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What Is The Wave Function?

Celso Luis Levada , Tabata Vidal[1,2] , Huemerson Maceti[1,2] , Bruno Sagioro Zaniboni[1,2]

Ivan José Lautenschleguer[1]

(1) FHO | HERMÍNIO OMETTO FOUNDATION - ARARAS / SP - BRAZIL - NUCLEUS OF ENGINEERING

(2)COLÉGIO PURÍSSIMO CORAÇÃO DE MARIA - HIGHSCHOOL - RIO CLARO / SP - BRAZIL – PHYSICS TEACHING

celsolevada@yahoo.com.br

ABSTRACT

Microscopic particles, like electrons, do not move following the classical laws of motion, given by Newtonian Mechanics. These particles, however, follow other laws that are associated to the propagation of waves. This becomes qualitatively clear when we observe an interference pattern arise in an experiment in which an electron beam passes through a double slit. In this brief study, we will deal with the quantum analysis of the dynamics of particles, by means of its postulates and its precise mathematical formulation. That is, we intend to introduce the wave function and the Schrödinger equation, as well as to interpret physically such a function. The scientific bases of this essay[(1),(2),(3),(4),(5)] can be found in the books listed in the bibliographic references.

Keywords: Schrödinger equation, wave function, probabilities

INTRODUCTION

Let us consider a microscopic particle, for example, an electron, which moves in three dimensions. Let us assume, as a postulate, that the state of this particle, at an instant of time t, is completely defined by a wave function which is denoted by the symbol $\Psi(x, y, z, t)$, where x, y, z represent the spatial coordinates. What do we mean by the expression "state of a particle"? In classical mechanics, the state of a particle is known by means of its position and velocity at a given instant. This information added to the knowledge of the force (or of the potential energy) acting on this particle allows the complete description of its subsequent trajectory through the integration of Newton's Second Law. Even a movement related to the waves will be fully characterized if the spatial and temporal dependence of the wave function is known. For example, in the case of waves at the water surface an appropriate wave function is obtained by considering the height of the water level. Note that, in the case of quantum particles, the mathematical description is much more similar to that of the waves than to that of the classical particles. In the case of classical waves, the wave function is the solution of a partial differential equation known as wave equation. Therefore, it is reasonable to assume that the wave function associated to a quantum particle must also satisfy a wave equation.

WAVE EQUATION

Suppose that a quantum particle has mass m and moves under the influence of a potential energy V(x, y, z, t). It is postulated that the wave function satisfies the following partial differential equation

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]\Psi = i\hbar\frac{\partial}{\partial t}\Psi, \quad (1)$$

where ħ represents the Planck constant. This is the famous Schrödinger Equation proposed by the Austrian physicist Erwin Schrödinger in 1926. Erwin Schrödinger explored analogies between geometric optics and classical mechanics and was inspired by the relation between the momentum of a particle and the length of a waveguide posited by Louis de Broglie, generating an equation that seems a little more complicated than the classical wave equation. Note that we are postulating that the study of a microscopic system consists of finding the wave function ψ, which satisfies the Schrödinger equation. In other words, quantum physics based on these assumptions correctly describes all the phenomena to which it has been applied.

There are, in the literature, presentations of the Schrödinger equation as being derived from the wave equation, making, with this, several considerations that try to show its plausibility. We prefer, however, to treat it as a postulate. It is not possible to arrive at quantum physics from classical physics only by a logical argument. Let us make a particular analysis that consists of restricting to the one-dimensional case, where x is the only spatial coordinate. In addition to bringing simplicity, this case will suffice to study most of the applications that will be considered in this study. In the one-dimensional case, Equation (1) is written as:

$$\frac{-\hbar^2}{2m}\nabla^2\Psi(x,t) + V(x,t)\Psi(x,t) = E\Psi(x,t) \quad (2)$$

PHYSICAL INTERPRETATION OF THE WAVE FUNCTION

Let us better understand the meaning of the wave function. So far, it looks just like an abstract amount. Since the wave function is a complex quantity, it cannot be measured directly by any physical instrument in such a way there is no immediate physical sense to this function. Therefore, let us make it well established that, in fact, the wave function of a system is nothing more than an abstract mathematical representation of the state of the system. It only has meaning in the context of quantum theory. So, what is this function for? May we use it in any way to describe the physical world? Max Born, in 1926, postulated that the probability density P(x, t) obeys the following relation

$$P(x,t) = |\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t) \quad (3)$$

So that the probability of finding the particle between the positions x and x + dx, at time t is given by

$$P(x,t)dx = |\Psi(x,t)|^2 dx = \Psi^*(x,t)\Psi(x,t)dx \quad (4)$$

This result is known as "probabilistic interpretation of the wave function". Moreover, the probability must be normalized, that is, the probability of finding the particle in any region of space at a given instant of time must be equal to 1, that is

