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TEACHING INTRODUCTORY QUANTUM PHYSICS AND CHEMISTRY: CAVEATS FROM THE HISTORY OF SCIENCE AND SCIENCE TEACHING TO THE TRAINING OF MODERN CHEMISTS¹

ILEANA M. GRECA & OLIVAL FREIRE JR.

Departamento de Didácticas Específicas, Facultad de Humanidades y Educación, Universidad de Burgos, C/Villadiego s/n- 09001, Burgos, Spain; E-mail: ilegreca@hotmail.com

Instituto de Física, Universidade Federal da Bahia, Campus de Ondina, Salvador, BA, 40210-340 Brazil; E-mail: freirejr@ufba.br

ABSTRACT

Finding the best ways to introduce quantum physics to undergraduate students in all scientific areas, in particular for chemistry students, is a pressing, but hardly a simple task. In this paper, we discuss the relevance of taking into account lessons from the history of the discipline and the ongoing controversy over its interpretations and foundations in the search for new ways of improving the teaching of quantum physics. We also review and discuss the recent research in science education literature that proposes new ways of introducing quantum mechanics for undergraduate students. From these discussions, we suggest some possibilities – the inclusion of philosophical interpretations and their defense; the emphasis on strictly quantum features of the systems; an emphasis on formalism, without worrying about the ultimate ontological status of mathematics; the incorporation of quantum mechanics applications to real problems; and the need to introduce complementarity when using images - which can be taken into account when devising more effective ways of teaching introductory quantum mechanics for chemistry students.

I. INTRODUCTION

¹ This paper is a condensed and changed version, specially addressed for chemistry education, from the chapter Meeting the Challenge: Quantum Physics in Introductory Physics Courses to appear in Michael R. Matthews (ed.) History, Philosophy and Science Teaching Handbook, Springer, forthcoming.

The wide recognition of the relevance of quantum physics in current technologies, its role in science training and in the culture of science have enhanced research into new ways to present the subject in introductory physics courses (McDermott & Redish, 1999; Müller & Weisner, 2002, McKagan et al., 2010). In the case of chemistry, if some years ago it was said that chemists have had, or needed, only a superficial knowledge of quantum mechanics (Sánchez Gómez & Martín, 2003), because the application of quantum mechanics to chemical problems was very difficult, and the existence of a simple visual model of a molecular structure, partially independent of quantum mechanics (called Folk Molecular Model), was enough to solve a broad spectrum of problems, the situation has now changed. As pointed out by Sánchez Gómez & Martín (2003, pp. 132-133), the development of rich computational models that can be used to approximate solutions to the Schrödinger equation on PCs and the fading hegemony of the above-mentioned simple visual model for the resolution of several challenging quantum chemistry problems in the last twenty years, have changed the position of quantum mechanics in the training of modern chemists. Now, more than ever, it is an unavoidable issue that calls for new ways in which to make the quantum core concepts accessible to for students.

Nevertheless this is no simple task. The difficulties students encounter with quantum theory in advanced courses are legendary and several studies have shown that the difficulties are even greater in introductory courses in quantum mechanics in all scientific careers (see, for example, Fishler & Lichtfeldt, 1992; Tsaparis, 1997; Johnston et al., 1998; Singh, 2001; Cataloglou & Robinett, 2002; Taber, 2002).

We will argue in this paper that one of the main challenges related to introductory courses in quantum physics is to find a balanced way in which to introduce the most basic quantum concepts while taking into account interpretational issues as quantum theory is both technically and philosophically sensitive. Philosophical issues in quantum mechanics concern the interpretation of its mathematical formalism as well as its conceptual foundations, because the conceptual understanding of its formalism was still evolving at the time of its inception. Indeed, we now have a better understanding of what quantum physics is mostly from the ongoing controversy over its interpretation and foundations. However, most of the research into science education and instructional materials do not take the philosophical choices behind the subject into account, which might bias some results.

