

# INTRODUCTION TO QUANTUM MECHANICS

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## I. INTRODUCTION

Quantum Mechanics is the description of the behavior of matter in all its details, particularly, of phenomena at the atomic scale.<sup>1</sup> It turns out that on the very small (atomic) scale, physical phenomena behave in such a way that typically escapes our intuition (the latter developed observing macro-scale phenomena.) Quantum Mechanics constitutes a very general theory that includes the classical physics laws as special cases.

Newton thought that **light** was made out of *particles* (probably based on the sharp shadows created by macroscopic object intersecting the path travel of a light beam). It was discovered later that it behaves as a *wave* (based on the observed diffraction phenomena produced by small apertures.) Later on, however, it was found that light indeed sometimes behave like a *particle* (photoelectric effect).

The **electron** was considered to be a *particle* (J.J. Thompson discovered the electron in a set up conceived to bombard aluminum atoms in an aluminum foil). But later, it was found that when bombarding a crystal with electrons, diffraction patterns result (similar to what observed when bombarding the crystal with x-rays); that is, electrons behave as *waves*.

We have come to the conclusion that light and electrons are neither a particle nor a wave. But an accumulated number of experiments suggest that **electrons behave just like light**. More general, the quantum behavior of atomic objects (electrons, protons, neutrons, photons, etc) is the same for all; they are considered 'particle waves'.

The initial apparently confusing behavior of atomic objects was better understood when, in 1926 and 1927, Schrodinger, Heisenberg and Born provided a more consistent analytical description. The objective of this course is to describe such transition from classic to quantum concepts, and familiarize with the theoretical machinery that quantum mechanics uses to describe Nature.

## II. PHILOSOPHY of the COURSE

One might be inclined to rigorously postulate the Quantum Mechanics principles, and then deduce everything else. However, there is a risk in this

approach; as one of my classmates once said “*I know how to solve the mathematical equation, but I have no idea what I am doing.*”

**From the general to the particular.** As an alternative, in the first part of this course we will (or try to) follow Feynman’s lectures approach,<sup>1</sup> solving important problems in a very general format, emphasizing on the concept of quantum states, calculating probabilities that a physical system will transit from one state to another, but without worrying (initially) on the detailed analytical description of the quantum states themselves. Only in the later sections of the course we will provide a more analytical description of the quantum states.

The focus of the first part is then to learn how the quantum mechanics machinery works. We will realize that Feynman’s approach is of such generality that allows undertaking a variety of problems, including the ones beyond the scope of the Schrodinger equation (for example dealing with problems involving the spin of the particles) which are typically considered ‘advanced’ quantum mechanics chapters. The ‘sacrifice’ of rigorous analytical procedure by no means implies a drawback in the presentation. Rather it helps illustrate the generality of the Quantum Mechanics principles. Following these physics-rich examples, illustrating in a very straightforward manner the basic foundations of quantum mechanics, a more analytical formal description of the Quantum Mechanic will follow in the final chapters.

### III. ORGANIZATION of the COURSE

The course has been divided in 4 sections (each composed of a few chapters):

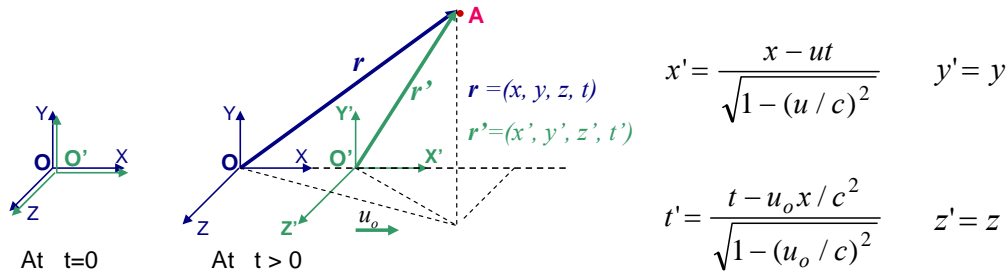
**PART I “The TRANSITION from CLASSICAL to QUANTUM PHYSICS”** provides a brief review of the classical physics atmosphere preponderant at the end of the 19<sup>th</sup> century (Chapter 2), followed by a description of important experiments (the blackbody radiation in particular) that put in evidence the limitation of classical physics and helped germinate the new quantum mechanics ideas (Chapter 3).