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, dx = 1 \quad (5)$$

In quantum mechanics we work with expected values (or mean values) of the dynamic quantities. The expected value of a quantity is defined as the average of the possible values, weighted by the respective probabilities of occurrence. In the case of the position, we have

$$\langle x \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t) x \Psi(x,t) \, dx \quad (6)$$

PROBABILISTIC INTERPRETATION OF MEASUREMENT RESULTS

Quantum mechanics, as it follows from the principles discussed above, is an inherently probabilistic theory: whereas in classical mechanics the result of each measurement can be predicted with precision, provided the initial state is known, quantum mechanics under the same conditions offers only probabilistic predictions. The nature of these probabilities, on the other hand, differs from those of classical physics: they do not happen due to lack of knowledge, because the wave function contains all the information about the state of a system, and the probability densities present terms of interference because they are the result of the squared module of amplitude sums.

In contrast to classical physics, the measuring device modifies the state of the system, which is usually, after conclusion of the measurement, in a different state. What happens to the system during the measurement? How should the measuring device be used to carry out the measurements? These questions, which do not appear in the classical case, constitute what is called the problem of the measure in quantum mechanics. What happens to the system during a measurement cannot be deduced from the previous principles, nor from the Schrödinger equation, which governs the behavior of quantum systems. The Schrödinger

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equation is a deterministic temporal evolution equation, that is, the final state is determined univocally by the initial state. Moreover, it is a reversible equation, from the final state one can in principle go back to the initial state, not being able to govern or describe an inherently probabilistic measurement process. Before the measurement, we cannot predict in which state the system will be after the measurement. The problems of measurement represent a matter of great complexity and in many of the books currently used were written not considering this problem as a relevant research topic.

OPERATORS AND EXPECTED VALUES

A quantum operator "operates" or acts on a wave function and the result is another function. This fact is represented by the result of the operation of the operator O on the wave function Ψ. In the simplest case, an operator can be a function f(x). When this happens, the result of the operation is simply the product of the function f by the wave function Ψ. However, in the more general case, a quantum operator may involve more complicated operations, such as differentiation. But, what are the quantum operators for? Certainly not just a mathematical curiosity, quite the contrary. Operators play a central role in the formalism of quantum physics, which is expressed by the following postulate: Each physical quantity is associated to a quantum operator. Moreover, supposing a particle in the quantum state defined by the wave function Ψ, the expected value of the measure of the physical quantity corresponding to the operator O is associated to the mean statistical value of many measurements of this quantity. In short, the quantum state of a particle is described by its wave function, which satisfies the Schrödinger equation. The squared module of the wave function gives us the probability amplitude of finding the particle in a certain position, with each physical quantity corresponding to a quantum operator.

FINAL CONSIDERATIONS

The behavior of a given wave function of a system is predictable in the sense that the Schrödinger equation for the corresponding potential energy will determine its form exactly at some later instant in terms of its form at some initial instant, but its initial form cannot be completely specified by an initial set of measures while its final form only predicts the relative probabilities of the results of the final set of measures, or in other words, the motion of the particles is in accordance with the laws of probability, but the probability propagates according to the law of causality.

In the teaching-learning of quantum mechanics, it is not enough to analyze the empirical facts and to develop the mathematical formalism. It is still necessary to reflect on the question of interpretation: what are the quantities present in the equations? How do they relate to the data that can be extracted from the experiments? What view of the physical world can one build from there? These questions have been debated between physicists and philosophers since the beginning of the theory and have been attracting a growing interest lately, both in the academic environment of the experts and even in the lay public. In partnership with relativity theory, quantum mechanics is the great star of the twentieth century. It represents the basis of nuclear, atomic, molecular and solid state physics, elementary particle physics and light theory. Nowadays quantum mechanics is associated with the most varied applications, benefiting even areas such as health sciences and engineering. Moreover, recent advances in electronic miniaturization and nanotechnology have introduced, even in the business world, devices that can only be developed from the principles of quantum mechanics. If this knowledge has been reserved for the students of physics and chemistry[6], it seems inevitable that most of the professionals of this new century must have a much deeper knowledge of this field than it was necessary until now.

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