INTRODUCTION TO QUANTUM MECHANICS

CHAPTER-1 OVERVIEW: CONTRASTING CLASSICAL AND QUANTUM MECHANICS FORMULATIONS

Contrasting the Classical Mechanics (deterministic) and Quantum Mechanics (probabilistic) theories

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References
Volume I, Chapters 30 and 38.
Chapter 1 exposes the contrast between the deterministic character of classical mechanics and the probabilistic character of quantum mechanics for predicting outcomes from a given experiment. Herein we address:

How is a classical state defined?
How is a quantum mechanics state defined?

Along this description we emphasize Landau’s view that a proper formulation of Quantum Mechanics should contain classical mechanics as a limit, which prepares the ground for a subsequent chapter addressing Feynman’s path integrals formulation.

1.2 Contrasting the (deterministic) classical and (probabilistic) quantum mechanics descriptions

1.2A Definition of a classical state

The deterministic character of classical mechanics to predict experimental results

i) Classical mechanics specification of a state of motion

The spatial configuration of a system composed by $\mathcal{N}$ point masses is completely described by $3N$ Cartesian coordinates,

$$(x_1, y_1, z_1), (x_2, y_2, z_2), \ldots, (x_N, y_N, z_N).$$

If the system is subjected to constraints, the $3N$ Cartesian coordinates are not independent variables. If $n$ is the least number of variables necessary to specify the most general motion of the system, then the system is said to have $n$ degrees of freedom.

The configuration of a system with $n$ degrees of freedom is fully specified by $n$ generalized position-coordinates $q_1, q_2, \ldots, q_n$.¹

The objective in classical mechanics is to find the trajectories,

$$q_\alpha = q_\alpha (t) \quad \alpha = 1, 2, 3, \ldots, n$$

or simply written as

$$q = q (t),$$

where $q$ stands collectively for the set.

1 See expression (13) below for a more complete summary to describe a classical state.
\[ q = (q_1, q_2, \ldots, q_n) \] called path or trajectory.

*What determines the particular path \( q \) followed by a system of particles?*

**ii) Time evolution of a classical state**

One of the most elegant ways of expressing the condition that determines the particular path \( q(t) \) that a classical system will actually follow, out of all other possible paths \( q(t) \), is the *Hamilton’s principle of least action*, which is described below.

![Figure 1 Possible motions for a system going from the fixed coordinate \((a, t_1)\) to the fixed coordinate \((b, t_2)\). The motion \( q(t) \) that makes the functional \( S \) an extreme (and represented by the solid path in the figure) is the one that the system actually takes.](image)

**The classical action \( S\)**

- One first expresses the Lagrangian \( L \) of the system in terms of the generalized position and the generalized velocities coordinates \( q_\alpha \) and \( \dot{q}_\alpha \) (for \( \alpha = 1, 2, \ldots, n \)).

\[
L(q, \dot{q}, t)
\] (2)

Typically \( L = T - V \), where \( T \) is the kinetic energy and \( V \) is the potential energy of the system. (For a particle moving in an electromagnetic field the Lagrangian is a bit more complicated. See the optional homework posted in the website, homework section, of this course). For example, in the case of a particle of mass \( m \) moving in a potential \( V(x, t) \), the Lagrangian is,
\[ L(x, \dot{x}, t) = \frac{1}{2}m \dot{x}^2 - V(x, t) \]  

- Then, for a couple of fixed end points \((a, t_1)\) and \((b, t_2)\) the classical action \(S\) is defined as,

\[
S(q) = \int_{(a, t_1)}^{(b, t_2)} L(q(t), \dot{q}(t), t) \, dt \quad \text{Classical action } S
\]  

Notice \(S\) varies depending on the arbitrarily-selected path \(q\) that joins the ending point \(a\) and \(b\), at the corresponding times \(t_1\) and \(t_2\). See figure 1.

### Hamilton’s principle of least action

- Out of all the possible paths that go from \((a, t_1)\) to \((b, t_2)\), the system takes only one.