*More specifically, Chapter 2 “CLASSICAL PHYSICS: ELECTROMAGNETISM and RELATIVITY (REVIEW)” briefly reviews the classical physics theories of Electromagnetism (Maxwell’s equations) and Special Relativity (Einstein’s postulates). The objective is to provide a proper context in which quantum mechanics emerged (as they both played preponderant roles in the quest for structuring a consistent scientific theory).*

*On one hand, although the Maxwell equations had placed on very solid theoretical foundations the wave nature of light, such interpretation was unable to explain the photoelectric effect. This shortcoming triggered Einstein’s interpretation of electromagnetic radiation as a statistical distribution of quantum packets of energy (later called “photons.”)*

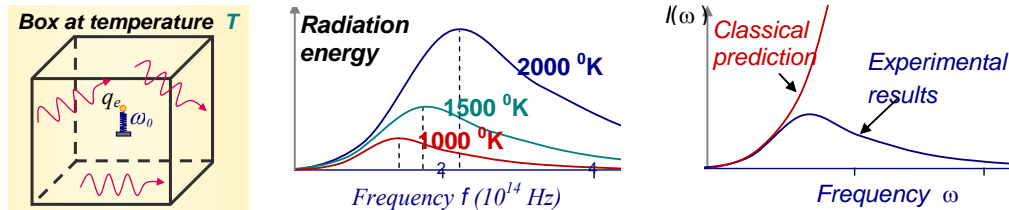
*On the other hand, electromagnetism also triggered the development of the Theory of Special Relativity at the end of the 19<sup>th</sup> century when scientists were trying to harmonize Maxwell equations with the general principles of relativity. It*

was found that the Maxwell equations were already intrinsically harmonious with the principles of relativity (as postulated by Einstein) and rather Newton's classical mechanics laws had to be modified. The corresponding correction, it turns out, was rather simple (although very intriguing):  $m = m(v) = (m_0) / \sqrt{1 - (v/c)^2}$ , where  $c$  stands for the speed of light. That is, the mass of a particle depends on its velocity  $v$ . Chapter 2 reviews how the expression for the velocity dependent mass is obtained from the conservation of energy and linear momentum principles. Years later, Dirac developed in 1930 a quantum mechanics theory compatible with relativity, in passing showing the relativistic character of the particles' spin.



By postulating that the speed of light is finite and independent of the motion of its source, the Lorentz transformation is obtained.

**Chapter 3 “The ORIGINS of QUANTUM PHYSICS”** describes (to a large extent) the blackbody radiation problem and (very briefly) other experiments (like the photoelectric effect, the Compton effect) that put in evidence the wave character of what is typically considered particles and the particle character of what is typically considered waves. They occurred at the end of the 19<sup>th</sup> century and the beginning of the 20<sup>th</sup> century. Hence resulted the de Broglie's dual-particle hypothesis (in 1923) which shortly later was confirmed experimentally (i.e. electron diffraction experiment.)



$$I(\omega) = \frac{1}{3\pi^2 c^2} \omega^2 \underbrace{\langle W \rangle}_{\text{Average energy of the oscillator at temperature } T}$$

$$\left\{ \begin{array}{l} \langle W \rangle_{\text{classic}} \sim k_B T \\ \langle W \rangle_{\text{Planck}}(\omega) = \hbar \omega \frac{1}{e^{\hbar \omega / kT} - 1} \end{array} \right.$$

Atom of natural frequency  $\omega$  in a bath of electromagnetic radiation of spectral density  $I(\omega)$ .  $\langle W \rangle$  is the energy of the atoms when in equilibrium.

