  $\hat{A}$  will denote the corresponding hermitian operator. The eigenvalues will be real and it is assumed that the eigenvectors have been *chosen* to be orthonormal. If we denote the eigenvalues of  $\hat{A}$  by  $\alpha_1, \alpha_2, \dots, \alpha_k, \dots$  and the corresponding orthonormal eigenvectors by  $|u_1\rangle, |u_2\rangle, \dots, |u_k\rangle, \dots$  then we have

$$A|u_k\rangle = \alpha_k|u_k\rangle, \quad \langle u_k|u_m\rangle = \delta_{km}. \quad (15)$$

1. The first part of the third postulate says that the only outcome of a measurement of a dynamical variable  $A$  is one of the eigenvalues of the corresponding operator  $\hat{A}$ . Thus, if an experiment to measure a dynamical variable  $A$  is performed, the result must be only one of the eigenvalues  $\alpha_k$ . In particular, an answer different, from every eigenvalue, cannot be the outcome of measurement of  $A$ .
2. The next part of the postulate tells that if a system is represented by one of the eigenvectors  $|u_n\rangle$ , a measurement of the dynamical variable  $A$  will give the corresponding eigenvalue  $\alpha_n$ .
3. The third postulate also tells us about the outcome of measurement of  $A$  when the state vector  $|\psi\rangle$  is not an eigenvector of  $\hat{A}$ . In this case, the result is some times one eigenvalue and sometimes another. We cannot predict the result of a single measurement fully. When repeated measurements are made, different eigenvalues  $\alpha_n$  will be obtained with different probabilities  $p_n$  which can be predicted.

To compute the probabilities  $p_n$ , we first expand the state vector  $|\psi\rangle$  in terms of the eigenvectors of the operator  $\hat{A}$  corresponding to the dynamical variable  $A$  which is being measured and write

$$|\psi\rangle = \sum_k c_k |u_k\rangle. \quad (16)$$

Then the probability  $p_k$  of getting value  $\alpha_k$  is given by  $|c_k|^2$ . We continue to assume that the state vector  $|\psi\rangle$  and the eigenvectors  $|u_k\rangle$  are orthogonal, *i.e.*,

$$\langle \psi | \psi \rangle = 1, \quad \langle u_k | u_k \rangle = 1 \quad (17)$$

4. How do we compute the coefficients  $c_k$  in Eq.(17)? The eigenvectors of a hermitian operator are orthogonal and this helps in computing the coefficients. Taking scalar product of Eq.(16) with  $|u_n\rangle$  gives

$$\langle u_k | \psi \rangle = \sum_n c_n \langle u_k | u_n \rangle = \sum_n c_n \delta_{kn} = c_k \quad (18)$$

Note that, in the right hand side of Eq.(18), only the term with  $k = n$  survives, all other terms where  $n \neq k$  will vanish due to orthogonality property of the eigenvectors.

$$\therefore \quad c_k = \langle u_k | \psi \rangle \quad (19)$$

and

$$p_k = |c_k|^2 = |\langle u_k | \psi \rangle|^2 \quad (20)$$

#### 5. The Parseval relation

$$\langle \psi | \psi \rangle = \sum_k |c_k|^2 \quad (21)$$

implies that

$$\sum_k |c_k|^2 = 1 \implies \sum_k p_k = 1. \quad (22)$$

if the state vector  $|\psi\rangle$  is normalised,  $\langle \psi | \psi \rangle = 1$ . This suggests that the interpretation of expressions  $|c_k|^2$  as probabilities  $p_k$  is consistent with the requirement that the sum of all probabilities be equal to unity. We shall call the coefficient  $c_k$  as the probability amplitude for obtaining a value  $\alpha_k$  for the dynamical variable  $A$  when the system is in state  $|\psi\rangle$ .

As a consequence of the dual nature of matter and radiation, we have indeterminacy in the theoretical predictions. The origin of this indeterminacy can be traced to the superposition principle which in turn is needed to incorporate the wave nature of matter. In classical mechanics the result of measurement of position, momenta, and every other dynamical variables, can be fully predicted. This is no longer true in quantum theory. Here is a summary.

#### Remarks

- A *single* measurement of  $A$  does not lead to a definite answer when the *state vector* is not an eigenvector  $\hat{A}$ .
- In general, a result of a measurement of  $A$  must be one of the eigenvalues. The outcome of a *single* experiment is *indeterminate*, and the quantum theory is probabilistic by its nature in contrast to the classical theory which is deterministic. When measurement is repeated several times, we will sometimes get an eigenvalue  $\alpha_j$  sometimes some other eigenvalue  $\alpha_k$ , and only the probabilities of each outcome can be predicted.
- A simple consequence of the above discussion is that a measurement of a dynamical variable  $A$  will give a value  $\alpha_m$  with probability 1 if and only if the state is represented by corresponding eigenvector  $|u_m\rangle$ .

