

QM-01 Lecture Notes

Classical Theories Revisited *

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§1 Concept of Waves and Particles in Classical Theory

§1.1 Introduction

From the times of Newton, it has been debated whether light is like a beam of corpuscles or is it a wave? It was believed that only one of these properties could be associated with a beam of light as the characteristic properties of classical particles and waves appeared to be incompatible. We briefly recall the differences between waves and particles.

A particle cannot be subdivided, whereas one can *subdivide* a wave indefinitely. For a wave, the intensity can be reduced continuously without any limit. The waves transfer energy and momentum in a continuous fashion. For a beam of particles, the intensity cannot be reduced indefinitely, beyond having one particle at “one time“. An exchange of energy momentum from particles takes place in a discrete fashion.

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A particles is localised in space where as the waves are, generally, not localised. A particle follows a well defined trajectory, but no trajectory can be associated with waves. A particle cannot bend round a corner, whereas waves exhibit the phenomena of diffraction.

The waves show phenomena of interference. Thus two waves of intensity I , meeting at a point, can give rise to resultant wave of intensity between 0 and $4I$. Clearly a similar situation for particles is not possible; two bullets meeting at point cannot destroy each other, nor do they create bullets giving rise to four bullets. A beam of bullets will not show phenomena of polarisation exhibited by (transverse) waves.

For a complete specification of the state of a particle we require a finite number of coordinates and momenta. The waves are specified by infinite number of "coordinates", an amplitude at each point of the medium. All waves, for example sound waves, can be thought of as a collection of an infinite number of oscillators. For sound waves these oscillators are just that particles of the medium. Light can also be thought of as a collection of infinite number oscillators, but without any medium being associated with it.

Some of the differences between wave and particle natures, outlined above, will be highlighted with the help of some *Gedanken experiments* (thought experiments) in the next few sections.

§1.2 Thought experiments with waves

Single Slit Experiment with Waves

The interference and diffraction are characteristic properties of waves. When a wave falls on a slit, a diffraction pattern is observed as the waves can bend round the corners of the slit. Consider the experimental set up of Fig.1 where a wave travelling along the z -axis passes through a slit and hits a screen where the intensity of waves is measured as a function of x . If a is the slit width and λ is the wave length, the intensity as a function of x is given by

$$I = I_0 \left(\frac{\sin \alpha}{\alpha} \right)^2, \quad (1)$$

where

$$\alpha = \frac{\pi a}{\lambda} \sin \theta, \quad \sin \theta \approx \tan \theta = \frac{x}{L}, \quad (2)$$

and L is the distance of the screen from the slit. The waves not only reach the point $x = 0$, but a significantly large part of the wave is received for large values of x . If the intensity of the incident wave is reduced, one would continue to get the same pattern, even for arbitrarily low values of the intensity of the incident waves.

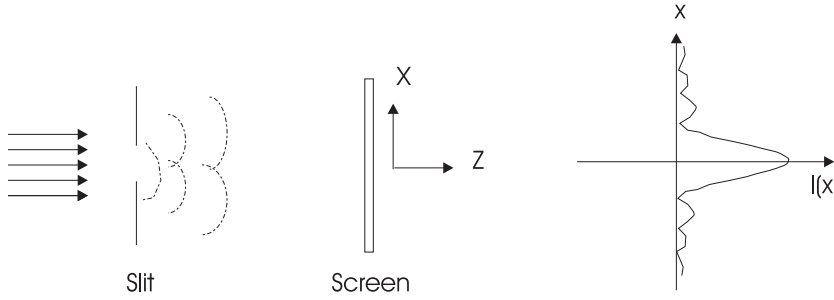


Fig. 1 Single Slit Experiment with Waves

Double Slit Experiment With Waves

In a double slit arrangement wave travels through each slit and on reaching a point, at position \vec{r} , on the screen, the two parts interfere and produce an interference pattern. This is because the waves travelling through different paths have a phase difference δ and the resultant amplitude ϕ at any point is given by the sum of the amplitudes, ϕ_1, ϕ_2 of the waves coming through the two slits :

$$\phi_1(\vec{r}, t) = A_1 \exp(i\vec{k} \cdot \vec{r}) \quad (3)$$

$$\phi_2(\vec{r}, t) = A_2 \exp(i\vec{k} \cdot \vec{r} + i\delta), \quad (4)$$

$$\phi = \phi_1 + \phi_2. \quad (5)$$

The resultant intensity is then given by

$$I_{12} = |\phi_1 + \phi_2|^2 = |\phi_1|^2 + |\phi_2|^2 + (\phi_1^* \phi_2 + \phi_1 \phi_2^*). \quad (6)$$

Here the first, the second and the third terms give the intensity due to the first slit, the second slit and the interference term, respectively. When the intensity of the incident waves is reduced, we continue to get the same intensity distribution pattern on the screen. Assuming that the detectors placed on the screen can measure arbitrarily low intensity by collecting waves received over a large period of time, the intensity pattern would look the same irrespective of the intensity of the incident beam.

