

What is the wave function?

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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 seem to be more appropriate for the propagation of waves. This becomes qualitatively clear when we see 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 superficial analysis of the dynamics of quantum particles, through their postulates and their 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 can be found mainly in the books of PESSOA, HALLIDAY, FEYNMAN and JAMMER, cited in the bibliographical references.

Keywords: schrodinger, wave function, probabilities

1. 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 complex quantity called the wave function, and denoted by the symbol $\Psi(x, y, z, t)$, Y, z are 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 knowledge, added to the knowledge of the force (or, if you prefer, of the potential energy) acting on this particle, allows the complete description of its subsequent trajectory through the integration of Newton's 2nd Law. Even an undulating movement, will be fully known, if we know the spatial and temporal dependence of the wave function.

For example, in the case of waves at the water surface, we have seen that an appropriate wave function was 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 derivative equation known as the wave equation. So it is reasonable to assume that the wave function of a quantum particle must also satisfy a wave equation.

2. What wave equation is this?

Suppose the 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 equation in partial derivatives:

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

Where h is 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 wave guide posited by Luis de Broglie, generating an equation that seems a little more complicated than the classical wave equation we know.

Note that we are postulating that the study of a microscopic system consists of finding the wave function ψ , which satisfies the Schrödinger equation. The only justification for the description of Quantum Physics to be based on these assumptions is that they work. 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 it really is, 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 which consists of restricting to the one-dimensional case, where x is the only coordinate. In addition to bringing simplicity, this case will suffice to study most of the applications we will consider in this study.

In the one-dimensional case, Equation (1) is written as:

$$\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V(r) \psi(r) = E \psi(r) \quad (\text{eq.2})$$

We see immediately that, because it is a solution of a complex equation in partial derivatives, the wave function will necessarily be a complex function. This fact will be discussed in the next item. The wave function $\Psi(x, t)$ is a continuous function and, whenever the potential $V(x, t)$ is finite, with continuous derivative as well.

3. Physical interpretation of the wave function

Before we begin to solve Schrödinger's equation in specific situations, what will be done in the next classes, we will better

understand the meaning of the wave function. So far, it looks just like an abstract amount. Is it really? Well, we see that, because the wave function is a complex quantity, it cannot be measured directly by any physical instrument. That means 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? Can we use it in any way to describe the physical world?

Max Born, in 1926, postulated that the probability density $p(x, t)$ of finding the particle at position x , at time t , obeys the following relation:

$$dP(x, t) = P(x, t)dx = |\Psi(x, t)|^2 dx \quad (\text{eq.3})$$

So that the probability of finding the particle in a region at time t is given by:

$$|\Psi(x, t)|^2 = \Psi^*(x, t)\Psi(x, t) \quad (\text{eq.4})$$

This result is known as "probabilistic interpretation of the wave function". Like all probability values, $P[a, b]$ must be real and positive, regardless of the interval considered. This is guaranteed by the fact that it is real and positive. Remember: this is the squared module of a complex number! 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,

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

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:

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

4. Probabilistic character 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 arbitrary 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.

Moreover, in contrast to Classical Physics, the measuring device modifies the state of the system, which is usually, after completion 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 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 are a matter of great complexity and in many of the books currently used were written in the decades in which this problem was not a relevant research topic.

5. Operators and expected values

A quantum operator "operates" or acts on a wave function, and the result is another function. We indicate 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.

This function is defined by the following postulate: Each physical quantity corresponds 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 , that is, the mean statistical value of many measurements of this magnitude.

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.

6. Final considerations

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 dwell on the question of interpretation: what are the magnitudes 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, Quantum Mechanics is the great star of the twentieth century. It is the basis of nuclear, atomic, molecular and solid state physics, elementary particle physics and light. Its practical impacts reach today's most varied applications, benefiting even areas of immediate practicality such as Health Sciences and Engineering. Moreover, recent developments in electronic miniaturization and nanotechnology have

introduced, even in the business world, devices that can only be appreciated from the principles of Quantum Mechanics. If until now this knowledge was reserved for the students of Physics and Chemistry, 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.

7. References

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