- It must be remembered that some obvious changes, described later at the end of the next section, will be needed when the eigenvalues of  $\hat{A}$  are continuous.
- Finally, we leave it as an exercise for you to convince yourself that the assumption about the probabilities, as stated above, is correctly contained in the the following statement. *Given that the system is in a state described by the state vector  $|\psi\rangle$ , the probability that it will be found in the state given by the vector  $|\phi\rangle$  is equal to  $|\langle\phi|\psi\rangle|^2$ .*

## §4.2 Probabilities and Average Values

Let  $A$  denote a dynamical variable and  $\hat{A}$  the corresponding hermitian operator representing  $A$  in quantum mechanics. Let  $|u_n\rangle$  be normalised eigenvector of  $\hat{A}$  with eigenvalue  $\alpha_n$ .

$$\hat{A}|u_n\rangle = \alpha_n |u_n\rangle \quad (23)$$

These eigenvectors, being eigenvectors of a hermitian operator, will satisfy the orthogonality relation

$$\langle u_m | u_n \rangle = \delta_{mn}. \quad (24)$$

If several repeated measurements are made on a system with *state vector*  $|\psi\rangle$ , one would get  $\alpha_k$  with probability

$$p_k = |c_k|^2, \text{ where } c_k = \langle u_k | \psi \rangle. \quad (25)$$

The average of results of measurements of  $A$  in the state  $|\psi\rangle$ , to be denoted by  $\langle A \rangle_\psi$ , will then be given by

$$\langle A \rangle_\psi = \sum_k p_k \alpha_k = \sum_k \alpha_k |c_k|^2. \quad (26)$$

We will now show that the above expression coincides with  $\langle \psi | \hat{A} | \psi \rangle$ . Without loss of generality, we may assume that the state vector  $|\psi\rangle$  and the eigenvectors  $|u_k\rangle$  are normalised. To prove this result we recall that  $c_k$  are the expansion coefficients

$$|\psi\rangle = \sum_k c_k |u_k\rangle \quad (27)$$

and make use of orthonormal property (24) to compute  $\langle \psi | \hat{A} | \psi \rangle$ .

$$\langle \psi | \hat{A} | \psi \rangle = (\psi, \hat{A} \psi) \quad (28)$$

$$= (\psi, \hat{A} \sum_k c_k u_k) = \sum_k c_k (\psi, \hat{A} u_k) \quad (29)$$

$$= \sum_k c_k (\psi, \alpha_k u_k) = \sum_k c_k \alpha_k (\psi, u_k) \quad (30)$$

$$= \sum_k c_k \alpha_k \bar{c}_k = \sum_k \alpha_k |c_k|^2. \quad (31)$$

which is seen to be equal to the average  $\langle A \rangle_\psi$  from Eq.(26). When the state vector  $|\psi\rangle$  is not normalised, the average value will be given by

$$\langle A \rangle_\psi = \frac{\langle \psi | \hat{A} | \psi \rangle}{\langle \psi | \psi \rangle}. \quad (32)$$

**Case of continuous eigenvalues:** So far our discussion has been restricted to the case when the eigenvalues of  $\hat{A}$  are discrete. Now consider the case when the eigenvalues  $\alpha$  of  $\hat{A}$  are continuous and the corresponding eigenvectors  $|\alpha\rangle$  are normalised to Dirac delta function

$$\langle \alpha | \alpha' \rangle = \delta(\alpha - \alpha'). \quad (33)$$

In this case the probability that a measurement of  $A$  will give a value in a small range  $\alpha$  and  $\alpha + d\alpha$  is equal to  $|\langle \alpha | \psi \rangle|^2 d\alpha$ . For probability of finding the result in between  $a$  and  $b$ , we would have the answer  $\int_a^b |\langle \alpha | \psi \rangle|^2 d\alpha$ .

## §5 Canonical Quantization

### §5.1 Introduction

The first three postulates of quantum mechanics give a general framework applicable to any physical system. The first and the second postulates are about the mathematical structure of the quantum theory. These two postulates furnish a description of states and dynamical variables of quantum systems. The third postulate makes contact with experiments and talks about the possible outcomes of result of a measurement. Recall that while the second postulate says that the dynamical variables of a theory are represented by hermitian operators, no clue is provided in the first three postulates about properties of these operators. For example, the generalised coordinate and canonical momentum variables in quantum theory are replaced by operators, which we denote will by  $\hat{q}$  and  $\hat{p}$ . However, the rules to manipulate these operators must be formulated. In general, the product of two operators depends on the order in which they are multiplied, so information about their commutator will be useful.

The canonical quantisation rules(CCR) are important assumptions about the commutation relations of operators that represent position and momentum, and more generally, about the commutation relations obeyed by a pair of operators representing generalised coordinate and canonical conjugate momentum.

The CCR are extremely powerful statements about the operators. In principles CCR together with other postulates make almost all computations in quantum mechanics possible using algebraic methods, and no further information is needed.

## §5.2 Canonical commutation relations

Let  $q_1, q_2, \dots, q_N$  be generalised coordinates of a classical system having  $N$  degrees of freedom and let the corresponding canonical conjugate momenta be denoted by  $p_1, p_2, \dots, p_N$ . The canonical quantisation procedure consists in assuming that the corresponding operators satisfy the following canonical commutation relations (CCR).

$$[\hat{q}_i, \hat{q}_j] = 0; \quad [\hat{p}_i, \hat{p}_j] = 0, \quad (34)$$

$$[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij}. \quad (35)$$

It should be noted that  $\hbar$  has the correct dimension of product  $q_k p_k$  and that the commutators in Eq.(34)-(35) are  $i\hbar$  times the corresponding Poisson brackets in the classical theory.

The canonical commutation rules for a particle in one dimension, the operators  $\hat{q}, \hat{p}$ , corresponding the generalised coordinate and momentum take the form

$$[q, p] = i\hbar. \quad (36)$$

For a particle in three dimensions the position and momenta are  $x, y, z, p_x, p_y, p_z$  and the nonzero commutators are

$$[\hat{x}, \hat{p}_x] = [\hat{y}, \hat{p}_y] = [\hat{z}, \hat{p}_z] = i\hbar, \quad (37)$$

and the commutators of all other pairs of operators are zero. For general dynamical variables, other than coordinates and momenta, one has the following correspondence between the commutators and Poisson brackets in the limit  $\hbar \rightarrow 0$ .

$$\lim_{\hbar \rightarrow 0} [\hat{F}, \hat{G}] = i\hbar \{F, G\}_{\text{P.B.}}. \quad (38)$$

Here  $\hat{F}, \hat{G}$  represent operators associated with the classical dynamical variables  $F, G$  which will be functions of the generalised coordinates and canonical momenta.