Double slit experiment with only one slit open at a time

Let us now consider a variation of the double slit interference experiment, keeping only one slit open at a time. Let us assume that only one slit is kept open for time $0 < t < T$ and the second slit is closed. During the time $T < t < 2T$, the second slit is kept open and the first slit is kept closed. In this case what intensity pattern do you expect to see on the screen? Would one get the interference pattern

$$I_{12} = |\phi_1 + \phi_2|^2 \quad (7)$$

or simply the sum of intensities due to the two slits:

$$I = I_1 + I_2 = |\phi_1|^2 + |\phi_2|^2? \quad (8)$$

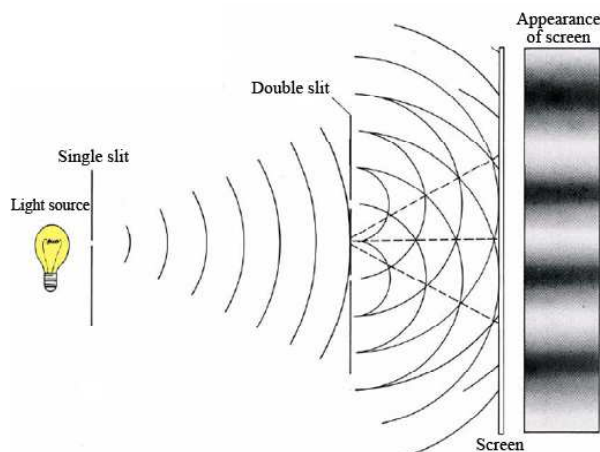


Fig. 2 Source:Internet

Interference can take place only between parts of a wave arriving simultaneously at a point with a phase difference. This happens when different parts of a wave arrive taking different paths. When only each slit is kept open for half the time, we expect to observe the intensity pattern $I_1 + I_2$ which is just the sum of intensities due to the two individual slits. While there is no doubt about the conclusion, the issue has to be settled only by doing an experiment. Primary reference for a discussion of waves and particle concepts is [1].

§1.3 Thought experiments with bullets

Waves can turn around the corners but not particles, certainly not the bullets. Consider an experiment with bullets fired along the z -axis from a gun and hitting a wall with a slit. Next to the wall there is a screen where all bullets are stopped and are collected in containers placed at different positions. The number of bullets, $N(x)$, received in a container placed at x , in a given time t , is counted. We plot the number of bullets as function of x . Assuming an ideal parallel beam of bullets, travelling in the z -direction, only the containers with positions in the range $d \leq x \leq d$ will receive the bullets, where $2d$ is the slit width. The container placed at far away positions will not receive any bullet. We should expect to see a distribution as in Fig.1.2. The bullets cannot bend round the corners of the slit and cannot reach containers at positions $|x| > d$.

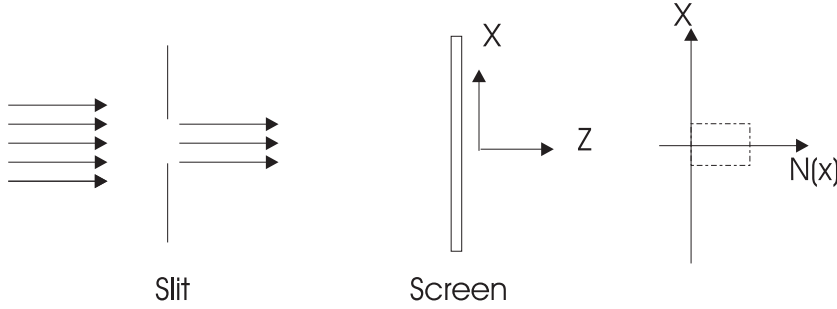


Fig. 3 Single slit experiment with bullets

Double slit experiment

If a double slit experiment is performed with two slits, one would get a count distribution pattern, $N(x)$, which is just the sum of the patterns corresponding to the two individual slits.

$$N(x) = N_1(x) + N_2(x). \quad (9)$$

Note that each bullet must pass through one of the slits, unlike waves where parts of the incident wave could pass through each slit and produce an interference pattern. The result will remain unchanged if the experiment with the bullets is repeated with each slit open only half the time.

A probabilistic description

The classical theory is deterministic in the sense that, knowing the initial position and momentum of a bullet, one can predict where it will hit the screen. Now imagine a gun firing the bullets randomly at different angles, with a maximum number of bullets along the z -axis. In this case, the bullets would reach positions outside the range $(-d, d)$ and the number of bullets reaching a point x will be as shown above. Assuming that the angle between the z -axis and the initial direction of a bullet is random, and not known a priori, it will not be possible to predict where the bullet would hit the screen. For a small number of bullets the distribution $N(x)$ of the bullets on the screen cannot be predicted. But, if the experiment is repeated sufficiently many times we expect to see the same distribution $N(x)$, irrespective of the rate of firing the bullets. In such a case, how do we describe the outcome of an experiment with a single bullet? We associate a probability distribution $P(x)$ that a bullet will hit the screen at a position x . If N_0 is the total number of bullets in the experiment, then

$$P(x) = \frac{N(x)}{N_0} \quad (10)$$

In a double slit experiment we would expect to see a distribution

$P_{12}(x)$:

$$P_{12}(x) = P_1(x) + P_2(x), \quad (11)$$

where

$P_{12}(x)$ = Probability that a bullet reaches position x when both the slits are open,

$P_1(x)$ = Probability that a bullet reaches position x when only the first slit is open,

$P_2(x)$ = Probability that a bullet reaches position x when only the second slit is open.

