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Teaching the Philosophical Interpretations of Quantum Mechanics and Quantum Chemistry Through Controversies

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Abstract This study has the key premise of teaching history and philosophy of physical sciences to illustrate how controversies and rivalries among scientists play a key role in the progress of science and why scientific development is not only founded on the accumulation of experimental data. The author is a defender of teachers who consider philosophical, historical and socio-scientific issues. In particular, the disputes can be used in science teaching to promote students awareness of the "historicity" of science and to facilitate the understanding of scientific progress beyond that of inductive generalizations. The establishment of a theory is accompanied with philosophical interpretations all the way. The author will try to show that it gives excellent results in teaching and learning to bring to the foreground the complexity that surrounds the development of ideas in science, illustrating how controversies, presuppositions, contradictions and inconsistencies find a place in the work of scientists and philosophers alike. In this sense, the case of quantum mechanics and quantum chemistry is very solid because it is historically full of controversies among their heads: Einstein, Bohr, De Broglie, Heisenberg, Schrödinger, Born, Lewis, Langmuir, Bader, Hoffmann and Pauling, at least.

1 Introduction

The objective of this study is to reconstruct historical episodes, and analyse controversies and rivalries among scientists that have been important in quantum mechanics and quantum chemistry progress. Philosophical interpretations of the first years of quantum mechanics will be also debated—the reader is referred to the work of Freire (2003) for the more recent debate that includes David Bohm "hidden variables" interpretation, Bell Inequality, Aspect experiment and Everett's Many Worlds Interpretation, that will not be

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taken up in this study. Hence notions of the Nature of Science will be investigated through history and philosophy of physical sciences (HPS), mainly to convince teachers of Quantum Mechanics and Chemistry, as readers of this journal, that Copenhagen's Interpretation is not the only one on the nature of electrons and chemical bonds.

Although quantum mechanics was created to describe an abstract atomic world far away from daily experience, its actual impact on our lives could hardly be greater, because of its impact on modern technology—lasers, transistors and semiconductors, for example.

The outstanding recent scientific advances could not have occurred without the instruments that quantum mechanics has made possible. Without quantum mechanics there would be no global economy to speak of, because the electronics revolution that brought us to the computer age is a child of quantum mechanics. So is the photonics revolution that brought us to Internet and the Information Age. The creation of quantum physics has transformed our world, bringing with it all the benefits—and the risks—of a scientific revolution.

Quantum theory is the most precisely tested and the most successful theory in the history of science. Its applications in chemistry explain the chemical bonding either via the valence bond—by John C. Slater and Linus Pauling—or the molecular orbital models—by Friedrich Hund and Robert Mulliken; bizarre phenomena such as superconductivity and superfluidity; also exotic forms of matter such as the ones existing in neutron stars; and Bose-Einstein condensates. Quantum mechanics provides essential tools for all of the sciences and for every advanced technology (Kleppner and Jackiw 2000). That is why, due to its growing importance, it becomes imperative to offer to the future professionals courses on the foundations of quantum theory. Given the controversial nature of the philosophical interpretations on the subject, in this paper a historical-philosophical focus is recommended for its teaching. The author of this article has been teaching quantum chemistry for almost 40 years with a historical focus; using, among others, a textbook written by him within this approach (Cruz-Garritz et al. 1986).

Though, there is a debate also in the way recommended to pedagogically present the topic. It has been argued that the historical presentation—beginning with blackbody radiation, photoelectric effect, and Bohr's hydrogen atom model—may be inconvenient (Greca and Herscovitz 2002) because these cases use a classical behaviour as a starting point (electrons with a given path). Facts are presented chronologically with the questionable pedagogical objective of persuading students that quantization is an "obvious" conclusion rationally attained as a consequence of a series of experiments. It has also been said that the emphasis on Bohr's model is inconvenient, because it is almost a 100 years old model that overemphasizes classical physics conceptions, adding the learning difficulties inherent in the quantum description (Fischler and Lichtfeld 1992). Kragh (1992) call these presentations as "quasi-historical". Exceptions to this rule are the proposals of *Feynman's Lectures on Physics* (Feynman et al. 1966) and *Berkeley Physics Course* (Wichmann 1967), both derived from Dirac's (1930) idea of discussing quantum concepts from quantum mechanics, directly.

However, James Conant's (1949) idea of using case histories in science to teach how scientists approach and conduct scientific research is a very good one in fostering learning that scientific development is not based on accumulation of data or constitutes a simple linear process. Conant believed that studying the work of great scientists can illustrate the "tactics and strategy of science" (Chapter IV, p. 94). Selected seminal cases from the early days of a discipline require the least amount of factual or technical background on the part of the students; at the same time, these early cases are the best examples of the intellectual groping involved in scientific research (Giunta 1998).

Williams (2003) reflects on the value of conflicts in the process of knowledge: “Disasters are revelations… We never understand a technological system better than when it collapses” (p. 216). Niaz (2009a, p. 1) says:

> Many major steps in science, probably all dramatic changes, and most of the fundamental achievements of what we now take as the advancement or progress of scientific knowledge have been controversial and have involved some dispute or another. Scientific controversies are found throughout the history of science. While nobody would deny that science in the making has had many controversies, most science textbooks and curricula consider it as the uncontroversial rational human endeavour.

This author has extended the view to the quantum mechanics models of the atom and molecules. He has been involved about the covalent bond with Lewis (Chapter 10); quantum mechanics with Bohr and Bohm (Chapter 11), wave-particle duality with De Broglie, Einstein and Schrödinger (Chapter 12) in his discussions.

The use of controversies to form chemistry teachers, in particular, has been also brilliantly treated by Niaz (2009b). In another paper, Niaz (2010) has argued that in order to facilitate an understanding of science-in-the-making, we need to write science textbooks within a HPS perspective. Chemistry and physics textbooks rarely use an historical controversy to present the Nature of Science. The Vienna Circle, cradle of the positivist vision, has dominated curricula and textbooks, considering science as an uncontroversial human endeavour.