**Question for You:** How do you understand that a factor  $i\hbar$  should appear in the righthand side of Eq.(38)?

## §5.3 General Form of Uncertainty Relation

For a particle in one dimension, the Heisenberg uncertainty relation

$$\Delta x \Delta p \geq \frac{\hbar}{2}, \quad (39)$$

using the canonical commutation relation

$$[\hat{x}, \hat{p}] = i\hbar\hat{I}, \quad (40)$$

where  $\hat{I}$  is the identity operator. The position momentum uncertainty relation is a special case of generalised relation

$$(\Delta A)_\psi(\Delta B)_\psi \geq \frac{\hbar}{2} |\langle \psi | C | \psi \rangle| \quad (41)$$

for two hermitian operators  $A, B$  having the commutator  $[A, B] = iC$ .

### Definitions and properties of uncertainty $\Delta X$

Several definitions and properties of uncertainty will be presented.

**Definition 1:** Assuming state vector  $|\psi\rangle$  to be normalized, the average of a dynamical variable in the state  $|\psi\rangle$  is given by  $\langle \psi | X | \psi \rangle$ . The uncertainty of a physical quantity  $X$  in a state  $\psi$  will be denoted as  $(\Delta X)_\psi$  and is defined by

$$(\Delta X)_\psi^2 = \langle \psi | \hat{X}^2 | \psi \rangle - (\langle \psi | \hat{X} | \psi \rangle)^2 \equiv \overline{X^2}_\psi - \overline{X}_\psi^2, \quad (42)$$

where notations  $\overline{X}_\psi$  and  $\langle X \rangle_\psi$ , both will be used to denote the average of an observable  $X$  in state  $\psi$  and omit the suffix  $\psi$  to simplify intermediate steps.

**Definition 2:** The uncertainty  $\Delta X$ , as given in (42) can be written in alternative form as

$$(\Delta X)_\psi^2 = \langle (\hat{X} - \overline{X})^2 \rangle_\psi. \quad (43)$$

TO see this note that

$$(\Delta X)_\psi^2 = \langle (\hat{X} - \overline{X})^2 \rangle_\psi \quad (44)$$

$$= \langle \psi | (\hat{X} - \overline{X})^2 | \psi \rangle \quad (45)$$

$$= \langle \psi | \hat{X}^2 - \hat{X}\overline{X} - \overline{X}\hat{X} + \overline{X}^2 | \psi \rangle \quad (46)$$

$$= \langle \psi | \hat{X}^2 - 2\overline{X}\hat{X} + \overline{X}^2 | \psi \rangle \quad (47)$$

$$= \langle \psi | \hat{X}^2 | \psi \rangle - \langle \psi | 2\overline{X}\hat{X} | \psi \rangle + \langle \psi | \overline{X}^2 | \psi \rangle \quad (48)$$

$$= \langle \psi | \hat{X}^2 | \psi \rangle - 2\overline{X} \langle \psi | \hat{X} | \psi \rangle + \overline{X}^2 \langle \psi | \psi \rangle = \overline{X^2} - 2\overline{X}^2 + \overline{X}^2 \quad (49)$$

$$= \overline{X^2} - \overline{X}^2 \quad (50)$$

**Definition 3:** The above alternate definition can be cast in a useful form. Remembering the  $X$  is a physical quantity and hence  $\hat{X}$  is hermitian. Therefore the average value of  $\hat{X}_\psi$  will be real and hence

$$(\hat{X} - \overline{X})^\dagger = (\hat{X}^\dagger - \overline{X}^*) = (\hat{X} - \overline{X}). \quad (51)$$

We will now show that uncertainty  $\Delta X$  can be also defined as

$$(\Delta X)_\psi = \|(\hat{X} - \bar{X})\psi\| \quad (52)$$

Consider the right hand expression and then we have

$$\|(\hat{X} - \bar{X})\psi\|^2 = ((\hat{X} - \bar{X})\psi, (\hat{X} - \bar{X})\psi) \quad (53)$$

$$= (\psi, (\hat{X} - \bar{X})^\dagger (\hat{X} - \bar{X})\psi) \quad (54)$$

$$= (\psi, (\hat{X} - \bar{X})^2\psi) \quad (55)$$

$$\therefore \langle (\hat{X} - \bar{X})^2 \rangle_\psi = \|(\hat{X} - \bar{X})\psi\|^2 \quad (56)$$

Substituting the above expression in the right hand side of (43), we get the third expression (52) for the uncertainty  $\Delta X$ .

It follows from the (52) that the uncertainty of a dynamical variable  $X$  in a state  $|\psi\rangle$  is zero if and only if Norm equals to zero iff vector equals to zero ,

$$(\hat{X} - \bar{X})|\psi\rangle = 0 \quad (57)$$

$$\text{or } \hat{X}|\psi\rangle = \bar{X}|\psi\rangle. \quad (58)$$

This implies that the state  $|\psi\rangle$  must be an eigenstate of the operator  $\hat{X}$ .

### Generalized uncertainty relation

We will now prove the generalised uncertainty relation given in Eq.(41). To simplify our notation we drop the suffix  $\psi$  in expressions for uncertainties and averages. We also stop using  $\hat{A}$  etc for operators. Thus in the following  $A, B, C$  appearing in mathematical expressions will stand for the operators.