The discussion of this issue is the main focus of this paper. In the second section, we examine a pair of historical examples, in order to show how interpretational and conceptual issues have been (and are) relevant for the development of quantum mechanics and why interpretational issues cannot be avoided in its teaching. In section 3, we present and discuss the classical teaching of quantum mechanics from this perspective and review papers published in the area of undergraduate education that propose new ways of introducing it. In the final section, we present some points informed by the literature on the history of science and science teaching that can be taken into account when devising more effective ways of teaching quantum mechanics.

We shall focus on introductory physics subjects where basic quantum mechanics concepts are as a rule first introduced on all scientific undergraduate courses. We are convinced that it is necessary to modify these introductory subjects, in order to help students to understand quantum concepts better, because the technical nature of advanced courses are of little help in overcoming conceptual difficulties. In the case of chemistry, although it is known that chemistry students tend to compartmentalize their chemistry learning separately from physics and do not appreciate the laws of physics at work in chemistry, which is an impediment to effective learning (Taber, 2001), we are convinced that fundamental quantum

concepts must be dealt with in these introductory subjects or alternatively in the first chemistry/physics subjects (as discussed, for example, in de Souza & Iyengar, 2013)

II. LESSONS FROM THE CONTROVERSY OVER QUANTUM PHYSICS

While the basic mathematical formalism has remained essentially the same since the inception of quantum theory around 1925–1927, our understanding of the implications of this formalism has grown dramatically in the last fifty years in particular. This deeper knowledge has resulted from both theoretical and experimental developments enabling the testing of quantum theory in extreme situations and from a new attitude towards its foundations and interpretations.

However, from the inception of quantum mechanics until the late 1960s concerns over its foundations were mainly centered on theoretical grounds. Some of the founding fathers of the new theory, such as Erwin Schrödinger, Albert Einstein and Louis de Broglie, neither accepted some of the features of the new physical theory, nor its interpretation in terms of the principle of complementarity suggested by Niels Bohr. Since the 1950s complementarity has no longer reigned supreme because alternative interpretations have begun to appear, such as those proposed by David Bohm and Hugh Everett. Indeed, since the 1950s shortcomings of complementarity came to the fore due both to its inadequacy to deal with issues such as the quantum measurement problem and quantization of gravity and to the rising of realism as worldview among philosophers and physicists dealing with foundations of quantum physics. Following on from Bohm's and Everett's works, finding alternative interpretations has become an industry for physicists and philosophers, populating many technical journals and books. These are, however, conspicuously absent from physics teaching and from most research on physics teaching. Nevertheless, as we will briefly illustrate with a couple of related examples from the recent history of quantum mechanics, from which it is possible to extract important lessons for the teaching of quantum mechanics, the discussion of these interpretations and their experimental tests have increased our conceptual understanding in an unforeseen way. It is worth stressing that most of these alternative interpretations lead to the same experimental predictions (an exception being the spontaneous collapse theory), at least in the non relativistic domain, representing one of the best examples of the so-called Duhem-Quine thesis, at least in one of its weaker version: the underdetermination of theories by the currently available empirical data.

While these theoretical discussions delved into the foundations of quantum theory, it was the possibility of bringing some of these issues to the laboratory benches that most contributed to increasing our knowledge of the quantum world. No case is more telling of this increased knowledge than the statement that local realism is incompatible with the predictions of quantum mechanics. The problem may be traced back to 1935, when Einstein, Podolsky, and Rosen suggested a gedanken experiment to demonstrate the incompleteness of quantum mechanics, which Bohr in turn rebutted. The issue was shelved until the middle of the 1960s when John Bell realized that quantum physics predictions could be contrasted with any theory sharing the same 1935 assumptions of Einstein – physical objects should have well defined properties, regardless of whether they are under observation, and no measurement of a system could change the state of a distant one, unless, of course, there is an interaction between these two systems propagating at a speed less or equal to the speed of light. According to Aspect (1999) *“Bell's theorem changed the nature of the debate”*. The creation of Bell's theorem was only the preamble to many thrilling activities after 1969, when a string of experiments has been carried out leading to the confirmation of a weird quantum property: quantum non-locality holds even for distances as lengthy as 100 kilometers, as recent experiments by Zeilinger and his team (Scheidl et al., 2010) have confirmed.