  On what basis such a path is chosen?

  **Answer:** The path followed by the system is the one, let’s call it \(\bar{q}\), that makes the functional \(S\) an extreme (i.e. a maximum or a minimum).

\[
\delta S \bigg|_{q = \bar{q}} = 0 \quad \text{Principle of Least Action} \quad (5)
\]

\((\delta S\) evaluated at the path \(\bar{q}\) is zero)

### Finding the extremum path (1-dimension case)

To simplify the calculations, let’s consider the particular case of one dimensional motion. The extremum path is determined with the usual procedures of the calculus of variation. Accordingly, we have to find the extremum path \(\bar{x}\) of the functional \(S\),

\[
S(x) = \int_{(a, t_1)}^{(b, t_2)} L(x(t), \dot{x}(t), t) \, dt \quad (6)
\]
Consider an arbitrary path $x$ that differs from the path $\bar{x}$ by an arbitrary “small” path-increment $\delta g$ (here $\delta g$ is a function, not a number),

$$x = \bar{x} + \delta g \quad \text{(functions)}$$

or equivalently

$$x(t) = \bar{x}(t) + \delta g (t) \quad \text{(numbers)}$$  \hfill (7)'

Since in (6) all the paths have the same end points, the requirement for the function $\delta g$ is that it vanishes at the extreme points,

$$\delta g (t_1) = \delta g (t_2) = 0$$

\hfill (8)

Figure 2. An arbitrary function $g$ generates a trial path $x(t) = x_C(t) + g(t)$ that is used to probe the action $S$ given by expression (6). Different trial functions can be used; a particular one is shown in the figure.

The condition that the function $\bar{x}$ is an extremum of $S$ means,

$$\delta S = S (\bar{x} + \delta g ) - S (\bar{x} ) = 0 \quad \text{Hamilton’s variational principle} \quad \text{(9)}$$

\textit{to first order variations in $\delta g$.}

We emphasize that in (6) and (9),

- $x$ stands for a function
  Indistinctly we will also call it a “path”.

- $x(t)$ is a number.
  It is the value of the function $x$ when the argument is $t$.

- $\dot{x}$ stands for the derivative of the function $x$.

- $S$ is the Action (a functional).
  $S$ is evaluated at a function $x$, which gives $S(x)$.
  $S(x)$ is a number.
is evaluated at a number \((1\text{-dimension case})\), or at a set of numbers (in the \(n\)-dimension case).

\(\delta g\) is a function

\(\delta g(t)\) “the function \(\delta g\) evaluated at \(t\)” is a number

Using the definition (6),

\[
S(x + \delta g) = \int_{(a,t_1)}^{(b,t_2)} L(x + \delta g, \dot{x} + (\delta g)^*, t) \, dt
\]

Notice, on the left side, \(S\) is evaluated on a path \(\bar{x} + \delta \bar{g}\).

On the right side, we have written \(x, \delta g, \dot{x}, \dot{(\delta g)}\) just for simplicity, BUT we should have written \(x(t), \delta x(t), \dot{x}(t),\) and \((\delta g)(t)\) respectively.

Also, we know that for a general function of two variables \(f = f(x, y)\), and for small values of \(\delta\) and \(\Delta\), we can make the following approximation:

\[
f(x + \delta, y + \Delta) \approx f(x, y) + \frac{\partial f}{\partial x} \delta + \frac{\partial f}{\partial y} \Delta.
\]

We apply this result to the function \(L\).

\[
S(x + \delta x) - S(x) = \int_{(a,t_1)}^{(b,t_2)} \left[ \frac{\partial L}{\partial x} \delta g + \frac{\partial L}{\partial x^*} (\delta g)^* \right] dt
\]

Integrating by parts the second integral,

\[
\int_{(a,t_1)}^{(b,t_2)} \left[ \frac{\partial L}{\partial x} \delta g \right] dt = \frac{\partial L}{\partial x} \left[ \delta g \right]_{t_1}^{t_2} - \int_{(a,t_1)}^{(b,t_2)} \left( \frac{d}{dt} \frac{\partial L}{\partial x} \right) \delta g \, dt
\]