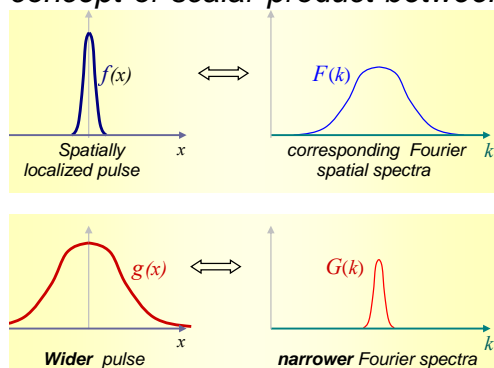
**PART II, entitled “MAKING PREDICTIONS IN QUANTUM MECHANICS and THE HEISENBERG’S PRINCIPLE”** aims at familiarizing with the underpinning concepts of quantum mechanics, with a focused interest in obtaining an understanding of the Heisenberg’s Uncertainty Principle. The latter constitutes one of the cornerstones of quantum mechanics.

First, it is shown that a wavepacket (a bunch of waves of different spatial frequencies  $p$  within a certain range  $\Delta p$ ) is needed even in the simplest case of describing the motion of a free particle. A single frequency wave is not enough. A wavepacket inherently reflects, then, the uncertainty in the values of a physical variable (in this case  $p$ ) associated to a particle.

Later, to illustrate the critical perturbation-role played by a measurement a relatively simple experiment is considered where particles (photons or electrons) pass through a screen containing two slits. A puzzle arises when trying to determine which aperture a particle uses to cross the screen. The no apparent direct answer helps illustrate the peculiar behavior displayed by microscopic objects.

Finally, an insight of the Quantum Mechanics machinery is gained with the introduction of the concept of “Amplitude Probability,” which is applied (in particular) to solve the puzzle of the two-slit experiment.

Since a particle’s quantum state of motion is described as a linear combination of given (fixed) base-states, **Chapter 4 “WAVEPACKETS DESCRIPTION of a FREE-PARTICLE’S MOTION”** reviews the Fourier’s spectral-decomposition analysis, and generalizes the concept to other types of spectral decompositions. Incidentally, this description also serves the purpose of familiarizing with the use of complex variables, which is the bread and butter in quantum mechanics. The concept of scalar product between functions is introduced, along with the widely



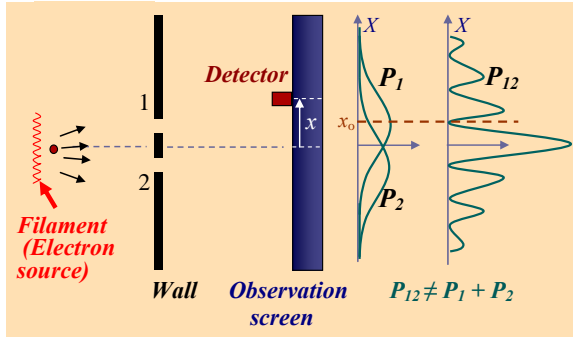
Wavefunctions and their spectral Fourier decomposition. It helps to illustrate the Heisenberg principle.

*uncertainty principle (one of the cornerstones of quantum mechanics), since an uncertainty  $\Delta p$  in the values of  $p$  is associated with the wavepacket.*

used bracket notation (adopted in most quantum mechanics books.) This framework of spectral decomposition allows the description of wavepackets, which was used by de Broglie when he enunciated his wave-particle hypothesis. Chapter 4 shows the necessity of associating a bunch of spatial spectral components  $p$  within a range  $\Delta p$  (and not just one) with the motion of a free particle. This preliminary result marks the beginning (in this course) in gaining an understanding of the Heisenberg’s