As a first step, in derivation of Eq.(41), we use the Cauchy Schwarz inequality

$$\|f\|^2 \|g\|^2 \geq |\langle f|g \rangle|^2, \quad (59)$$

with  $|f\rangle = (A - \bar{A})|\psi\rangle$ , and  $|g\rangle = (B - \bar{B})|\psi\rangle$ . So we have , since  $A$  and  $B$  are hermitian ,

$$\langle f| = \langle \psi|(A^\dagger - \bar{A}^*) = \langle \psi|(A - \bar{A}) \quad (60)$$

$$\langle g| = \langle \psi|(B^\dagger - \bar{B}^*) = \langle \psi|(B - \bar{B}) \quad (61)$$

and therefore

$$\|f\|^2 = \langle f|f \rangle = \langle \psi|(A - \bar{A})^2|\psi\rangle, \quad (62)$$

$$\|g\|^2 = \langle g|g \rangle = \langle \psi|(B - \bar{B})^2|\psi\rangle, \quad (63)$$

$$\langle f|g \rangle = \langle \psi|(A - \bar{A})(B - \bar{B})|\psi\rangle. \quad (64)$$

Inserting these expressions into Cauchy Schwartz inequality, Eq.(59), we get

$$(\Delta A)^2 (\Delta B)^2 \geq |\langle \psi|(A - \bar{A})(B - \bar{B})|\psi\rangle|^2 \equiv |\langle \psi|X|\psi\rangle|^2, \quad (65)$$



where we have used  $X$  to denote the operator expression  $(A - \bar{A})(B - \bar{B})$ . We write the operator  $X$  as a sum of commutator and anticommutator of operators  $(A - \bar{A})$  and  $(B - \bar{B})$ :

$$X = (A - \bar{A})(B - \bar{B}) = \frac{1}{2}[(A - \bar{A}), (B - \bar{B})] - + + \frac{1}{2}[(A - \bar{A}), (B - \bar{B})]_- \quad (66)$$

$$\text{using } XY = \frac{1}{2}[X, Y]_+ + \frac{1}{2}[X, Y]_- \quad (67)$$

$$= \frac{1}{2}[(A - \bar{A}), (B - \bar{B})]_+ + \frac{i}{2}C. \quad (68)$$

This splitting of  $X$  into two parts allows us to separate the real and imaginary parts of  $\langle\psi|X|\psi\rangle$  and to compute its absolute square needed in Eq.(65):

$$\langle\psi|X|\psi\rangle = \frac{1}{2}\langle\psi|[(A - \bar{A}), (B - \bar{B})]_+|\psi\rangle + \frac{i}{2}\langle\psi|C|\psi\rangle. \quad (69)$$

Both the quantities marked with braces, being average values of hermitian operators, are *real*. Hence

$$|\langle\psi|X|\psi\rangle|^2 = \frac{1}{4}|\langle\psi|[(A - \bar{A}), (B - \bar{B})]_+|\psi\rangle|^2 + \frac{1}{4}|\langle\psi|C|\psi\rangle|^2. \quad (70)$$

Therefore, the inequality Eq.(65) becomes

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}|\langle\psi|[(A - \bar{A}), (B - \bar{B})]_+|\psi\rangle|^2 + \frac{1}{4}|\langle\psi|C|\psi\rangle|^2 \quad (71)$$

$$\therefore (\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}|\langle\psi|C|\psi\rangle|^2. \quad (72)$$

This gives us the desired generalised form of uncertainty relation

$$\Delta A \Delta B \geq \frac{1}{2}|\langle C \rangle_\psi|. \quad (73)$$

For position and momentum  $[\hat{x}, \hat{p}] = -\hbar$ , and hence we have

$$(\Delta x)_\psi (\Delta p)_\psi \geq \frac{\hbar}{2} \cdot \langle\psi|C|\psi\rangle \quad (74)$$

### Minimum uncertainty states

Let us now ask, "Which states will have the minimum value of the uncertainty product?" Going back to the first step and analysing the proof, for equality to hold in the uncertainty relation (73), the Cauchy Schwarz inequality, Eq.(59), must become equality. This will be the case if and only if  $|f\rangle = \lambda|g\rangle$ , for some complex number  $\lambda$ . In addition to this, the average of the anticommutator in Eq.(71) should zero. Thus necessary and sufficient conditions for state  $|\psi\rangle$  to be state with minimum uncertainty becomes

$$(A - \bar{A})|\psi\rangle = \lambda(B - \bar{B})|\psi\rangle, \quad [(A - \bar{A}), (B - \bar{B})]_+|\psi\rangle = 0. \quad (75)$$

## §6 Simultaneous Measurement

### §6.1 Compatible Observables

Let  $A$  and  $B$  be two dynamical variables,  $\hat{A}, \hat{B}$  be the corresponding operators,  $\alpha_j, j = 1, 2, \dots$  and  $\beta_k, k = 1, 2, \dots$  be their eigenvalues.

Let us assume that  $A$  and  $B$  can be measured simultaneously. This means there are states in which these variables have definite values  $\alpha_j, \beta_k, j, k = 1, 2, \dots$ . The corresponding vectors  $|\alpha_j, \beta_k\rangle$  must then be simultaneous eigenvectors of the two operators.

$$\hat{A}|\alpha_j, \beta_k\rangle = \alpha_j|\alpha_j, \beta_k\rangle, \quad \hat{B}|\alpha_j, \beta_k\rangle = \beta_k|\alpha_j, \beta_k\rangle \quad (76)$$

In order that the probability of getting pair of values  $\alpha_j, \beta_k$  for all pairs  $j, k$  be given by the postulate III, it should be possible to write an arbitrary vector  $|\psi\rangle$  as linear combination of these vectors  $\mathcal{B} = \{|\alpha_j, \beta_k\rangle | j = 1, 2, \dots, k = 1, 2, \dots\}$  and these states must form a basis.