Since \(\delta g(t_1) = \delta g(t_2) = 0\) the first term cancels out
\[ S(x+\delta g) - S(x) = \int_{(a,t_1)}^{(b,t_2)} \left( \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} \right) \delta g \, dt \]

Therefore, (10) adopts the form,

\[ S(x+\delta g) - S(x) = - \int_{(a,t_1)}^{(b,t_2)} \left( \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} \right) \delta g \, dt \]

The principle of least action requires that when \( x = \bar{x} \), the right-hand side of (11) will be zero, for any arbitrary path \( \delta g \). This implies, the classical path \( \bar{x} \) must satisfy the following equation,

\[ \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0 \] (11’)

The procedure can be generalized for the more general case of a system with \( n \) degrees of freedom,

\[ \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_\alpha} - \frac{\partial L}{\partial q_\alpha} = 0 \quad \alpha = 1, 2, 3, \ldots, n \] (12)

These are the equations to be satisfied by the classical trajectory \( \bar{q}(t) \), which constitutes the trajectory we are looking for.

Here \( \bar{q}(t) \) stands collectively for the set \((\bar{q}_1(t), \bar{q}_2(t), \ldots, \bar{q}_n(t))\)

**iii) Determinism in the evolution of a classical state**

Classical mechanics tell us:

"the motion \[^{\text{\textbf{\textit{\bar{q}(t)}}}}\] of the system, i.e. the trajectories followed by each coordinate, are obtained by solving the set of equations given in expression (12)."

As occur in any system of differential equations, solving (13) will give us a very general solution containing parameters to be determined by the initial conditions, i.e. position and velocity at a specific time \( t=t_0 \). Once the initial conditions are incorporated, the solution predicts the position and velocity at any other future time. That is,
there exists determinism on the time evolution of the classical path $\overline{q}(t)$.

(However, as we will explain below, the above is not this kind of determinism that distinguishes classical mechanics from quantum mechanics, since, as we will see later, QM states also evolve deterministically. The difference between Classical Mechanics and Quantum Mechanics lies in that they predict different physical outcomes from a given experiment, as addressed in the next sections.)

iv) Determinism in the prediction of other classical physical quantities

Once $\overline{q}$ is uniquely determined for the system under study, the other various physical quantities can also be completely determined at any time (since they depend on $\overline{q}$). One can predict with certainty the result of any measurement (kinetic energy, angular momentum, linear momentum, ..., etc.) to be performed on the system at any time $t$. This is the type of deterministic prediction in classical mechanics, which, as we will see later, differs from quantum mechanics.

In summary:

- The state of a classical system at a given time $t_0$ is defined by specifying
  $n$ generalized coordinates $q_\alpha(t_0), \alpha = 1, 2, 3, \ldots, n$; and
  $n$ generalized velocities $\dot{q}_\alpha(t_0), \alpha = 1, 2, 3, \ldots, n$

- The time evolution of the state of the system is determined through the Lagrangian equations,
  \[
  \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_\alpha} - \frac{\partial L}{\partial q_\alpha} = 0, \quad \alpha = 1, 2, 3, \ldots, n,
  \]
  which, once solved, tell us how $q=\overline{q}(t)$ changes with time.
  A unique solution $\overline{q}(t)$ exists for a given set of specified initial conditions \{ $q_\alpha(t_0), \dot{q}_\alpha(t_0), \alpha = 1, 2, 3, \ldots, n$ \}

- Knowing the state at an arbitrary time $t$, one can predict with certainty the result of any measurement performed at that time $t.$
1.2B Absence of trajectories in the quantum behavior of particles. 

In the quantum description, in contrast to the classical one, there are no trajectories.

We know that the assumption of trajectories leads to predictions that do not corroborate reality. Under a classical electromagnetism description, the existence of trajectories implies instability of the atom.