In this sense Kuhn (1970), who is generally supposed to have been a harbinger of radical changes and even perhaps an iconoclast in the social sciences, in the case of science education, however, has had an influence in favour of traditional approaches to teaching. Kuhn (1970) insists that textbooks to be good “pedagogical vehicles” to transmit the “normal science” vision:

> Textbooks, however, being pedagogical vehicles for the perpetuation of normal science, have to be rewritten in whole or in part whenever the language, problem-structure, or standards of normal science change (p. 137).

Tsaparlis (1997b) emphasizes the historical method of teaching as a way of understanding better the atomic and molecular structure. He says that “the view that the history of scientific discoveries shows the natural route of human thinking and matches the cognitive development of the human mind” (p. 924). Teixeira et al. (in press) have recently report a synthesis of didactic strategies that have been used within the HPS perspective in physics teaching, including quantum mechanics.There are only a few of the textbooks of quantum mechanics and chemistry that uses a HPS strategy and present the topic with the debate of interpretations on it. And when the authors include them (Blinder 2004, for example), they do it in a final chapter out of the presentation of the content in itself; that is, those books are mainly permeated with the flavour of the Copenhagen interpretation.

In the book of Cruz-Garritz et al. (1986) the author of this article has written in its chapter 6 a summary on two of the interpretations of quantum mechanics (the Copenhagen and the Stochastic; sections 6.5.2 and 6.5.3), that have been used to exercise argumentation in the college level course “Structure of Matter”—lectured in second semester at National University of Mexico—that will be detailed below.

1.1 Difficulties in the Teaching and Learning of Quantum Mechanics and Quantum Chemistry at College Level

Students have difficulty understanding the concepts of atomic and molecular structure because of the abstract nature of the sub-micro world:

> This is an unobservable world, accessible only by imagination. Imagination is such a key component of advances in chemistry at the research level, as well as of rich student understandings, that its significance cannot be underestimated, and we would do well to rise our students' consciousness of it in order that they might try to develop their visualization abilities (Bucat and Mocerino 2009, p. 12).

Many authors have been discussing in several studies the difficulties or misconceptions in students' learning about bonding. For example, those related to bonding in general (Hund 1977; Kutzelnigg 1984; Boo 1998; Birk and Kurtz 1999; Özmen 2004; Magnasco 2004); the history of the concept (Sutcliffe 1996); on geometry and polarity (Furió and Calatayud 1996); the covalent bonding model (Peterson et al. 1989; Niaz 2001; Coll and Treagust 2002); the metallic bonding model (de Posada 1999; Coll and Treagust 2003a); and the ionic bonding one (Butts and Smith 1987; Taber 1994, 1997; Coll and Treagust 2003b).

Other studies have reported students' difficulties in grasping the fundamental issues of quantum mechanics and quantum chemistry in college level (Paoloni 1982; Johnston et al. 1998; Hadzidaki et al. 2000; Greca and Moreira 2001; Wittmann et al. 2002; Kalkanis et al. 2003), in particular the following concepts: "probability and energy quantization" (Park and Light 2009); "quantum numbers" or "electron configurations of chemical elements" (Scerri 1991; Ardac 2002; Niaz and Fernández 2008; Melrose and Scerri 1996); "orbital ideas" (Ogilvie 1994; Tsaparlis 1997a; Scerri 2000; Taber 2002a, b; Conceicao and Koscinski 2003; Taber 2005); "uncertainty and complementarity" (Pospiech 2000); and the "Schrödinger equation" (Tsaparlis 2001).

From the point of view of teaching, the elementary, qualitative and pictorial coverage of quantum chemical concepts is approached with certain reservations or with strong opposition by many chemical educators (Bent 1984; Gillespie 1991; Hawkes 1992).

Physicists have also recognized the difficulties involved in understanding quantum mechanics (Einstein 1926; 1944; 1948; Feynman 1985; Styer 2000; Laloë 2001). Feynman (1985, p. 129) was categorical when he said: "I can safely say that nobody understands quantum mechanics". Philosophers of science have argued that quantum mechanics is particularly difficult to understand; due to the controversial nature of the different interpretations [e. g. Copenhagen School "indeterminacy", Bohm's "hidden variables", and Everett's Many Worlds Interpretation].

According to physicist–philosopher Shimony (1985, p. 109), "I must confess that after 25 years of attentive—and even reverent—reading of Bohr, I have not found a consistent and comprehensive framework for the [Copenhagen] interpretation of quantum mechanics". In contrast, in a recent critical review, Laloë (2001), a physicist, has conceded that:

> At the turn of the century, it is probably fair to say that we are no longer sure that the Copenhagen interpretation is the only possible consistent attitude for physicists… Alternative points of view are considered as perfectly consistent; theories including additional variables (or "hidden variables") (p. 656).

Kleppner and Jackiw (2000) mention on quantum mechanics: "today some of the luminaries of science remain dissatisfied with its foundations and its interpretation, even as they acknowledge its stunning power". The conclusion of this section is that Quantum Mechanics and Chemistry are hard nuts to crack for students as well as for scientists.

1.2 A Brief Scientific and Philosophical Account

In 1900 Max Planck postulated that a black body does not absorb or emit radiant energy in arbitrary quantities but in quanta. More precisely, electromagnetic energy of frequency υ exchanges energy with matter in an integral multiple of the quantum of energy $h\upsilon$, where

$h = 6.626 \times 10^{-34}$ J s, is the famous Planck's constant (Planck received the Physics Nobel Prize in 1918 "by his discovery of energy quanta"). It was in 1905 when Albert Einstein solved the photoelectric effect conundrum postulating that something similar holds for electromagnetic radiation in free space (the quantum hypothesis of light): the total energy of a light quantum of frequency υ is $h\upsilon$ (he received the Nobel Prize in Physics in 1921 "especially for his discovery of the law of the photoelectric effect"). In other words, radiation is composed of photons, or electromagnetic field quanta. In 1911 Ernest Rutherford explained the result of his scattering experiments by assuming that an atom is made up of a positively charged hard core surrounded by electrons. In 1913, Niels Bohr mathematized Rutherford's model and gathered it with Planck's and Einstein's ideas about radiation. As it was pointed out by Wilson and Sommerfeld, Bohr postulated that in an atom the action (energy × time) is quantized and, more precisely, that it is an integral multiple of the Planck constant h. All these developments are known as the "Old Quantum Theory".