Experiments on Bell's theorem have created a widely shared feeling among physicists that local realism should be abandoned, even though more precise tests can be done in the future, particularly by improving the efficiency of photo detectors. This perception led physicists to unearth the term entanglement, coined by Schrödinger in 1935, to name this new quantum physical property of quantum correlations between systems far away from each other. The feeling that local realism should be abandoned had a strong philosophical implication at first, as stated by Clauser and Shimony as early as 1978: *"Either one must totally abandon the realistic philosophy of most working scientists, or dramatically revise our concept of space-time."* Later different experiments were developed in this line, for example, Gröblacher et al. (2007) and Paterek et al. (2007) both examples of what Shimony has called "experimental metaphysics", that is, theoretical and experimental research on the foundations of physics with huge philosophical implications. It is worth stressing that these developments caused a stir beyond philosophy and basic science and nowadays entanglement (recent examples can be found in Hofmann et al., 2012 or van Loos et al., 2013) lies at the core of a great deal of research into quantum information, as scientists and engineers attempt to harness quantum features for more reliable cryptography and for speedier information processing. For those physicists and philosophers who are interested in a better understanding of the kind of world described by quantum theory, entanglement brought with it a new challenge: how to cope with the implicit Weltanschauung of this weird quantum property. The challenge for teachers involved in teaching basic quantum concepts is even greater. If the purpose of this teaching is not just to hone calculus skills, how does the teacher convey an understanding of this seminal quantum property, if neither an intuitive perception nor a clear image of it can be presented?

One may consistently argue that entanglement is implied in mathematical quantum formalism. However, the discovery of these new properties was only possible more than fifty years after quantum formalism was established and as a result from the ongoing controversy on interpretations of quantum physics and its basic concepts. Furthermore, an important part of this development was the work of scientists who were uncomfortable with the conceptual implications of this theory, critical of the complementarity view (Freire, 2009) and attempting to demonstrate absurd consequences of quantum formalism. A list of these authors would include some from the older generation, such as Einstein, but mainly from the new generation, such as Bohm, Everett, Bell, Clauser, and Shimony. One lesson for the teaching of quantum mechanics that this historical example brought with it is the relevance of the conceptual discussion of quantum formalism when the subject is presented to students and that this conceptual discussion should not avoid interpretational issues, as will be discussed later on.

However, quantum mechanics has survived their criticisms and their related experimental tests and as a result recent generations of physicists have learned that the object of quantum theory must be described by its own quantum mathematical formalism and that we should make no independent assumptions, however reasonable they may appear. This practical and epistemological lesson is important because this formalism, embedded as it is in a very abstract mathematical structure, means that we cannot grasp it through pictures or mental images, important cognitive resources for the understanding of physics concepts, as will be discussed. However, it appears to be one way to get around this. We may use images of phenomena, such as waves and particles, but by doing so we are obliged to make explicit reference to Bohr's complementarity principle. A case that exemplifies this is Aspect's 1986 experiment with wave particle duality for single photons. After presenting his results Aspect interpreted them in two different ways (Grangier, Roger & Aspect, 1986, 178). The first was based on complementarity, although he remained cautious about its interpretation: *"if we want to use classical concepts, or pictures, to interpret these experiments, we must use a*

particle picture for the first one, [...] on the contrary, we are compelled to use a wave picture, to interpret the second experiment. Of course, the two complementary descriptions correspond to mutually exclusive experimental set-ups."