Below we present further arguments on the impossibility to ascribe trajectories-of-indefinite-accuracy to the motion of an atomic particle.

Another example where one cannot predict specific trajectories to be followed by a particle is shown in Fig. 3.

After passing the first aperture, the particle may be found angularly deflected, at best, at any point within this angular range.

Attempt to know the vertical position better: we place an aperture of size \( a \).

Uncertainty in the vertical position: \( \Delta y \approx a \)

Uncertainty in the vertical momentum \( \Delta p_y \approx p\theta = p\lambda/a \)

Figure 3 Electrons incident with a definite momentum \( \vec{p} = p_x \hat{i} \) (i.e. with \( \Delta p_x = 0 \)) “diffract” after passing through an aperture of size \( a \). From diffraction theory we learn that first minimum of a diffraction pattern is located at an angular position \( \theta = \lambda/a \). The profile shows that for a given incident electron, there are many possible values of its vertical momentum \( p_y \) when it strikes the screen.
Electrons (initially travelling horizontally) being diffracted after passing through a small aperture of size “a” (in a similar way to the double slit experiment using light.) That is, there is a probability different from zero that the electron arrives at any vertical position on the screen (some places with higher probability than others.) The highest probability lies within a cone of angular-aperture $\lambda/a$. ($\lambda$ is the de Broglie wavelength associated to the particle). This means, for a particular electron, it is unpredictable to determine what would be its vertical position upon hitting the screen.

An attempt to measure velocities. In those circumstances, if we attempted to measure the vertical component of the velocity of an incident particle at a position right after the aperture ($x=0$), we would have to measure (following a typical classical procedure of finding a time derivative of a vertical position) the position of the particle at $x=0$ and $x=\Delta$ (as suggested in Fig. 4 below) and then divide that difference by $\Delta t$. Accordingly, we could place two small apertures of size “a” at those positions. However, notice that after passing the first aperture at $x=0$ (which already has an uncertainty “a” on the y-position), there is an uncertainty about the y-position of the particle at $x=\Delta$ of the order of $\theta \Delta \sim (\lambda/a)\Delta$ or greater. We wouldn’t be able to determine, then, the classically expected change in the y-position coordinate since there is no way to establish a value for $\Delta y$, and hence neither be able to calculate $\Delta y/\Delta t$.

Figure 4 Limitations to ascribe trajectories to the motion of a quantum particle. The higher precision of the particle’s vertical position at $x=0$ (using apertures of smaller values for “a”), the less precise its vertical position at $x=\Delta$, which makes impossible to apply the classical mechanics definition of velocity $\Delta y/\Delta t$ because the value of $\Delta y$ is unpredictable to determine with high precision.
We see that an attempt to attain a \( y = y(t) \) trajectory would require tracking the motion of the particle choosing apertures with very small value of \( a \); but that would further worsen the range of possible values for the \( y \)-coordinate at \( x = \Delta \) (the smaller the value for “\( a \)” the larger uncertainty \( \theta = \lambda / a \). Hence, it is not possible to establish differences like \( \text{(final vertical position)} - \text{(initial vertical position)} \), because such difference can have scattered values; the smaller the value of \( a \) the more scattered the values of \( \Delta y \).

In short, when describing the motion of an atomic particle, one finds that it is not possible to establish trajectories, and as a consequence, neither velocities.\(^2\)

The theory to describe atomic phenomena must be therefore fundamentally different than the classical mechanics theory. In quantum mechanics there is not such concept as path of a particle. The example given above illustrates the content of the uncertainty principle, one of the fundamental principles of quantum mechanics, discovered by W. Heisenberg in 1927.

1.2C Requirement that the new atomic theory has to confront:

**Viewpoint-1**

- **Classical Mechanics should be obtained as a limiting case of a Quantum Mechanics formulation.**\(^1\)

Even though in quantum mechanics there is no such a concept as “the velocity of a particle” in the classical sense, still (as we will see in the coming chapters) the new theory provides a reasonable definition of the likely range of velocities a particle could have at a given instant. This is a reflection of the fact that, when formulating a quantum mechanics theory it must contain classical mechanics as a limit. That is to say, it is in principle impossible to formulate the basic concepts of quantum mechanics without any reference to classical mechanics; Landau supported this view.