Louis de Broglie, Werner Heisenberg, Max Born, Pascual Jordan, Erwin Schrödinger, Paul A. M. Dirac and a few others built the modern quantum physics between 1924 (De Broglie's wave-corpuscular nature of particles) and 1928 (Dirac relativistic equation). All started with De Broglie's idea of a pilot wave guiding the trajectory of a particle. This is a way of introducing integer numbers to represent the quantization of particles.[1]

The De Broglie expression relating the wavelength of the pilot wave and the momentum of the particle is an inversely proportional equation: $\lambda = h/p$. This theory gave up the classical concepts of position, linear and angular momentum, and energy because there is an explicit relation between a wave property, λ, and a particle one, p. Instead, the Schrödinger formulation introduced operators that act on the famous state function, Ψ, formally similar to a classical wave, which is why it is also called the "wave function". This formal resemblance suggested, at the beginning, that matter is wavelike. In 1927 Clinton J. Davisson and Lester H. Germer in USA, and George Paget Thomson and Alexander Reid in UK, confirmed experimentally this conjecture under certain conditions, measuring the wavelength from the diffraction patterns of electrons passing through a crystal (Davisson) or a metallic film (Thomson). However, under different conditions the wave aspect stands out and the De Broglie wavelength was confirmed. One therefore talks about the particle-wave duality since then.

2 The Copenhagen Interpretation of Quantum Mechanics and its Opposition

The key elements of the Copenhagen interpretation of quantum mechanics are the probabilistic description of matter, and the reconciliation of the wavelike and particlelike natures through Bohr's 'principle of complementarity'. It is an extension for particles of the complementarity of light. Measurements made on identical systems that are identically prepared will not yield identical results. Rather, the results will be scattered over a range described by the wave function, Ψ. Consequently, the concept of an electron having a particular location and a particular momentum loses its foundation. The Uncertainty

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[1] The determination of the stable motion of electrons in the atom introduces integers, and up to this point the only phenomena involving integers in physics were those of interference and of normal modes of vibration. This fact suggested to me the idea that electrons too could not be considered simply as particles, but that frequency (wave properties) must be assigned to them also.

(Louis V. de Broglie, 1929, *Nobel Prize Lecture*, p. 247).

Principle quantifies this: To locate a particle precisely, the wave function must be sharply peaked (that is, not spread out). However, a sharp peak requires a steep slope, and so the spread in momentum will be great. Conversely, if the momentum has a small spread, the slope of the wave function must be small, which means that it must spread out over a large volume, thereby portraying the particle's location less exactly (Kleppner and Jackiw 2000).

Bunge (2003) has argued that, "the wave-particle duality pops up clearly in Heisenberg's inequality, popularly misnamed "indeterminacy" or even "uncertainty relation". According to it, the position and the linear momentum have distributions whose variances (or mean standard deviations) are inversely proportional to one another. More precisely, $\Delta x \cdot \Delta p \geq \mathrm{h}/4\pi$. Thus, the sharper the position (small Δx), the more spread out the momentum is (large Δp), and *vice versa*" (p. 449).

Niels Bohr (1928) headed the Copenhagen School with the usual or orthodox interpretation of quantum mechanics, and almost universally accepted by chemists, physicists, philosophers and textbook authors, based on the concepts of "complementarity" (wave-particle duality), "indeterminism" and "nonrealism". The complementarity principle states that some objects have multiple properties (wave and particle-like ones) that appear to be contradictory. Complementarity and Uncertainty dictate that all properties and actions in the physical world are therefore non-deterministic to some degree.

In 1926 Max Born proposed that the central role of the wave function is to determine the probability of a certain outcome, by means of its square. When a quantum superposition is observed or measured, we see one or the other of the alternatives at random, with probabilities controlled by the square of function Ψ. When the wave function "collapses" a single outcome is observed, with the distribution shown by $|\Psi|^2$.

The interpretation in question reads thus: the quantity $|\Psi(x, t)|^2$ is the probability of *finding* (cursives by the author) the particle inside the unitary volume placed at point x when its position is measured at time t . This postulate shows, among other things, that the probability concept is basic in quantum mechanics. It also suggests that the probability in question depends upon the observer as much as upon the object observed (Shimony 1963). But, what happens when no position measurement is being performed? "According to the Copenhagen interpretation, in this case the quanton *has* no position, not even inside the volume element being considered. The idea is that you won't find unless you search and what is not found does not exist" (Bunge 2003, pp. 451–452).

It was decisive in the formulation of the Copenhagen interpretation its thesis that every microphysical event is the product of some measurement, so that every probability one calculates must be the probability of *finding* something upon performing a measurement. In general, the experimenter would create the world as one measures it. "To be is to measure or to be measured. Clearly, this view is anthropomorphic and even magical. It collides head-on with the realism inherent in both common sense and the practice of science" (Bunge 2003, p. 452).

Quantum phenomena, according to the orthodox interpretation, are located in the intersection of the observer and his observing setups. In addition, it is the observer who is supposed to play the active part therein. As long as the physical object was thus denied an autonomous existence, as long as laws of nature were not regarded as objective patterns, but their meaning was confounded with the mode of their verification, physical causation could merrily be swept aside. Thus, the role of the observer is crucial for the Copenhagen school. One cannot really discount the effect of observations in order to obtain an observer independent picture of the world. "There are not autonomous quantum events but only observer dependent quantum items: the observation or measurement operations generate the entities in given states" (Bunge 1973, p. 89).

Bunge (1982) writes on the field of modern science causality principle:

> Causality had been a casualty of two profound intellectual revolutions in the 1920s, namely the quantum theory and logical positivism… Besides, the quantum theory was basically probabilistic. No wonder, then, that causality seem scientifically and philosophically dead… The arguments against causality have lost much of their force in recent years. For one thing, the Copenhagen interpretation of quantum mechanics is no longer accepted without qualifications: more and more physicists are becoming dissatisfied with its subjectivist aspects (pp. 134–137).