**Chapter 5 “QUANTUM BEHAVIOR of PARTICLES and the HEISENBERG’S UNCERTAINTY PRINCIPLE”** covers more in depth the Heisenberg’s uncertainty principle, emphasizing on the perturbation role played

by the act of performing a measurement. The passage of particles (photon or electrons) through a screen containing two small apertures (better known as the Young's experiment) is used to illustrate the peculiar (and somewhat intriguing) quantum behavior of microscopic particles. A puzzle arises when asking "which of the two apertures an incident particle uses to cross the screen?" In an attempt



Which aperture an electron passes through?

to answer this question it is proposed to use photons to watch the passage of electrons. But, it turns out, this mere attempt disturbs completely the original Young's interference pattern. This places in evidence the limited information that can be obtained from a quantum system. This example helps to set the stage to enunciate the Heisenberg's Uncertainty Principle, which relates the relationship between the

particle's uncertainty position and uncertainty linear momentum:  $\Delta x \Delta p \geq \hbar / 2$ , (where  $\hbar = h / 2\pi$  and  $h$  is the Planck's constant.) When applied to the Young's experiment, the uncertainty principle means that if an electron is perturbed by a photon in order to gain accuracy in their position (and thus to know which aperture it passes through), its momentum is perturbed (thus spoiling the diffraction phenomena.)

The second part of Chapter 5 is devoted to illustrate the uncertainty principle pertaining to the measurement of the energy content uncertainty  $\Delta E$  of a light pulse and the time  $\Delta t$  required for the measurement. This aspect of the Heisenberg's uncertainty principle is relatively very little explained in most textbooks; so we decided to describe it in a bit more depth in order to attain a better grasp of its meaning. As an experimental framework for this description we exploit the working principle of an optical grating to decompose a pulse into its spectral frequency components. Thus relatively lot of time is invested to familiarize with the working principle of a grating, the method of phasors (complex numbers) to add waves, the parameter that limit the resolution of a grating to differentiate waves of different frequency; all of which will allow interpreting better the meaning of  $(\Delta E)(\Delta t)_{\text{measurement}} \geq \hbar / 2$ .

The introduction of the uncertainty principle sets the basis for a statistical interpretation of the wavefunction that describes the state of motion of a particle (or system of particles.) This interpretation is better understood in the context of statistical ensemble, which is defined at the end of Chapter 5. The statistical interpretation of the quantum wavefunction did not come without causing controversy (Einstein nor de Broglie accepted that interpretation.)

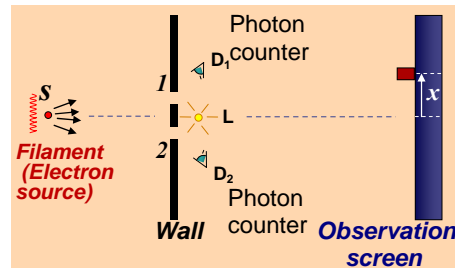
**Chapter 6 "THE CONCEPT of AMPLITUDE PROBABILITY"** introduces the concept of "amplitude probability", complex variable numbers that help evaluate



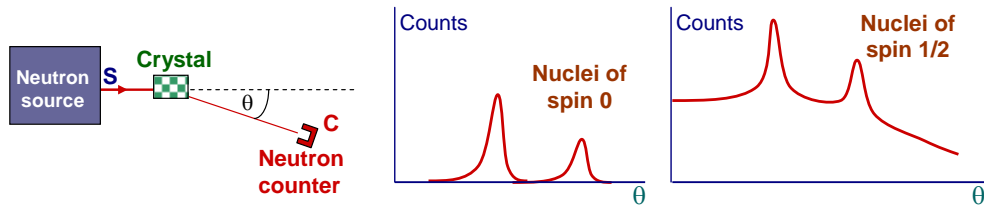
the interference between the different paths available for a particle (or a system of particles) to transit from an initial state to a final state. This concept is applied in great detail to the two-slit Young's experiment undertaken in the previous Chapter 5. This example helps illustrate how to apply quantum concepts, arriving to conclusions that have been verified experimentally. As a second example, amplitude probabilities are also applied to the description of scattering of neutrons by a crystal.