Aspect preferred the other explanation he had suggested. It was an explanation based on a direct interpretation of the quantum mathematical formalism, without appealing to pictures, using concepts that had just emerged in quantum optics: *"from the point of view of quantum optics, we will rather emphasize that we have demonstrated a situation with some properties of a 'single-photon state'"*. While presenting the second explanation, he remarked that a logical conflict only appears if one appeals to classical concepts, such as waves and particles. *"If, on the contrary, one is restrained to the quantum mechanics formalism, the descriptions of the light impulses are the same. It is the same state vector (the same density matrix) that one must use for each experiment. The observable changes but not the description of light"* (Aspect, Grangier & Roger, 1989, 128). Thus the quantum formalism is self-sufficient, it describes both experiments without appealing to pictures or classical concepts.

If the history of research in the foundations of quantum mechanics appears to favor the interpretational trend, as suggested by Paty (1999), which assumes only quantum formalism to grasp quantum phenomena, then the same history also suggests a different lesson. Indeed, it seems to us that the need for pictures/images, thus of classical concepts, persists even among the best working physicists; a point that is perhaps more evident in chemistry – as nicely described by Gavroglu & Simões (2012) in a recent history of quantum chemistry. Its development at the epistemic level can be seen as the history of using conceptual, mathematical, experimental and visualizability procedures in a complementary way, the latter being intrinsic to the thinking of chemists. Here the case of John Clauser, who conducted the first experimental tests on Bell's theorem, is enlightening. He reminisced that he always disliked abstract reasoning *"I am not really a very good abstract mathematician or abstract thinker. Yes, I can conceptualize a Hilbert's Space, etc. I can work with it, I can sort of know what it is. But I can't really get intimate with it. I am really very much of a concrete thinker, and I really kind of need a model, or some way of visualizing something in physics"*. Clauser's recollections may be useful for researchers, facing the challenge of teaching introductory quantum physics. He goes on to say: *"There exists a set of numbers with algebraic structure of such and such, and we will define a particle as being something for which this operator commutes with that operator, etc. I haven't the foggiest idea what any of that means. But an electron is a charge density which may be Gaussian in shape and its shape, and it's about this big, and it's held together by various forces, and this is how the forces work that kind of hold it together. The difference between those two [concepts] are very dramatic differences of thinking. Now there's a whole class of physicists who can only think in the former method. I can only think in the latter mode."* We should add that insofar as Clauser also disliked Bohr's complementarity, he expressed persistent discomfort with the habitual presentations of quantum physics; a discomfort that is relevant in our discussion of the teaching of quantum physics.

Therefore, the question of visualization has an interpretational base: it seems that is not possible to use images if we do not adopt a complementary vision. If we do not explicitly adopt this interpretation when using images, we will think in terms of classic physics and we will not be able to understand quantum concepts properly. At the very beginning of the development of quantum chemistry, Pauling and Wilson (1935, p. iii) stressed, *'quantum mechanics is essentially mathematical in character, and an understanding of the subject, without a thorough knowledge of the mathematical methods involved and the results of their application, cannot be obtained'*. Despite the mathematical complexity of quantum mechanics, the tendency to use more phenomenological approaches very close to images has

led many practicing chemistry researchers to give a quasi-quantum character to the quantum chemistry tools they employ (Sánchez Gómez & Martín, 2003). Also, some conceptual difficulties detected in chemistry students, for example their non-discrimination between orbits and orbitals, could be associated with a similar tendency, because of the visual simplicity of Bohr's atomic model (Tsapalis & Papaphotis, 2009). Nevertheless, the complementary principle seems not to play a central role in quantum chemistry. The book by Gavroglu & Simões (2012) extensively discusses how visualization has permeated the development of quantum chemistry, yet there is not a single entry about the complementary principle.