Bryce DeWitt, the driving force of Hugh Everett's Many Worlds Interpretation of Quantum Mechanics has mentioned in relation with the overwhelming majority of physicists defending the Copenhagen Interpretation.[2]

2.1 Einstein Versus Bohr-Born Debate

Alongside numerous advances, however, fierce debates were taking place on the interpretation and validity of quantum mechanics. Foremost among the protagonists were Bohr and Heisenberg, who embraced the new theoretical interpretation, and Einstein and Schrödinger, who were dissatisfied with it. Einstein kept a long controversy with Bohr, in particular. It is clearly revealed in the sentence "God does not throw dice" in the December 4th 1926 letter to Max Born:

> Quantum mechanics is certainly imposing. But an inner voice tells me that it is not yet the real thing. Quantum theory says a lot, but does not really bring us any closer to the secret of the Old One. I, at any rate, am convinced that He [God] does not throw dice (Einstein in letters to Max Born December 1926).

In another famous phrase, Einstein says "The quanta really are a hopeless mess" (Einstein 1926; On doing Quantum Theory calculations with Pauli). Almost two decades after that sentence, in 1944, Einstein claims for a more realistic way of interpreting the quantum theory.[3]

Dirac shared the 1933 Nobel Prize for physics with Schrödinger and the Nobel Committee also announced the award of the 1932 Prize to Heisenberg. All three physicists went to Stockholm in December 1933. Those were squally years in Germany because Adolf Hitler became Chancellor on January 1933, and the government introduced laws forbidding Jews from holding academic positions in German universities. Max Born and James Frank were displaced. And, although he was not Jewish, Schrödinger left Berlin for exile in Oxford, and Einstein moved to the Institute for Advance Study in Princeton, USA.

Following the description of the debate, Einstein—with two young scientists, the Russian Boris Podolsky and the American Nathan Rosen, that were invited to work in Princeton with him—managed to construct a Gedankenexperiment (thought experiment) of an idealized two-atom system in an "entangled" state in which the properties of both atoms are shared with each other (Einstein et al. 1935). If the atoms are separated, information

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[2] If a poll were conducted among physicists, the majority would profess membership in the conventionalist [Copenhagen] camp, just as most Americans would claim to believe in the Bill of Rights, whether they had ever read it or not (DeWitt 1970, p. 34).

[3] You believe in the God who plays dice, and I in complete law and order in a world which objectively exists, and which I, in a wildly speculative way, am trying to capture. I hope that someone will discover a more realistic way; or rather a more tangible basis than it has been my lot to find. Even the great initial success of the Quantum Theory does not make me believe in the fundamental dice-game, although I am well aware that our younger colleagues interpret this as a consequence of senility. No doubt the day will come when we will see whose instinctive attitude was the correct one (Einstein in letters to Max Born September 1944).

about one is shared, or "entangled", in the state of the other. The authors say as a conclusion: "a description of reality as given by a wave function is not complete" (p. 777). One of the lacks of this paper was its description of "reality" because it unnecessarily exposed the EPR argument to a powerful counter-argumentation.

The challenge was answered strongly by Bohr (1935) with a paper with the same title as EPR: "It is shown that a certain 'criterion of physical reality' formulated in a recent article with the above title by A. Einstein, B. Podolsky and N. Rosen contains an essential ambiguity when it is applied to quantum phenomena" (p. 696). The physical community has accepted fully Bohr's arguments even if Einstein did not changed his standpoint till the end of his life, having been aware of the correctness of his conclusions. The year 2010 was the 75th anniversary of this dispute and, nowadays, the literature is full of analysis about it yet. The effects are so surprising that they are the focus of study by a small but active theoretical and experimental community even today (Fine 2009; Peres 2005; Krüger 2004).

The issues are not limited to questions of principle, as entanglement can be useful: entangled states have already been employed in quantum communication systems, and underlie all proposals for quantum computation (Nielsen and Chuang 2000; Mermin 2007; Amador and Aspuru-Guzik 2008; Yuan and Gui-Hua 2009). For example, a book on quantum computing (Nielsen and Chuang 2000) quotes the following two sentences about EPR paradox in relation to Bell's (1964) entangled states and the correlated quantum bits (or qubits):

> These correlations have been the result of intense interest ever since a famous paper by Einstein, Podolsky and Rosen, in which they first pointed out the strange properties of states like the Bell state. (p. 17)
>
> Many physicists rejected this new view of Nature [Copenhagen]. The most prominent objector was Albert Einstein. In the famous 'EPR paper'… proposed a thought experiment which, he believed, demonstrated that quantum mechanics is not a complete theory. (p. 112)

In 1948, Einstein is still not convinced of the statistical status of the Copenhagen interpretation of the matter:

> I am well aware that no causality exists in relation to the observable; I consider this realisation to be conclusive. But in my opinion one should not conclude from this that the theory, too, has to be based on fundamental laws of statistics. It is, after all, possible that the [molecular] structure of the means of observation involves the statistical character of the observable, but that it is expedient in the end to keep the basis of the theory free from statistical concepts (Einstein in letters to Max Born 1948).

Tittel et al. (1998) of the University of Geneva informed a violation of Bell's inequalities with entangled photons, measured in Bellevue and Bernex in Swiss, 11 km apart. More recent experiments have been developed at greater distances. When Einstein and Schrodinger developed their now infamous thought experiments, they had sought to use entanglement and a "spooky" action at a distance to undermine the foundations of the interpretation of quantum theory laid down by the Copenhagen school. It would have been quite impossible to imagine that their arguments would become a basis of an entire new quantum technology.

2.2 Schrödinger's Cat

The famous paradox of the Schrödinger's cat (1935) goes as follows. A live cat is locked up for a while in a steel cage containing a phial filled with a lethal poison that may be released by the disintegration of a single atom present in a very small sample of radioactive material. Obviously, the disintegration may or may not occur during the time interval concerned. If it does, it is sure to kill the cat. But the observer won't know what happened until s/he opens the box and takes a look inside. Assume that the cat is a quantum-mechanical system and that while confined in the box, it is in a state superposition of its two possible macrostates: alive and dead. That is, its state is the linear combination:

$$\Psi = a\Psi_{\mathrm{L}} + b\Psi_{\mathrm{D}} \quad \text{with } |a|^2 + |b|^2 = 1$$

where $|a|^2$ and $|b|^2$ are the probabilities that the cat be alive or dead, respectively. According to the Copenhagen interpretation, these are the chances that the cat is *found* in either state when an observer opens the cage and looks into it.