### $\langle x|s \rangle$ Amplitude Probability

Complex number whose magnitude squared  $|\langle x|s \rangle|^2$  gives the probability that a system initially in the state  $|s\rangle$  will be found in the state  $|x\rangle$  after the measurement.



**Left:** The concept of amplitude probability. **Right:** Description of the two slit experiment setup (where electrons are being watched by photons, the latter monitored by two photon detectors) using the amplitude probability formalism.



The amplitude probability formalism will be used to predict potential results in an experiment involving scattering of neutrons from a crystal of atoms having spin 1/2

## NOTE

At this stage of the course we will find ourselves in the advantageous position of presenting the basics of quantum mechanics via two approaches, each offering complementary perspectives.

- i) The first approach introduces right away the concept of the Hamiltonian Operator (a concept encountered while trying to figure out how a quantum state evolves with time.) This approach goes along with the style presented so far, reach in physics concept despite not being too precise on the specific (point to point coordinate) spatial-dependence of the wavefunction. A great advantage in this formulation is its generality, allowing to acquire a conceptually wider view of quantum mechanics problems, including the ones involving spin (the latter a concept where the wavefunction does not admit spatial-variable dependence.) We will present this approach in Part-III.
- ii) The other approach is a more analytical one, which pursues obtaining a differential equation (to be satisfied by the quantum state wavefunction) while

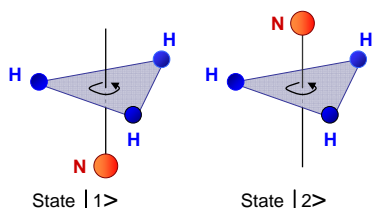
requiring compatibility of such procedure with the de Broglie's hypothesis and the conservation of energy. The result is the Schrodinger Equation. This approach is presented in Part-IV. The more analytical version of the Schrodinger equation is used to obtain the wavefunctions of the harmonic oscillator and the hydrogen atom.

**Part III “The HAMILTONIAN EQUATIONS and the SCHRODINGER EQUATION”** involves a more formal formulation of Quantum Mechanics. In the context of trying to find *how quantum states evolve with time*, the Evolution Operator and the Hamiltonian Operator are introduced in Chapter 7. The ammonia molecule is used as a specific example to illustrate the preponderant role played by the Hamiltonian Operator. The concept of the Hamiltonian operator is later generalized for any quantum system. A two-state system is solved in general terms, including cases where an electric and magnetic fields are applied. The problem of a spin one-half particle in a magnetic field is solved, and later expressed in terms of the Pauli's spin matrices. These particular problems are solved in a general way (calculating probabilities for a system to transit from state to another) without the need of a detailed analytical description of the states.

Chapter 8 shows an analytical transition from a general description to a more detailed analytical description of the wavefunction. A quantum state is obtained by first solving the problem involving the motion of an electron in a discrete crystal lattice of atoms. Then, by making the lattice constant (the separation between atoms) to approach a zero limiting value, the resulting limiting case ends up with an equation of motion for the electron quite similar to the Schrodinger equation.

Such a limiting case transition allows gaining a better interpretation of the wavefunction (analytical solutions of the Schrödinger equation.)

**Chapter 7 “THE HAMILTONIAN EQUATIONS How Do States Change with Time?”** undertakes the task of finding how the quantum state of a system evolves with time. Recognizing the complexity that a real problem can be, a few



The ammonia molecule. The figure shows two possible states for the molecule.