\(^1\) A blurred and imprecise path could be obtained if the coordinates of the particle were measured with a low degree of accuracy. For instance using apertures of large values for “\( a \)” in the example above. But what we are addressing here is the impossibility to define quantum mechanically a trajectory of arbitrary precision.
“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 formulation”.

In perspective, this is different than Relativity (enunciated based on the constant speed of light in any inertial system of reference), which does not need classical mechanics for its formulation but reproduces the latter in the limit of low velocities.

- The fact that a quantum object does not have a definite trajectory means that it has also no other (classically interpretable) dynamic motion characteristics. Therefore, for a system composed only of quantum objects (system of atomic dimensions) it would be impossible (for a classical guy) to construct a logically independent mechanics theory.

It results plausible, then, to conceive that a quantitative description of the dynamics of a *quantum system* has to include its interaction with a *classical object*.

That way as a result of the interaction between the *quantum system* and the *classical object*, a classical signature will be registered on the latter which could reveal information about the former.

*The nature and magnitude of the change on the classical object depends on the state of the quantum object, which can serve to characterize the latter quantitatively. The classical object is usually called apparatus, and its interaction with the quantum object is referred to as measurement.*

More specifically (viewpoint-1),

*in quantum mechanics a measurement refers to any process of interaction between classical and quantum objects, occurring apart from, and independent of, any observer.*

The accuracy of the apparatus plays a role here; if the accuracy is very poor then the quantum object may behave as a *classical object*. (See the footnote included at the end)

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#### Footnotes

3 *Viewpoint-2.* The viewpoint-1, expressed above, is found in the Landau book reference. However, newer experiments, developed in the context of quantum entanglement, do not share that drastic distinct view. The following is an interesting reference intended for the general public: Anton Zeilinger, “DANCE OF THE PHOTONS. From Einstein to Quantum, Teleportation.”
of the previous section.) However an experimenter is typically driven to obtain the maximum accuracy possible. But,

measurement always affects the dynamics of the quantum object, and it is in principle impossible to make its affect arbitrarily small.

This is a logic consequence of the fact the dynamic characteristics of a quantum object is revealed by the measurement itself; if no modification occur on the quantum object dynamics, then no signature is left on the apparatus. A signal on the apparatus implies a modification on the dynamics of the quantum object.

Thus, whereas in classical mechanics a particle has definite position coordinates and velocity at a given instant, in quantum mechanics the situation is quite different; the better we know the position, the worse we know its momentum, and vice versa (as shown in Fig.3). A simultaneous existence of the coordinates and velocity would imply the existence of a definite path, which the QM particles do not have.

1.2D The less detailed quantum mechanics description

- As mentioned above, a complete description of the classical state of a physical system is obtained by giving all its position-coordinates and velocities at any given instant. With these initial conditions, the equations of motion completely determine the behavior of the system at all subsequent times and one can predict with certainty the result of any measurement performed at any given time.

- In contrast, in quantum mechanics the prediction of results with such an unrestricted precision is not possible, since position and velocities cannot be known simultaneously.

- As we will see later, the description of a state in QM is specified by a smaller number of quantities than in classical mechanics, i.e. it is less detailed than a classical description. This has important consequences regarding the nature of the predictions made in QM. Whereas a classical description predicts the future of a mechanical system with complete accuracy, QM gives a less detailed prediction.
Even if the QM-state of a system is described in the most complete manner, the values of, for example, position and momentum at subsequent instances will be uncertain. For a given initial state of an electron, a subsequent measurement can give various results. QM tackles this uncertainty.

The task in QM consists in determining the probability of obtaining some given results upon performing some measurements.

Comment:
It should be kept in mind that in some cases the probability of a given result may be equal to unity, i.e. there is a certainty that the result of the measurement will be unique).

