

Is Quantum Chemistry a neo-science?

¿Es la química cuántica una nueva ciencia?

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Abstract In this discussion is intended to explore a philosophical point of view about quantum mechanics, proposing quantum chemistry as neo-science, this philosophical approach to our view is certainly much neglected in many textbooks. The importance of creating new concepts in chemistry and propose new methodological tools motivate to the scientist to create new concepts and interpretations in theoretical chemistry.

Keywords quantum mechanics; philosophical approach; theoretical chemistry.

Resumen En esta discusión se pretende explorar un punto de vista filosófico sobre la mecánica cuántica, proponiendo la química cuántica como neo ciencia, este enfoque filosófico de nuestra visión está ciertamente muy descuidado en muchos libros de texto. La importancia de crear nuevos conceptos en química y proponer nuevas herramientas metodológicas motiva al científico a crear nuevos conceptos e interpretaciones en química teórica.

Palabras clave mecánica cuántica; enfoque filosófico; química teórica.

1 Introduction

Despite many considerations, the natural and exact sciences are not based on any recognized philosophy. Science is based only on experimental facts and on human performance that evolve with the growth of experience in doing science. If there several positions about interpretations of the outcomes of an experiment this does not lead to different predictions of experimental results, but some time dependent on a philosophical point of view. We can give different philosophical interpretations about experimental facts and on nature around. For instance, the double slide experiment has been object of many philosophical interpretations such as the Copenhagen school analysis or Einstein and Schrödinger interpretation. Only to mention some of the many possible interpretations with the same outcomes for a single experiment.

Basic human experience together with the training supply the strengths for working into reality. Human experience have the role of facilitating the unformulated elaboration with theory is brought into relation with experience for example in laboratory and the observation of physical facts and science singularities.

In this order of ideas mathematical or computer calculations are mere aids in imaging what is going on, this depends not only on learning mathematics but also on the training of scientifics who have learned, how to communicate their experiences and connect with mathematical concepts and other concepts such as social issues. Mathematical achievement has been successfully along with the history of science with application very well elaborate and tested by experiments. When mathematics and abstract concepts are applied for example to enterprise theoretical model of reality and methods for handling microphysical phenomena, we are deprived of the supports on with. We have been habituated to rely on our raw approach to nature and our treatment of atoms, nuclei and elementary particles seem to present them disembodied in space and time.

Quantum mechanics (QM) is a highly mathematized theory. The building of a theoretical model in quantum mechanics means developing a consistent mathematical framework in which the mathematical processes that mimic the physical reality. The predictions of quantum mechanics are right and their nature is abstracted. The outcome obtained correspond a mean values or expecting values of the properties of system. These facts have led to not simple interpretations of the theory, in fact, there are several interpretations of QM some of them with clears contradictions with other interpretations.

The use of a specific theoretical model using computers machine to calculate some chemical or physical properties that can be measure with an adequate set of mechanical devices in experimental way. In this case is possible to compare the computer machines results with the experimental date such as quantum chemistry made. Using computers to simulate reality is possible to perform a large number of numerical calculations.

Quantum Mechanics perhaps is the most successful and revolutionary theory in the history of science, with multiple consequences and applications in the real world. The use and application of quantum mechanics have changed our view of what the world is like. The impact and applications of quantum mechanics theory has touched many fields in science one of them is chemistry through quantum chemistry.

Quantum chemistry gives a rigorous description of chemical methods at its most essential level, for usual chemical processes. Quantum chemistry calculations have made a remarkable progress during the last decades. A development that have run parallel to the upgrading in hardware and software improvement. At the same time, quantum chemistry with its series of programs that calculate a variety of molecular properties have become standardized and automatized tool. Quantum chemistry customers when performed their calculations have in mind that their theories and theoretical models must be compatibles with experimental facts.

Here, we have the first problem, because of Dirac statement point of view, chemistry can be explained and reduced to quantum mechanics in an easy

way [1a]]. The Dirac's statement expresses a position that counts against the autonomy of chemistry and its status as a scientific discipline. From Dirac's point of view, chemistry is only a branch of physics. This point of view has been object of several critics especially for those whom believe that chemistry is an autonomous science [1(b-h)]. But The remarkable predictive power of quantum mechanics and successful when is applicable to solve problem in chemistry, led to most chemists, physicists and scientific in general to think that chemistry can be reduced to physics. This reductionist way of thinking is due to the achievement of quantum mechanics. For this reason, quantum chemists and physicists tend to reduce chemistry to physics.