This result is rightly regarded as paradoxical, because the idea that a cat can be half-alive and half-dead is plainly false. Schrödinger and Einstein took this result as an indication that something is seriously wrong about quantum mechanics and, in particular, the superposition principle. Bunge (1999) mentions that the cat paradox is definitively dissolved because it originates in the unwarranted tacit assumption that the cat is a quantum-mechanical entity that can be adequately described in terms of macrostates (live and dead), that are not specified in quantum mechanical terms (Ψ_{L} and Ψ_{D} are not eigenfunctions of any hermitian operator, and are not solutions to the Schrödinger equation for the cat-phial system, but only part of the imagination in the paradox). The Many Worlds Interpretation solve the trouble by saying that in half of the universes the cat is dead and in the other half is alive.

Now there is also controversy in the convenience of bringing Schrödinger's cat to life (Yam 1997) or breaking the phial and leaving it dead (Bunge 1999). In taking a decision we can relax with the following verse (Alda 1999):

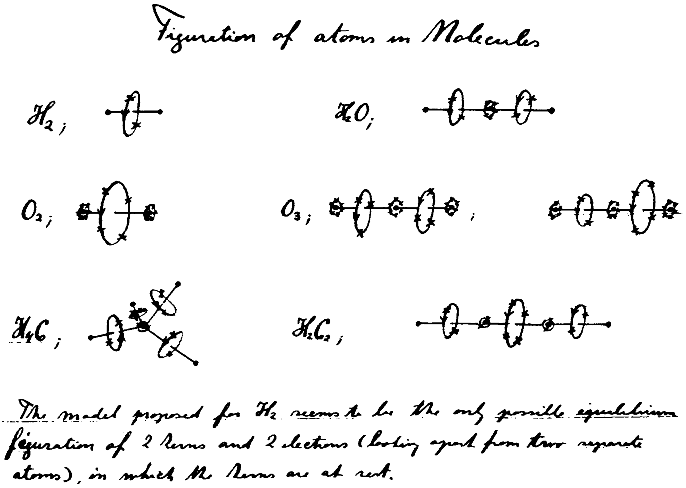
> His cat was both dead and alive
> Till Schrödinger's guests would arrive
> Then he'd open the box
> And toss in some lox—
> And the cat would both lay there and thrive.

3 Conceptions and Rivalries in Quantum Chemistry

In this section the point of view of physicists will be separated from that of chemists, because both have a different perception of the importance of quantum phenomena. Chemical bond is fundamental for a chemist as well as the electron nature is for a physicist.

We shall start in the Old Quantum Theory years, when Niels Bohr published his third work on the electronic model of atoms (and also molecules) in 1913. In it, Bohr presented a diagram of a H_2 molecule with two electrons orbiting in a circle perpendicular to the line connecting both nuclei, and O_2 molecule as four electrons in that circle (See in Fig. 1 the interesting, and almost present day diagrams for water, methane and acetylene besides the strange three electron bonds proposed for ozone, in "resonance"—I would say—with a second configuration with a single and a double bond). It is incredible the chemical knowledge and intuition that Bohr had being a physicist. He was the first who propose a way to predict electronic configurations of atoms that would explain the periodic table, in 1920, with the aufbau principle.

In 1916, the physicist Walter (Ludwig Julius Paschen Heinrich) Kossel developed an electrostatic model of the heteropolar chemical bond (ionic bond). In this case it was the transfer of electrons the responsible of the formation of ions and the multiple coulomb interactions between ions what achieves the bonding. Of course, the stability of ions was


Figuration of atoms in Molecules

The model proposed for H_2 seems to be the only possible equilibrium figuration of 2 kerns and 2 electrons (looking apart from two separate atoms), in which the kerns are at rest.

Fig. 1 Molecular configurations as sketched by Niels Bohr, from an unpublished 1912 manuscript, intended as an appendix to his 1913 papers (taken from Svidzinsky et al. 2005)

explained by the octet rule, fully familiarized afterwards by Gilbert Newton Lewis work. Lewis had presented its first cubic atom model since 1902 (mentioned in Lewis 1923, pp. 29–30) and his sharing electron model for the covalent bond (1916), which is based in the fact that atoms form bonds in order to achieve stable electronic configurations (variously referred to as octets, full outer shells or noble gas configurations).[4] In the absence of careful explanations of how bonds came about, and in the presence of some dubious diagrams and explanations in many text books, pupils find the octet rule as a rationale in what they are taught. The octet or full outer shell framework becomes elevated to the prime explanatory principle for chemistry, but nowadays it is considered as a pedagogic learning impediment (Taber 2000).

Lewis cubic atom was first conceived as a teaching device to illustrate the octet rule and can be considered as "speculative" (Niaz 2009a, p. 142). Lewis model—with its kernel and outer electrons; that is, its dotted structures—provides a useful way of describing and communicating much important chemistry yet today. Years later, the sharing of couples of electrons by atoms been bonded was attributed to Pauli Exclusion Principle, mixing ideas of chemists with ideas of physicists, at last. The exchange energy that maintains coupled different spin electrons remains a useful explanation of Lewis shared pairs in most of the written deep chemistry textbooks.

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[4] The third postulate of Lewis is very clear on the "octet rule":

> The atom tend to hold an even number of electrons in the shell, and especially to hold eight electrons which are normally arranged symmetrically at the eight corners of a cube (Lewis 1916, p. 768).

And the sixth on the non-applicability of Coulomb interaction for the electrons of the cube atom contrasts with its existence in polar compounds because of the larger distance between the charges:

> When a molecule owing to the displacement of an electron, or electrons, becomes a bipole (or multipole) of high electrical moment, that is, when its charged parts are separated by an appreciable distance, its force of attraction for another molecular bipole will be felt over a considerable intervening distance, … (Lewis 1916, p. 764).

It is remarkable the Lewis' (1916, p. 768) 6th postulate saying[4] "Electric forces between particles which are very close together do not obey the simple law of inverse squares", because it points out a difference between physicists and chemists. Bohr made use of the Coulomb attraction between nucleus and electron as a central force in his hydrogen atom model, and he based his arguments on the paradoxical stability of the Rutherford planetary model, in spite of the electrodynamics that forces a charge to radiate when subject to acceleration (Heilbron and Kuhn 1969). Nevertheless, Coulomb force was inconvenient for the polielectronic atoms of Lewis' model so he decided its non-existence by a postulate.