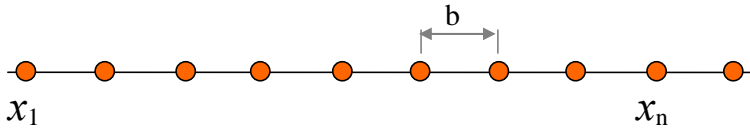
$$i\hbar \frac{d}{dt} \begin{pmatrix} A_1(t) \\ A_2(t) \end{pmatrix} = \begin{pmatrix} H_{11}(t) & H_{12}(t) \\ H_{21}(t) & H_{22}(t) \end{pmatrix} \begin{pmatrix} A_1(t) \\ A_2(t) \end{pmatrix}$$

examples help illustrate how to judiciously isolate the important parts of a given system and select, accordingly, the proper base states.

A highlighting feature in this chapter is the Hamiltonian operator, whose mathematical ‘appearance’ changes depending on which base states (for the same problem) are chosen; but the operator is the same. The Hamiltonian operator plays the important role in determining how a quantum system evolves with time. Suffice to say that, in order to find out how a system evolve with time (and hence obtained

all its dynamic characteristics) all we have to do is to find the corresponding Hamiltonian. The ammonia molecule, as complex as it may appear, is solved as a two-state system. This sets the stage to solve any two-stage system including the case in which an external electric field and magnetic fields are applied, respectively. For the latter, the problem is solved with such generality that it allows considering the case of a spin and the Pauli's spin matrices (typically treated in most books only in their more advanced chapters.)

**Chapter 8 “From the HAMILTONIAN EQUATIONS to the SCHRODINGER EQUATION. The case of an electron propagating in a crystal lattice”** considers the propagation of an electron in a one dimensional lattice. Two cases are studied. First, stationary states in which each atom oscillates with the same frequency (a state of motion better known as mode); and then the scattering of an electron by an impurity, thus generation transmitted and reflected waves. The former case is extrapolated to one in which the separation between atoms is taken progressively equal to zero, leading to an equation for the amplitude probabilities, coincident with the Schrodinger Equation. It provides another perspective of how to interpret the wavefunctions (the solutions of the Schrodinger equation.)



...

$$i\hbar \frac{dA_{n-1}}{dt} = -W A_{n-2} + E_o A_{n-1} - W A_n$$

$$i\hbar \frac{dA_n}{dt} = -W A_{n-1} + E_o A_n - W A_{n+1} \quad (5)$$

$$i\hbar \frac{dA_{n+1}}{dt} = -W A_n + E_o A_{n+1} - W A_{n+2}$$

...

**Chapter 9 “WAVEFUNCTIONS and OPERATORS”** Quantum theory is based on two mathematical items: **wavefunctions and operators**. a) The state of a system is represented by a wavefunction. An exact knowledge of the wavefunction is the maximum one can have of the system: all possible information about the system can be calculated from this wavefunction. b) Quantities such as position, momentum, or energy, which one measures experimentally, are called observables. In classical physics, observables are represented by ordinary variables. In quantum mechanics observables are



*represented by operators; i.e. by quantities that operate on the wavefunction giving a new wavefunction.*

**SECTION IV “THE SCHRODINGER EQUATION”** presents the non-relativistic version of the Schrodinger Equation, which is used to solve in great analytical detail a number of important microscopic systems, particularly the harmonic oscillator and the hydrogen atom. The latter is also use to introduce the properties of the angular momentum operator.

**Chapter 10** The Schrodinger equation is solved for problems that can be reduced to one dimension.

**Chapter 11** The Schrodinger equation is solved for the three dimensional case, applicable for problems involving one-electron atoms. The decoupling between the radial dependence and the angular dependence serves the basis to undertake the eigenvalue problem of the angular momentum.

**SECTION V “IDENTICAL PARTICLES”** describes the interesting consequences when a physical situation happens in several indistinguishable ways. In those situations we have to let the amplitude probabilities to interfere before evaluating the probability of these equivalent events to occur. It turns out that for some type of identical particles (bosons) the interference is evaluated by adding the wavefunctions, while for others (fermions) a mixture of positive and negative sign are involved. We will consider, in some detail, the case for n bosons.

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<sup>1</sup> Richard Feynman, “The Feynman Lecture on Physics,” Vol-III, Addison-Wesley, 1963.