Now it is easy to show that the action of  $\hat{A}\hat{B} - \hat{B}\hat{A}$  on each of these vectors in the set  $\mathcal{B}$  is zero. In fact

$$(\hat{A}\hat{B} - \hat{B}\hat{A})|\alpha_j, \beta_k\rangle = \hat{A}\hat{B}|\alpha_j, \beta_k\rangle - \hat{B}\hat{A}|\alpha_j, \beta_k\rangle \quad (77)$$

$$= \hat{A}\beta_k|\alpha_j, \beta_k\rangle - \hat{B}\alpha_j|\alpha_j, \beta_k\rangle \quad (78)$$

$$= \alpha_j\beta_k|\alpha_j, \beta_k\rangle - \beta_k\alpha_j|\alpha_j, \beta_k\rangle \quad (79)$$

$$= 0. \quad (80)$$

Thus we have proved that the action of commutator  $[\hat{A}, \hat{B}]$  on every element of basis  $\mathcal{B}$  results in zero. This implies that  $[\hat{A}, \hat{B}] = 0$  and the two operators  $\hat{A}, \hat{B}$  must commute.

Conversely, if two hermitian operators commute, one can select a basis of orthonormal vectors which are simultaneous eigenvectors of the two operators.

The above considerations generalize to several dynamical variables.

A set of operators  $\{\hat{A}_k, k = 1, 2, \dots\}$  is called *commuting set* if every pair of operators  $\hat{A}_\ell, \hat{A}_m$  commute, *i.e.*

$$[\hat{A}_\ell, \hat{A}_m] = 0 \quad \text{for all pairs } \ell, m. \quad (81)$$

A set of dynamical variables  $\{A_k, k = 1, 2, \dots\}$  is called a compatible set if the corresponding set of operators  $\{\hat{A}_k, k = 1, 2, \dots\}$  is a commuting set of operators. It then follows that

#### REMEMBER

"A set of dynamical variables can be measured simultaneously if and only if they commute pairwise. In other words they should form a compatible set."

## §6.2 Functions of Operators

Let  $\hat{X}$  be an operator which has eigenvalues and eigenvectors  $\{\lambda_k, |u_k\rangle | k = 1, 2, \dots\}$ . Let us further assume that the span of eigenvectors of  $\hat{X}$  is entire vector space. Then a function  $\hat{F}(X)$  of the operator  $\hat{X}$  is defined by specifying its action on the basis formed by the eigenvectors  $\mathcal{B} = \{|u_k\rangle | k = 1, 2, \dots\}$

$$\hat{F}(X)|u_k\rangle \equiv F(\lambda_k)|u_k\rangle, \quad k = 1, 2, \dots \quad (82)$$

The action of the function  $\hat{F}(X)$  on an arbitrary vector  $|\psi\rangle$  is obtained, as usual, by expanding the vector  $|\psi\rangle$  in the basis  $\mathcal{B}$ :

$$|\psi\rangle = \sum_k c_k |u_k\rangle \quad (83)$$

$$\hat{F}(X)|\psi\rangle = \sum_k c_k F(\lambda_k) |u_k\rangle. \quad (84)$$

As the hermitian operators and unitary operators have a complete set of orthonormal eigenvectors, their functions are defined by the method outlined above.

It is a simple exercise to show that if an operator  $\hat{Y}$  commutes with  $\hat{X}$ , it commutes with every function of  $\hat{X}$ .

**Complete commuting set:** A set  $\mathcal{S}$  of operators is called *complete commuting set* if it is a commuting set and if any operator which commutes with every member of the set  $\mathcal{S}$  can be written as function of the operators in the set  $\mathcal{S}$ .

The concept of complete commuting set is important in choosing a basis and working with representations as against with abstract vector space.

For more details, we refer the reader to

T. F. Jordan, *Linear Operators for Quantum Mechanics*, John Wiley and Sons, New York (1969)

## §6.3 Setting up a Representation

Section on representation to be brought here

## §7 Time Evolution

### §7.1 Time development in quantum mechanics

Description of state of a quantum mechanical system at one time is by state vector in the Hilbert space. As the system evolves this state vector will change. General requirements on time evolution lead to time evolution governed by unitary operator and for short times by a hermitian operator  $H$  which will be identified with Hamiltonian of the system.

Let  $|\psi t_0\rangle$  represent the state of system at time  $t_0$  and  $|\psi t\rangle$  represent the state at time  $t$ . We assume that  $|\psi t_0\rangle$  at time  $t_0$  determines the state at time  $t$  completely. The principle of superposition should apply at these two times  $t_0$  and  $t$ . If we have a relation at time  $t_0$

$$|\psi t_0\rangle = \alpha|\chi t_0\rangle + \beta|\phi t_0\rangle \quad (85)$$

between three possible states,  $|\psi\rangle, |\chi\rangle, |\phi\rangle$ , the same relation must hold at all times  $t > t_0$  when the system is left undisturbed

$$|\psi(t)\rangle = \alpha|\chi t\rangle + \beta|\phi t\rangle \quad (86)$$

Thus if we write

$$|\psi t\rangle = U(t, t_0)|\psi t_0\rangle \quad \text{etc.} \quad (87)$$

Then  $U(t, t_0)$  must be a linear operator independent of  $\psi$ . Obviously  $U$  must reduce to the identity operator at time  $t = t_0$

$$U(t_0, t_0) = I \quad (88)$$

Next we demand that the norm of vector  $|\psi t\rangle$  should not change with time and hence

$$\langle\psi t|\psi t\rangle = \langle\psi t_0|\psi t_0\rangle \quad \text{for all } t \quad (89)$$