The later development of quantum mechanics, and its early successes in explaining the bonding in the hydrogen molecule led Dirac to make his much quoted remark:

> The fundamental laws necessary for the mathematics treatment of large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved" (Dirac 1929, p. 714).

This assertion has led to the philosophical debate of the reduction of chemistry into physics (Weininger 1984). Chemists continue to rely on electronic configurations for atoms and molecules that cannot themselves be strictly predicted fully from quantum mechanics. For example, they use three principles to deduce the configuration of any atom. These are the aufbau, Hund, and Pauli principles, none of which have themselves been deduced from quantum mechanics (Scerri 1998, 2007).

With the triumph of quantum mechanics there has been an inevitable tendency to exaggerate its success, especially on the part of practicing quantum chemists and physicists. There is no such thing as a completely *ab initio* calculation and, if one looks far enough back at the history of any scientific theory, one finds that it began with the assumption of at least some experimental data. Scerri (2004) asks to what extent the periodic table of the elements can be explained strictly from first principles of quantum mechanics without assuming any experimental data whatsoever. He arrives to the conclusion that the electronic configurations of atoms cannot be predicted by quantum calculations (Scerri 2007b, a book on the periodic table fully based in HPS). As Roald Hoffmann's (Nobel Prize in Chemistry 1981) title at the Rosenfeld memorial meeting stated, "Most of what's interesting in chemistry is not reducible to physics".

On the other hand, HPS has been defended for teaching by several authors in themes of Quantum Chemistry. For example, Blanco and Niaz (1998) have arrived to the following conclusions for the first quantum models of the atom:

1. History of science can be conceived as that of competing rival research programs;
2. Some of the greatest scientific research programs progressed on inconsistent foundations;
3. In actual scientific practice, counter-examples would be considered as mere anomalies;
4. Work of Thomson, Rutherford and Bohr led to the postulation of atomic models based on competing frameworks of understanding.

These authors have used Lakatos' methodology of competing research programs as a useful framework for the reconstruction of students' and teachers' understanding of the science content. Likewise, Justi and Gilbert (2000) established the use of HPS through models in the case of atomic structure. These authors have outlined their strategy based on six worthy assertions that have to be considered for teaching this topic:

1. Models are a suitable basis for HPS in science education;
2. Historical models can be characterized;

3. A finite number of models of the atom exist;
4. School curricula do not clearly refer to historical models;
5. Textbooks do not make appropriate use of historical models; and
6. Hybrid models are often used in teaching.

Teachers have also to realize that "atomic orbitals" are mathematical constructs and strictly speaking are only genuine wave functions in one-electron systems such as the hydrogen atom. In many-electron atoms orbitals serve as a useful approximation for the solution of the Schrödinger equation and that is all. The orbital approximation is the basis of a great deal of the work conducted in quantum chemistry, but here it is recognized that orbitals are mathematical constructs and do not possess any independent physical status (Scerri 2000).

Sanchez-Gomez and Martin (2003) have also adopted a historical perspective, focusing on the work of Gilbert N. Lewis and Linus Pauling as the main sources of modern chemical theory. Lewis theory brought along a model of the electronic distribution in the molecule that took into account most of the chemical experimental evidence that had been accumulated during the nineteenth century and the beginning of the twentieth. The initial work of Lewis appeared in 1916 and was extended in depth in a work with an explicit vocation for a textbook (Lewis 1923) and by Irving Langmuir since 1919, with his paper "The Arrangement of Electrons in Atoms and Molecules".[5]

The nature of the chemical bond, as well as the chemical properties resulting from this same nature, can be determined by chemists by means of several models and semi-empirical rules ["Lewis dot structures"; "atomic orbitals hybridization rules" (Pauling 1960); "Valence Shell Electron Pair Repulsion model" (Gillespie and Nyholm 1957); "Molecular orbitals" by Hund and Mulliken (Locke 1996)], most of them being old models of molecular structure, without a rigorous base on quantum mechanics. Those models are nowadays used by chemists even today, but with a progressively use of quantum mechanics and chemistry through personal computers. Quantum chemistry calculations that required a supercomputer can now be done with a much more accessible kind of devices and procedures.

Furthermore, if one focuses among the 1980s to 2000s issues of a referential journal for chemists, such as *Journal of Chemical Education*, the number of published papers on quantum chemistry (both on basics and on applications) have steadily increased. This growing importance of quantum chemistry can also be detected in the current chemistry curricula of most universities. Padilla and van Driel (2011) have captured the pedagogical content knowledge (PCK)—and its components and their relationship—of university professors teaching quantum chemistry. There are only a few papers on PCK that take university professors as their object of study (Padilla et al. 2008). Padilla and van Driel selected some questions on basic concepts taught in quantum chemistry courses: atom model, wave-particle duality, and atomic orbital. One of the questions had to do with an historical topic: "Could you tell how wave-particle duality was developed in the history of science? Do you pay attention to this historical development in your lessons?" All of the professors considered the subject to be quite complicated for students and seem to have almost identical views on what is important and what is unimportant. They tended to think

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[5] The problem of the structure of atoms has been attacked mainly by physicists who have given little consideration to the chemical properties which must ultimately be explained by a theory of atomic structure. The vast story of knowledge of chemical properties and relationships, such as is summarized by the Periodic Table, should serve as a better foundation for a theory of atomic structure than the relatively meager experimental data along purely physical lines. (Langmuir 1919, p. 868).

that thorough and careful explanations are required during lectures. It is interesting that one professor splits up his theoretical-experimental course into three parts: The first is an introductory course where he explains new ideas and concepts. The second is a workshop where he, together with students, solves problems that, initially, students had to work on by themselves. The third part is a lab session, which is held twice during the semester.

Although there are a lot of ways of probing bonding experimentally, the nature of chemical bond remains certainly obscure: distances (from X-ray, neutron and electron diffraction, microwave spectroscopy); bonding electron densities from diffraction experiments; dissociation energies; force constants, vibrational frequencies; magnetism; magnetic resonance (shifts and coupling constants); ionization potentials; spectroscopic criteria; scanning tunneling microscopy, atomic force microscopy. All that can be said through all different bonding models is that it is an electrostatic consequence of Coulomb interaction among atoms' particles, starting from here a pack of different bonding models: covalent, ionic, metallic, polar, residual, coordinate covalent, network covalent, *et cetera*.