In fact, measurement processes in QM may be divided into two groups:

- In one group (which contains the majority of cases) the measurements do not lead with certainty to a unique result.
- The other group contains measurements where there is an absolute accuracy to obtain a given result (provided that the possible values of the physical quantity are discrete). When this occurs, one says that the system is in a stationary state.

1.2E The Non-relativistic quantum mechanics description

So, how does QM describe the dynamic of a system with 

\( n \) 

degrees of freedom, which is classically specified by \( n \) generalized position coordinates \( q_1, q_2, \ldots, q_n \)?

- In QM such a system is specified, at a fixed instant of time, by a wave function

\[
\psi( q_1, q_2, \ldots, q_n ) ,
\]

which satisfies,

\[
\int |\psi(q_1, q_2, \ldots, q_n)|^2 \, dq_1 \, dq_2 \ldots \, dq_n = 1 \quad \text{Normalization condition} \tag{15}
\]

where the integration extends over all the accessible values of the generalized coordinates \( q_1, q_2, \ldots, q_n \).
The set of all such wave functions satisfying (15) form a vector space called the Hilbert space \( G \).

- In addition to depending on the coordinates \( q_1, q_2, \ldots, q_n \), the wave function depends also on the time \( t \). But the dependence of the wavefunction on the spatial coordinates \( q_s \) and on temporal-coordinate \( t \) are essentially different. Since the Hilbert space \( G \) is formed with respect to the spatial coordinates \( q_1, q_2, \ldots, q_n \) only, states of the system at different instants of time \( t, t', t'' \ldots \), are then given by the corresponding different wave functions:

\[
\psi_t(q_1, q_2, \ldots, q_n),
\]

\[
\psi_{t'}(q_1, q_2, \ldots, q_n),
\]

\[
\psi_{t''}(q_1, q_2, \ldots, q_n), \ldots
\]

of the Hilbert space.

A less cumbersome notation,

\[
\psi(q_1, q_2, \ldots, q_n, t), \text{ or simply } \psi(q, t),
\]

is typically used instead.

Such a description that treats the time variable different than the position coordinates results from a non-relativistic formulation of the quantum mechanics.

- The normalization (15) responds to the probability-character in the interpretation of \( |\psi(q)|^2 \), as described in the next section. Notice two wave functions differing by a phase factor \( e^{i\alpha} \) give the same probability (probability to obtain a value in an experimental measurement). Thus, the choice of that phase factor is arbitrary.

- It is a postulate in QM that a complete knowledge of the wave function \( \psi(q, t) \) represents the maximum information about the system. Every property of the system can be derived from its wave function. We should emphasize, however, that even knowing the wave function, the result of measurement is still uncertain; only probabilistic predictions can be made.
In summary

A system, classically described as one of $n$ degrees of freedom, is completely specified in quantum mechanics by a normalized wave function $\psi( q_1, q_2, \ldots, q_n )$ which contains an arbitrary factor of modulus 1. All possible information about the system can be derived from this wave function.

How to build the QM wave function $\psi( q_1, q_2, \ldots, q_n, t )$?

How to use the classical measurements of the physical properties of a system to build the QM wave function?

It turns out the state of a system, specified by a wave function in the Hilbert space, represents a theoretical abstraction. One cannot measure the state directly in any way. What one does do is to measure certain physical quantities such as energy, momentum, etc., which Dirac referred to as observables; from these observations one then infers the state of the system.

Strategy followed in this course,

i) We will postpone the presentation of a logical procedure to write down explicitly the QM states until we introduce the concept of QM operators (which are quantities corresponding to the classical observables) and their commutation properties until Lecture 10.

ii) Instead, we will focus first in the evolution of a QM system.

Following Feynman approach, we will then present a plausible demonstration of the Schrodinger equation. Once the latter is established, then we will build the operators and define the observables. Once we have those tools, we will address a logical description of how to express explicitly a quantum state.

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1 L. Landau, page 3.