The above requirements (2) and (5), respectively, imply that the operator  $U$  must be a linear operator and that it must be unitary.

$$UU^\dagger = U^\dagger U = I \quad (90)$$

We shall now derive a differential equation satisfied by the state vector at time  $t$ . We, therefore, compute

$$\begin{aligned} \frac{d}{dt}|\psi t\rangle &= \lim_{\Delta t \rightarrow 0} \frac{|\psi t + \Delta t\rangle - |\psi t\rangle}{\Delta t} \\ &= \lim_{\Delta t \rightarrow 0} \frac{(U(t + \Delta t, t) - I)}{\Delta t} |\psi t\rangle \end{aligned} \quad (91)$$

$$\text{or } \frac{d}{dt}|\psi t\rangle = \hat{X}|\psi t\rangle \quad (92)$$

$$\begin{aligned} \text{where } \hat{X}(t) &= \lim_{\Delta t \rightarrow 0} \frac{U(t + \Delta t, t) - I}{\Delta t} \\ &= \frac{d}{dt'} U(t, t')|_{t'=t} \end{aligned} \quad (8'')$$

The operator  $\hat{X}$  can be shown to be anti-hermitian and hence with notation  $H(t) \equiv X/(i\hbar)$ ,  $H(t)$  will be hermitian. We therefore write Eq.(92) as

$$i\hbar \frac{d}{dt}|\psi t\rangle = \hat{H}(t)|\psi t\rangle \quad (93)$$

where

$$\hat{H}(t) = \frac{1}{i\hbar} \frac{\partial}{\partial t} U(t, t')|_{t'=t} \quad (94)$$

We shall now check that  $H(t)$  must be a hermitian operator. Consider

[Link\[?\]](#)

$$U^\dagger(t, t')U(t, t') = I \quad (95)$$

Differentiating w.r.t.  $t$  we get

$$\left\{ \frac{\partial}{\partial t} U^\dagger(t, t') \right\} U(t, t') + U^\dagger \left\{ \frac{\partial}{\partial t} U(t, t') \right\} = 0 \quad (96)$$

Setting  $t' = t$  and using  $U(t, t) = I$  we have

$$\frac{d}{dt} U^\dagger(t, t')|_{t'=t} + \frac{d}{dt} U(t, t')|_{t'=t} = 0 \quad (97)$$

$$\text{or} \quad \left( \frac{1}{i\hbar} \hat{H} \right)^\dagger + \frac{1}{i\hbar} \hat{H} = 0 \quad (98)$$

$$\text{or} \quad -i\hat{H}^\dagger + \hat{H} = 0 \quad (99)$$

$$\text{or} \quad \hat{H}^\dagger = \hat{H} \quad (100)$$

Thus the time evolution of a quantum system is governed by the equation

$$i\hbar \frac{\partial}{\partial t} |\psi t\rangle = \hat{H}(t) |\psi t\rangle \quad (101)$$

Using correspondence with classical mechanics, Dirac shows that the operator  $\hat{H}$  represents the energy (or the Hamiltonian) of the system. ( See §2 below and the discussion in the end of this section.) Using (3) in (18) we get

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) |\psi t_0\rangle = \hat{H}(t) U(t, t_0) |\psi t_0\rangle \quad (102)$$

This equation must hold for all vectors  $|\psi\rangle$ . Hence the time evolution operator  $U$  must satisfy the differential equation

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) = \hat{H}(t) U(t, t_0) . \quad (103)$$

## §7.2 Time development of averages

### Time variation of average values

The time evolution of a quantum system is governed by the Schrodinger equation

$$i\hbar \frac{d}{dt} |\psi t\rangle = \hat{H} |\psi t\rangle . \quad (104)$$

We will obtain an equation for time development of averages of a dynamical variable  $\hat{F}$ . The result will turn out to have an obvious correspondence with the classical equation of motion for dynamical variable  $F$ . This then will suggest the identification of  $\hat{H}$  as the operator representing the Hamiltonian of the system.

Let  $F(q, p, t)$  be an dynamical variable of the system and let  $\hat{F}$  denote the corresponding operator. We are interested in finding out how the average value

$$\langle \hat{F} \rangle \equiv \langle \psi t | \hat{F} | \psi t \rangle \quad (105)$$

changes with time. The time dependence of the average value comes from dependence of the three objects, the operator  $\hat{F}$ , the bra vector  $\langle \psi t |$ , and the ket vector  $|\psi t\rangle$ , present in Eq.(105). The equation conjugate to the Schrodinger equation

$$i\hbar \frac{d}{dt} |\psi t\rangle = \hat{H} |\psi t\rangle \quad (106)$$

is given by

$$-i\hbar \frac{d}{dt} \langle \psi t | = \langle \psi t | \hat{H}^\dagger \quad (107)$$

Since the operator  $\hat{H}$  is hermitian, the above equation takes the form

$$-i\hbar \frac{d}{dt} \langle \psi t | = \langle \psi t | \hat{H} \quad (108)$$

Therefore

$$\frac{d}{dt} \langle \hat{F} \rangle = \left( \frac{d}{dt} \langle \psi t | \right) \hat{F} |\psi t\rangle + \langle \psi t | \frac{d\hat{F}}{dt} |\psi t\rangle + \langle \psi t | \hat{F} \left( \frac{d}{dt} |\psi t\rangle \right) \quad (109)$$