The molecular structure hypothesis—that a molecule is a collection of atoms linked by a network of bonds—was forged in the crucible of XIXth century experimental chemistry (Archibald Couper in 1856 with his lines in chemical formulas; Alexander M. Butlerov: with the concept of chemical structure in 1861; and Friedrich A. Kekulé, with the structural formulas during the 1860s). It has continued to serve as the principal means of ordering and classifying the observations of chemists. The difficulty with this hypothesis is that it is not related directly to quantum mechanics. Richard Bader and Beddall (1972), Bader (1990) proposed a theory to make quantum mechanics compatible with the atoms in molecules paradigm, the "Quantum Theory of Atoms in Molecules".

The electron density describes the manner in which the electronic charge is distributed throughout real space. The electron density is a measurable property and it determines the appearance and form of matter. This is illustrated in Fig. 2. To determine what physics has to say about this property one must consider not the density itself but the field one obtains by following the trajectories traced out by the gradient vectors of the density. This theory continues receiving attention (Nasertayoob and Shahbazian 2010).

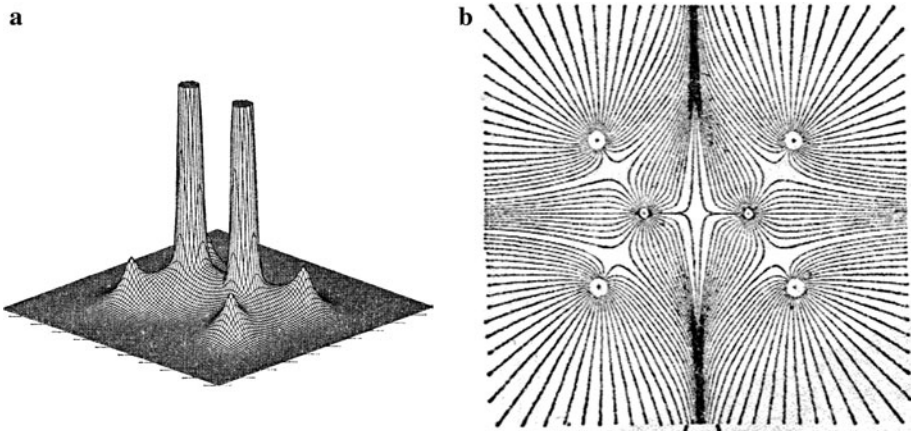

Fig. 2 Bader diagrams. **a** Electron density of C_2H_4. **b** A display of the trajectories that terminate at the nuclei in C_2H_4. Each trajectory is arbitrarily terminated at the surface of a small circle centered on the nucleus. The set of trajectories that terminate at a given nucleus (attractor) cover the basin of the attractor

Nevertheless, the “reality” on the structure of molecules has been questioned by complexity and the existence of fluxional molecules (Löwdin 1991; Mainzer 1997; Del Re 1998; Zeidler 2000; Ault 2001). That is why Roald Hoffmann (2011, final slide) finished a recent conference on the chemical bond by saying:

> I think that any ‘rigorous’ definition of a chemical bond is bound to be impoverishing, leaving one with the comfortable feeling, ‘yes (no), I have (do not have) a bond’, but little else. And yet the concept of a chemical bond, so essential to chemistry, and with a venerable history, has life, generating controversy and incredible interest. Even if we can’t reduce it to physics.

4 Argumentation, a Strategy to Confront the Controversies on Quantum Phenomena in the Classroom

The conceptualization of science learning as argument has been proposed by Duschl (1990), Kuhn (1993), and Driver et al. (2000), as well as others. A review on the topic has recently been published (Erduran and Jiménez-Alexander 2008).

As Jiménez-Alexander et al. (2000) mention, “Argumentation is particularly relevant in science education since a goal of scientific inquiry is the generation and justification of knowledge claims, beliefs, and actions taken to understand nature” (p. 758). That is why science education should give the opportunity to develop, among others, the capacities of reason and argument. It is also a way to form people within tolerance, to acknowledge especially opinions or behaviour one may not agree with.

Andree Tiberghien (2007) summarises the place of argumentation in science education in terms of three goals: knowledge about nature of science; developing citizenship more specifically; concerning socio-scientific issues and developing higher order thinking skills. Duschl (2007) says “Thus, learners need to have opportunities to discuss, evaluate, and debate the processes, contexts, and products of inquiry. Such discussions and debates expose the members of the community to each other’s ideas, opinions, sources of evidence, and reasoning” (p. 159). This author also remembers us that argumentation has three generally recognized forms: analytical, dialectical, and rhetorical (van Eemeren et al. 1996).

Edgar Morin (1998) speaks of the need of connecting knowledge to doubt, because education must be based on “the necessity of reinforcing critical thinking by linking knowledge to doubt, by integrating particular knowledge in a global context and using it in real life, by developing individuals’ ability to deal with fundamental problems with which they are confronted in their own historical epoch” (p. 17).

Erduran et al. (2004, p. 918) made an analysis on argumentation based in Toulmin’s (1958) point of view. The definitions to several keywords of Toulmin’s Argument Pattern are the following (It is important to mention all this new words to students, to set up an organized debate, calling things by its name during its development):

- “A claim is an assertion put forward publicly for general acceptance”.
- Grounds are “the specific facts relied on to support a given claim”.
- Backings are “generalizations making explicit the body of experience relied on to establish the trustworthiness of the ways of arguing applied in any particular case.”
- Rebuttals are “the extraordinary or exceptional circumstances that might undermine the force of the supporting arguments”.
- Toulmin further considers the role of qualifiers as “phrases that show what kind of degree of reliance is to be placed on the conclusions, given the arguments available to support them”.