The outcome of an experiment with waves can also be described in probabilistic terms. We normalise the intensity of waves at a position x by the intensity of the incident waves, I_0 , and associate a probability $P(x) = I(x)/I_0$, which would give the intensity pattern as a function of x . Here it must be emphasised that a probabilistic description for waves is purely a matter of taste or convenience, but for bullets we are forced to introduce the probabilistic description because of incomplete information about the initial momentum of the bullets. Even in this case, the classical theory is deterministic in the sense that each bullet takes a well defined trajectory which can be predicted if the initial position and momentum are known accurately. A knowledge of the probability distribution of the angle at which bullet is fired, will in principle permit us to compute $P(x)$ and the number of bullets reaching a container at position x .

§1.4 Waves versus particles

Waves vs particles

An analysis of single and double slit experiments with waves and beams of particles brings out the fact that a wave bends round the corners, whereas particles do not. Interference phenomenon seen in the double slit experiment emphasises that a part of a wave passes through one slit and another part passes through another slit and an interference pattern is produced when parts of waves from different paths meet on the screen. The bullets (particles) have a well defined trajectory and for a beam of particles, each particle must pass through one of the slits and no interference pattern is produced. While in interaction with other physical systems, the waves transfer energy and momentum in a continuous fashion, in contrast, the particles transfer energy and momentum in a discrete manner. Another important difference between the waves and particles is that a wave can be subdivided indefinitely by cutting down the intensity. For a beam of particles, the intensity cannot be reduced beyond having a single particle at a time.

The particle and the wave aspects appear to be incompatible and it would seem impossible that they could coexist for a physical system. However, the nature has its own way and it is amazing that all particles show a wave nature and all waves have a particle nature. First indications came from the photoelectric effect from its explanation in 1905 by Einstein. Next came the matter wave hypothesis by de Broglie and its confirmation by Davisson Germer experiments and it was established that the electrons exhibit wave

nature. It is now accepted that all matter has a wave nature associated with it. This lead to acceptance of 'every body' having a dual nature, behaving like both a wave and a particle.

§2 Structure and Formulations of Mechanics

§2.1 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

$$m_\alpha \frac{d^2 \vec{r}_\alpha}{dt^2} = \vec{F}_\alpha \quad (12)$$

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 Newtons 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.

§2.2 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

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}_k} \right) - \frac{\partial \mathcal{L}}{\partial q_k} = 0, \quad k = 1, 2, \dots \quad (13)$$

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 :

$$p_k = \frac{\partial \mathcal{L}}{\partial \dot{q}_k}. \quad (14)$$

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

$$\dot{q}_k = \frac{\partial H}{\partial p_k}, \quad \dot{p}_k = -\frac{\partial H}{\partial q_k}, \quad k = 1, \dots, n. \quad (15)$$

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

$$[F, G]_{\text{PB}} = \sum_k \left(\frac{\partial F}{\partial q_k} \frac{\partial G}{\partial p_k} - \frac{\partial F}{\partial p_k} \frac{\partial G}{\partial q_k} \right). \quad (16)$$

The Hamilton's equations, Eq.(16), written in terms of Poisson brackets assume the form

$$\dot{q}_k = [q_k, H]_{\text{PB}}, \quad \dot{p}_k = [p_k, H]_{\text{PB}}. \quad (17)$$

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

$$\frac{dF}{dt} = [F, H]_{\text{PB}}. \quad (18)$$

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.

§2.3 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.

§3 Concepts that changed from classical to quantum theory

In §1 several thought experiments have been discussed. The aim has been to bring out some aspects of wave and particles, that are going to change. The change in our understanding

of waves and particles is necessitated by wave particle duality, observed for electrons in 1924 and successful explanation of photoelectric effect by assuming electromagnetic waves to have particle nature as well.

During the first three decades of the twentieth century when quantum theory was 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.

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,

You will understand all this more clearly as you move on and learn the subject. Before moving on, I leave you with a quote from the quantum mechanics book by Landau and Lifshitz [2] 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 about ‘intriguing’ relation between the classical and quantum theories.

References

- [1] R. P. Feynman. *Lectures in Physics Vol. III*. B. I. Publishers, INDIA, 1969.
- [2] L. D. Landau and E.M. Lifshitz. *Quantum Mechanics*. Pergamon Press Ltd., London, 2nd edition, 1965.