Using Eq.(107) and Eq.(108) in Eq.(109) we get

$$\frac{d}{dt} \langle \hat{F} \rangle = -\frac{1}{i\hbar} \langle \psi t | \hat{H} \hat{F} |\psi t\rangle + \langle \psi t | \frac{d\hat{F}}{dt} |\psi t\rangle + \frac{1}{i\hbar} \langle \psi t | \hat{F} \hat{H} |\psi t\rangle \quad (110)$$

The above equation is rearranged to give the final form

$$\frac{d}{dt} \langle \hat{F} \rangle = \left\langle \frac{\partial}{\partial t} \hat{F} \right\rangle + \frac{1}{i\hbar} \langle [\hat{F}, \hat{H}] \rangle \quad (111)$$

This result is known as Ehrenfest theorem. Comparing the Eq.(111) with the equation of motion in classical mechanics for time evolution of dynamical variables

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \{F, H\}_{PB} \quad (112)$$

and remembering that the commutator divided by  $i\hbar$  corresponds to the Poisson bracket in the limit  $\hbar \rightarrow 0$ , we see that  $\hat{H}$  must be identified as the operator corresponding to the Hamiltonian  $H$  of the system.

### §7.3 Solution of time dependent Schrödinger equation.

A scheme to solve the time dependent Schrödinger equation

$$i\hbar \frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle \quad (113)$$

is described. The solution will be presented in the form

$$|\psi t\rangle = U(t, t_0)|\psi t_0\rangle \quad (114)$$

**For our present discussion, it will be assumed that the Hamiltonian  $\hat{H}$  does not depend on time explicitly. Let the state vector of system at initial time  $t = 0$  be denoted by  $|\psi_0\rangle$ .**

Since  $\hat{H}$  is always assumed to be hermitian, its eigenvectors form an orthonormal complete set and we can expand the state vector at time  $t$ ,  $|\psi t\rangle$ , in terms of the eigenvectors. Denoting the normalized eigenvectors by  $|E_n\rangle$ , we write

$$|\psi t\rangle = \sum_n c_n(t)|E_n\rangle. \quad (115)$$

where the constants  $c_n(t)$  are to be determined. Substituting (115) in (113) we get

$$i\hbar \frac{d}{dt} \sum_n c_n(t)|E_n\rangle = \hat{H}|\psi t\rangle \quad (116)$$

$$i \sum_n \hbar \frac{dc_n(t)}{dt} |E_n\rangle = \sum_n c_n(t) \hat{H} |E_n\rangle \quad (117)$$

Taking scalar product with  $|E_m\rangle$  and using orthonormal property of the eigenvectors  $|E_n\rangle$ , we get

$$i\hbar \frac{dc_m(t)}{dt} = E_m c_m(t). \quad (118)$$

which is easily solved to give

$$c_m(t) = c_m(0)e^{-iE_m t/\hbar}. \quad (119)$$

Therefore,  $|\psi t\rangle$ , the solution of time dependent equation becomes

$$|\psi t\rangle = \sum_m c_m(0)e^{-iE_m t/\hbar} |E_m\rangle. \quad (120)$$

The coefficients  $c_m(0)$  are determined in terms of the state vector  $|\psi_0\rangle$  at time  $t = 0$  by setting time  $t = 0$  in the above equation. This gives

$$|\psi_0\rangle = \sum_n c_n(0)|E_n\rangle. \quad (121)$$

The unknown coefficients  $c_n(0)$  can now be computed; taking scalar product of Eq.(121), with  $|E_m\rangle$  we get

$$c_m(0) = \langle E_m | \psi_0 \rangle. \quad (122)$$

Thus Eq.(120) and (122) give the solution of the time dependent Schrödinger equation as

$$\boxed{|\psi t\rangle = \sum_n c_n(0) \exp(-i\hbar E_n t) |E_n\rangle}. \quad (123)$$

The right hand side of the above equation can be rewritten as

$$\sum_n c_n(0) \exp(-i\hbar E_n t) |E_n\rangle = \sum_n c_n(0) \exp(-i\hbar H t) |E_n\rangle \quad (124)$$

$$= \exp(-i\hbar H t) \cdot \sum_n c_n(0) |E_n\rangle \quad (125)$$

Therefore Eq.(123) takes the form

$$|\psi t\rangle = \exp(-iHt/\hbar) |\psi_0\rangle. \quad (126)$$

In general, if the state vector is know at time  $t = t_0$ , instead of time  $t = 0$ , the result Eq.(126) takes the form

$$|\psi t\rangle = \exp(-iH(t - t_0)/\hbar) \sum_n c_n(t_0) |E_n\rangle \quad (127)$$

$$= \exp(-iH(t - t_0)/\hbar) |\psi t_0\rangle. \quad (128)$$

The time evolution operator  $U(t, t_0)$ , of Eq.(114), is therefore given by

$$\boxed{U(t, t_0) = \exp(-iH(t - t_0)/\hbar)}. \quad (129)$$

## §7.4 Stationary states and constants of motion

### Stationary states

Let us consider time evolution of a system if it has a definite value of energy at an initial time  $t_0$ . The value of the energy then has to be one of the eigenvalues and the state vector will be the corresponding eigenvector. So  $|\psi t_0\rangle = |E_m\rangle$ , then at time  $t$  the system will be in the state given by

$$|\psi t\rangle = U(t, t_0) |E_m\rangle = \exp(-iE_m(t - t_0)/\hbar) |E_m\rangle. \quad (130)$$

It must be noted that the state vector at different times is equal to the initial state vector times a *numerical phase factor* ( $\exp(-iE_m(t - t_0)/\hbar)$ ). Therefore, the vector at time  $t$  represents the same state at all times. Such states are called **stationary states** because



the state does not change with time. Every eigenvector of energy is a possible stationary state of a system. In such a state the average value of a dynamical variable,  $\hat{X}$ , not having time explicitly, is independent of time even if  $\hat{X}$  does not commute with Hamiltonian. In fact the probabilities of finding a value on a measurement of the dynamical variable are independent of time.