5 Example of Application of Argumentation Put in Practice in the Classroom

The author of this article thinks that arguments on quantum physics are grounded in premises that are not evidently true, that are complex and counter-intuitive, they are dialectical, although also have a rhetorical character. The argumentation developed in the classroom of the course "Structure of Matter" in the second semester of the Chemistry careers at National University of Mexico, involved the probability concept in quantum mechanics and its vision within Copenhagen and Stochastic interpretations. The argumentation is based on the reading of Sections 6.5.2 and 6.5.3 on chapter 6 of the book by Cruz-Garritz et al. (1986), made by students at home.

All starts with a short presentation of the teacher on the statistical interpretation of the square of the wave function given by Max Born (1926). He was the one who in a paper wrote a footnote referring to the following sentence:

> If one translates this result into terms of particles, only one interpretation is possible: $\Phi_{n,m}$ (α, β, γ) gives the probability* for the electron…
>
> Max Born (1926, p. 866)

The star in the word "probability" above refers to a footnote which reads:

> *Addition in proof: More careful consideration shows that the probability is proportional to the square of the quantity $\Phi_{n,m}$

The discussion open in Cruz-Garritz's book is the meaning of this "probability" mentioned by Born. It has been debated by the different interpretations of quantum mechanics, as the "probability of *finding*" the particle by the observer in the Copenhagen interpretation, or the "probability of *being*" by the stochastic interpretation of quantum mechanics (De la Peña-Auerbach 1969). The last one explains the probability distributions in terms of statistical ensembles. De la Peña and Cetto (2001) present the main features of Linear Stochastic Electrodynamics (LSED) and its resemblances to the matrix mechanics developed by Born, Heisenberg and Jordan in 1926. These authors discuss extensively the concept of "trajectory" in quantum mechanics.[6] And, with respect to Heisenberg's uncertainty principle they say: "LSED implies that one should consider the quantum properties of matter not as intrinsic (hence irreducible), but as acquired properties. More specifically, according to LSED, the Heisenberg inequalities could in principle be violated before the quantum regime settles, even if for very short intervals of time" (p. 1723).

It was asked to the students, after reading the two sections, to go to an Statistics book and find what kind of definition of probability they present, what it is an ensemble, and debate what do they think on these claims of *finding* vs. *being* in the two interpretations. Some students base her/his grounds on common sense and classical arguments, arguing that the electron existence must not depend on the fact of being observed. Others defend the Copenhagen interpretation even with the rebuttal of experimental confirmations of the entanglement of particles.

Afterwards, students read some paragraphs of Bunge (1973) introduction to Quantum Mechanics in his book *Philosophy of Physics*. Bunge says, as a summary, that this discipline is probably the most powerful of all scientific theories, but it is also the one with the weakest philosophy. Bunge adds: "This weakness resides mainly in the inability to state unambiguously and persuasively what the genuine referents of the theory are" (p. 87). This

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[6] That the notion of trajectory becomes unrecoverable within the quantum description does not mean that the quantum particles do not possess a trajectory by themselves; only the theory describes not these trajectories, but the mean 'noiseless' motion (p. 1722).

reading had no profit on our students because they do not understand what could be the referents of a theory, of what type they can be, and things like that.

Greca and Herscovitz (2002) have also used conceptual discussions at the university level with topics like quantum computing, teleportation, quantum tunneling, one particle self-interference, quantum jumps and the Schrödinger's cat paradox. These authors work in a collaborative environment with groups of 3 to 4 students to which they give a written essay to be read during the 2 h session, which also contained questions and problems to make it interactive.

We agree with those authors that students entering the university do not have a deep knowledge on this topic, but a set of isolated facts useful to pass exams instead; the mental models used by these students are technically advanced but structurally unsophisticated (Johnston et al. 1998). Nevertheless we conclude that the argumentation was useful at least to leave clear in students' mind that there exist tentativeness in the interpretations of quantum mechanics, one of the characteristics mentioned by the Nature of Science (Niaz 2009a, b).

6 Conclusions and Implications for Teaching

Issues in HPS have for decades been marginalized in the curriculum (Nashon et al. 2008). In this paper historical episodes are reconstructed, and the analysis of controversies and rivalries among scientists is presented as very important features in quantum mechanics and quantum chemistry teaching.

Many of Albert Einstein's contributions to the study of the quantum nature of matter (Bent 1980) need to be recovered by college level teachers. But also his controversies with Bohr school have to be presented in an historical framework to develop in students a real idea of scientific development through debates among the central physicists of the scene.

Science education should not only present the empirical dimension of science to students but also the heuristic principles that enable the progress of science: "science curricula and textbooks, by emphasizing the historical context in which ideas, hypotheses and theories develop, can be particularly helpful in facilitating conceptual understanding" (Niaz 2009a, p. 25).

From the point of view of chemists, the complexity of the concept of bonding is also important for students to evaluate the gradual construction of scientific models. The work by Pauling is also recoverable (Abe 1981), mainly because his contributions to the valence bond model of molecular structure, the concept of "resonance" (Truhlar 2007) and mainly that of electronegativity (Kutzelnigg 1984), which has produce tens of new scales (Cruz-Garritz et al. 1986). Although today the molecular orbital model (Magnasco 2004; Cass and Hollingsworth 2004; Harrison and Lawson 2005; David 2005) has acquired a better teaching consideration with respect to the valence bond alternative, both models have to be evaluated by students. Teachers also have to be alerted on new technologies, because the PCs' latest generation has computing performances which are at least as high as those of most workstations of the 1990s. In other words, the possibility for literally any chemist of producing high quality quantum chemistry information is now open. It could be said that quantum chemistry is absolutely democratised through better and more exact methods each day.

The peculiar relationship between quantum theory and the quantum approach to molecular structure implies a series of obstacles for the teaching/learning of the latter. Some of these difficulties are perhaps coming from the twofold, physical and chemical, character of quantum chemistry. But the bulk of the problem arises from the distinct orientations of Physics and Chemistry as disciplinary sciences. Chemistry's approach is inclusive: substances are studied from the point of view of their common properties, of their similarities, detail playing a secondary role. Using a thermodynamic metaphor, it could be said that chemistry is an *extensive* science. In contrast, Physics is an *intensive* science. Substances are studied from the point of view of their differences. Detail is precisely what modern physics is committed to explain. History can be used by the teacher to get a metadisciplinary analysis on the scientific didactic topics (Sanchez-Gomez and Martin 2003).

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