In these order of ideas, many concepts can be connected from physics to chemistry via quantum chemistry calculations, such as electron density or electric charge. In the electronic theory, the static and dynamic behaviors of molecules can be explained by the electronic effects that are based on nothing but the distribution of electrons in a molecule. For example, charge distribution in a molecule can be outlined to some degree by the use of the electronegativity concept. Also, this concept is supported by physical measurements of electron distribution and quantum calculations based on quantum theory.

The charge distribution is habitually represented by the total numbers of electrons in each atom and each bond, and it is a concept acceptable without trouble almost accept for everyone as having an acceptably realistic meaning. Chemists have employed the electron density as a key concept to explain or to understand a widely variety of chemical phenomena. In particular, for stimulating chemical investigations. Chemist usually rely on the similarities through familiarity, and the electron density is a very successfully and extensively used as the basic concept in that analogy [1 i)]. But the change of electron density distribution does not give answer to everything.

The question to be developed in the present contribution is "if quantum chemistry are eligible to be part of the natural sciences?", this question has been

addressed in different ways throughout the history of theoretical chemistry according to Bunge et al. [1(b)] According to Mario Bunge [1 j,k)] not all scientific research seeks objective knowledge. So, logic and mathematics, that is, the various systems of formal logic and mathematics are rational, systematic and verifiable but they are not objective, not give us information about reality: simply do not address the facts. A lot of work in mathematics or logicians often meets the needs of the physical or chemical. The material used by chemist-mathematicians is not factual is ideal, and a clear example of this idea is precisely the measurement system employing quantum chemistry governed by the ideal and the causality of the facts.

Moreover, QM as factual science has its empirical base. Because some of the theoretical facts can be checked experimentally. Verifiability is the essence of scientific knowledge, if it were not so, it could be said that scientists seek to attain objective knowledge, as example we have the abstract character of quantum chemistry.

This question in itself is not an easy question to answer considering that a scientific discipline is considered a science when complying with the scientific method and this is based on accurate measurement processes and it is precise which in the quantum chemistry missing, for this purpose in this paper is postulated answer to this concern through of recognition of the quantum chemistry as a science.

In classical mechanics is possible to define with precision arbitrarily large number of variables dynamic such as position coordinates, components of moment and angular momentum, or electric and magnetic field vectors and other properties that describe the stat of the system under consideration. For these kind dynamic variables are possible to assume that the evolution of a system over time is predictable with certainty, still less the knowledge of final state and initial state in the time obtained by the application of the equations of motion [2].

Despite of the big achievement made by quantum mechanics remain controversy in some point. For instance, the idea of measure in quantum mechanics continue being a controversial issue, since

Heisenberg uncertainty principle was established as universal principle in quantum mechanics [3]. This principle has been object of many philosophical interpretations. The most famous interpretation is the interpretation of the Copenhagen school. This school assumes that the uncertainty relation is a restriction associated with the process measurement that will never fade with subsequent advances in knowledge. Represents a fundamental limitation that applies permanently, and hence it is elevated to the status of the principle of nature. They affirm that science is the study of our observations and not the world itself is very well known from Heisenberg Principle [3] that is impossible to determine simultaneously with precision certain pairs of variables called "conjugate"(for example, the position and momentum, energy and time), does not mean simply abandoning the deterministic hypothesis and the idea that the "laws of nature" are inherently probabilistic, it also calls into question the classical notions of realism and physical location and makes the act of measuring something enigmatic, because it shows that any interaction between the system-object-apparatus system changed so as irreversible and unpredictable status-object system after the measurement. As was noted by E. Wigner, "all is well in quantum mechanics, while not wonder how the observation takes place". The magnitude of this transformation appears dramatically in the "paradoxes", for example in the paradox Einstein-Podolsky-Rosen (E.P.R) [4]. First formulated in 1935 by Einstein and collaborators, these events indicate that the quantum chemistry needs conceptualizations according with their probabilistic nature and this is a problem that has the theoretical quantum chemical not to know from the point of view of the theory of knowledge that underpins their measurements. Is very well known, that the Copenhagen interpretation was developed when quantum mechanics was still a developing theory, this interpretation was established principally by Bohr, Heisenberg and others in the 20's of last century. Try to explain the reason behind the collapse of the wave function. Copenhagen interpretation is considered until today as the standard interpretation of quantum

mechanics at least is the most used and known version [5-7].