### Constant of motion

Unless mentioned otherwise, we shall always assume that the Hamiltonian  $H$  of the system under discussion is independent of time.

If the dynamical variable  $F$  does not contain explicit time dependence, then we have  $\frac{\partial F}{\partial t} = 0$ . If such an operator  $\hat{F}$  commutes with the Hamiltonian operator  $\hat{H}$ , we will have

$$\boxed{[\hat{F}, \hat{H}] = 0}. \quad (131)$$

Eq.(111) shows that

$$\frac{d}{dt} \langle \psi t | \hat{F} | \psi t \rangle = 0$$

Therefore in an arbitrary state, the average value of  $\hat{F}$  does not change with time. Such a dynamical variable will be called a **constant of motion**.

### §7.5 Summary

- Given the state of the system at a time  $t_0$ , the state vector at any other time is related to it by a unitary transformation  $U(t, t_0)$ .

$$|\psi t\rangle = U(t, t_0) |\psi t_0\rangle$$

- The equation of motion of quantum system is the Schrodinger equation

$$i\hbar \frac{d}{dt} |\psi t\rangle = \hat{H} |\psi t\rangle$$

where  $\hat{H}$  is the Hamiltonian operator of the system.

- The time evolution operator satisfies the equation

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) |\psi t_0\rangle = \hat{H}(t) U(t, t_0)$$

- If the Hamiltonian does not depend on time, the evolution operator is

$$U(t, t_0) = \exp[-i\hat{H}(t - t_0)/\hbar]$$

- The average value of a dynamical variable,  $\hat{F}$ , satisfies

$$\frac{d}{dt} \langle \hat{F} \rangle = \left\langle \frac{\partial \hat{F}}{\partial t} \right\rangle + \frac{1}{i\hbar} \langle [\hat{F}, \hat{H}] \rangle$$

- A dynamical variable is a constant of motion if it commutes with the Hamiltonian.
- The energy eigenstates of a system are stationary; they do not change with time. The state vector of a stationary state at any time is equal to the initial state vector multiplied by a numerical phase factor.
- The average value of a *constant of motion*  $G$  is independent of time in every possible state of the system including *nonstationary states*.
- The average value of *every* dynamical variable is independent of time in *stationary* states.

## §7.6 Time Evolution of Quantum Systems

The state vector at a given time specifies the state of the system at a given time and the state at any time is obtained by solving the Schrödinger equation.

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle. \quad (132)$$

where  $H$  is the Hamiltonian operator. The reason for identification of  $H$ , in the above equation, with Hamiltonian is best brought out in by means of correspondence with equations in classical mechanics.

From now on we will assume that the Hamiltonian  $H$  does not depend on time. In this case the state vector at time  $t$  is related to the state vector at initial time  $t_0$  by

$$|\psi t\rangle = U(t, t_0)|\psi t_0\rangle \quad (133)$$

where

$$U(t, t_0) = \exp\left(-\frac{iH(t-t_0)}{\hbar}\right) \quad (134)$$

Since  $H$  is a hermitian operator, it follows that  $U(t, t_0)$  is a unitary operator.

The Hamiltonian operator being Hermitian leads to the following important consequences. In the table below a few examples of time evolution of states are given.

**Table : Time evolution energy eigenstates of a quantum system**

S.N.	State at time $t = 0$	State at time $t$
1.	$ E_n\rangle$	$e^{-iE_n t/\hbar} E_n\rangle$
2.	$c_1 E_1\rangle + c_2 E_2\rangle$	$c_1e^{-iE_1/\hbar} E_1\rangle + c_2e^{-iE_2/\hbar} E_n\rangle$
3.	$\sum_k c_k E_k\rangle$	$\sum_k c_k e^{-iE_k t/\hbar} E_k\rangle$
4.	If states $ \psi t_0\rangle,  \phi t_0\rangle$ then $c_1 \psi t_0\rangle + c_2 \phi t_0\rangle$	evolve into $ \psi t\rangle,  \phi t\rangle$ , evolves into $c_1 \psi t\rangle + c_2 \phi t\rangle$

- The first row in the table shows that the energy eigenstates

$$H|E_n\rangle = E_n|E_n\rangle \quad (135)$$

*i.e.* the states corresponding to a definite value of energy, have a very simple time evolution. The state vector changes by phase factor, a multiplicative constant of absolute value 1. Thus the state itself does not change with time. Therefore energy states are called *stationary states*.

- The time evolution preserves the superposition of states as is brought out by the examples in the second and last rows of the table.
- The time evolution is unitary and hence norm of the state vector is preserved. Mathematically this means that the norm  $\langle\psi t|\psi t\rangle$  is independent of time. In other words

$$\langle\psi t|\phi t\rangle = \langle\psi t_0|\phi t_0\rangle \quad (136)$$

$$\text{and } \frac{d\|\psi(t)\|^2}{dt} = 0 \quad (137)$$

Remembering that  $\|\psi(t)\|^2$  is just the sum of probabilities of all possible outcomes, The above result has a physical interpretation that the total probability of all possible outcomes of a measurement remains constant ( $= 1$ ) at all times.

Here the results given above are a consequence of Hamiltonian being hermitian.

In an alternate approach [?], one can start from requirements that superposition be preserved and the normalization of the state vector should not change with time and prove that this leads to an equation of the form (132) where  $H$  some hermitian operator.

Identification with operator corresponding to Hamiltonian can then be done by making use of classical correspondence.

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