2 Quantum Chemistry as Neo-science

For the formulation of the concept of quantum chemistry as Neo-science is taking into account the advantage of the autonomy of chemistry as a science widely studied in the epistemological theory of science, see ref. [8-14].

The new concept that is propose in this study is justified by the intrinsic nature of quantum mechanics through the story of understanding and interpretation of the wave function its probabilistic nature and its collapse when we make a measurement. On the other hand, very few Scientifics have accepted the philosophical exercise in the quantum chemistry, therefore is a widely neglected area according to Vivas-Reyes et al. [15]; which allow us to highlight the world of chemistry from the point of view anthropological and ontological.

However, the runaway success of classical mechanics and electromagnetics later gave rise to the idea that the concept of causality is only necessary in for a context in terms of physical determinism [16]. The necessity to present new concepts of quantum mechanics is evident from the point of view of the scientific naturalism that tends to adopt generalized positions and especially of the tradition [3, 7, 17-24], due to the pronounced mental inertia which adopts the ideas pre-conceited and natural. Taking into account the basic characteristics of original naturalism proposed by Willard Van Orman Quine et al. [13].

On the other hand, the philosophy of quantum chemistry emerge as a legitimate area of philosophical inquiry that demands our attention, the best work can be done now by the chemists in this neglected area is the attempt to understand this kind of thing to show importance in many scientific aspects of chemistry as something to help change the image of chemistry as an autonomous science, and often lose the context of it in the field of physics, making a more impartial communication between chemistry and

physics, which is vital to make a chemistry teaching that reaches a wider audience and that positively impact and this can be achieved by making it more friendly chemistry on issues such as the progress of applications physicochemical today more impact on our society.

Quantum physics tells us that all realities exist simultaneously in a potential that the subatomic world behaves incomprehensibly different from the physical laws we know and the mystery of life seems even more profound, but if we adopt their principles given the opportunity to renew and enjoy life more given that the assumptions of all the philosophies we know, many of them false, and do not serve us, because they do not value the power of man and the value of thought, quantum physics does not explain the mystery of the universe but encourages us to become more responsible for ourselves.

New concepts are presented in this contribution such as abstract such as quantum chemistry as Neo-science with mathematical-statistical abstract image using as evidence the experimental conditions, open new possibilities to reclassify and characterize the quantum chemistry from the point of view scientific and educational science, in which its mathematical fundamentalism has much coherence with experimental data, however little understood as is able to get his amazing successes, so this perspective presented in the study, show the uncertainty of their measurements and probabilistic intrinsic character.

Thus, quantum chemistry is oriented towards the future as a science that is able to recognize the probabilistic nature, with large expectation who every day between their theoretical prediction and experimental correlations, therefore understanding the epistemological sense of quantum chemistry is very important.

3 Conclusions and perspectives

In this paper, we propose a new perspective about quantum mechanics which states that it is science that seeks to determine the chemical principles from a

point of view physical, mathematical-statistical abstract image using the experimental conditions as evidence, this concept that we intend to present is motivated by the philosophical character of the relationship between Heisenberg and the behavior of the wave function, used the autonomous nature of the chemical to create concepts and arguments that allow us to give an identity to the chemical sciences and philosophical and scientific that this aspect of chemistry almost never mentioned. In addition, quantum physics calculates only possibilities and what or who choose this option and immediately we can realize that consciousness has something to do because we cannot ignore the observer is part of us, our spirits stay in the body, awareness controls us, the man was chosen from among the movements of consciousness at every moment the actual experience that manifests itself, so, instead of thinking about these things is to think of possibilities, because they are all possibilities of consciousness for all these reasons we propose to call quantum chemistry as Neo-science.

There is necessity to recognize the abstract nature of quantum chemistry as Neo-science is currently not recognized, taking into account the great successes of the chemistry quantum experiments which have been very consistent from the beginning [25, 26].

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