Summing up, quantum physics has passed the most severe experimental tests ever imagined for a physical theory. However, this does not mean that corroboration of the predictions of quantum physics, that is, predictions of quantum mathematical formalism, have implied corroboration of only one interpretation of this formalism. Therefore, perhaps the most important lesson from the history of physics, as regards the attempts to introduce quantum physics at more elementary levels, is that we should take into account the peculiar situation of the existence of a tension between a strong consensus over the formalism of this physical theory and meaningful dissension over its interpretation. Of course, students need first to learn the inherent formalism of quantum physics, in order to grasp such a controversy. However, at a certain moment in time we should convey the existence of the controversy to them, in order to enable them to grasp some understanding of the weird properties of the quantum world.

III. QUANTUM THEORY AND ITS TEACHING

A. The classical teaching of quantum physics

As we have indicated, teaching quantum physics is no easy task, because it is both technically and philosophically sensitive. It is interesting to note that its teaching is quite different from that of other topics in physics. It is perhaps the only topic that is most commonly introduced through the history of its origins in the late nineteenth century up until at least the first half of the twentieth century. This introduction is a typical example of what Kragh (1992) called quasi-history, a mystical history made to convince students of a particular point of view, the only "rationale" possible reached by physicists in the past. It is worth stressing that this historical approach has been criticized (Cuppari, Rinaudo, Robutti, & Violino, 1997; Fischler & Lichtfeldt, 1992; Michelini, Ragazzon, Santi, & Stefanel, 2000) for reinforcing classical concepts in students' minds, at a time when they should be moving on to more appropriate quantum models. Specifically, in the case of chemistry, the usual approach of introducing quantum theory through the models of the first two decades of the twentieth century (when the scientists themselves were still trying to move beyond their classical notions) acts as a learning impediment (Taber, 2001), because students rely on deterministic models of the atom derived from old quantum theory for understanding modern quantum concepts (Tsapalis & Papaphotis, 2009).

Advanced courses, while dispensing with this historical tour, repeat very similar material many times (Cataloglou & Robinett, 2002). The typical approach in advanced courses can be described as consisting of highly abstract rules and procedures (Shankar, 1994), in part because the mathematical tools necessary for applying it, even in the simplest cases, are so different from the ones usually used, that there is a tendency to present quantum concepts as inseparable from their mathematics (Bohm, 1951). Nevertheless, unlike other areas in physics, there is a wider variety of approaches to the teaching of quantum theory, even at undergraduate level. This is due to the lack of consensus among physicists about which are the most fundamental ideas in quantum physics and so there is a wider array of possible topics which one might consider as constituting the core ideas.

Although only in recent years it has also been possible to find textbooks designed to introduce updated views on undergraduate courses, including many physical examples, and making direct connections to experimental results (an example of this type of textbooks for chemistry students is Blinder, 2004, that in its final chapter discusses different interpretations of quantum mechanics), most of the traditional textbooks provide few, if any, physical insights. General chemistry textbooks appear to present a similar pattern, presenting quantum mechanics as a set of rules to allocate quantum numbers, which are later used to write electron configurations. This presentation is based on rules/algorithms (Niaz & Fernández, 2008) with very little discussion of what quantum mechanics can predict or explain that makes it a better explanation than the one offered by the Bohr model (Shiland, 1997). Niaz & Fernández (2008) also found that only two out of 55 of the textbooks they analyzed included alternative interpretations of quantum mechanics.

In fact, textbooks seem to prioritize what one could call an instrumentalist view of quantum mechanics, or what Redhead (1987) called the “minimal instrumentalist interpretation”; i.e. quantization algorithm, statistical algorithm plus the epistemological premise that “theories in physics are just devices for expressing regularities among observations”. This kind of approach reduces the cognitive reach of quantum physics and does not make it any easier to understand.

This “minimal instrumentalist interpretation” is so widespread among physics teachers that several authors consider that most of the difficulties students have with quantum mechanics are related to its characteristic formalistic teaching, which begins in the introductory disciplines (Jonston et al., 1998; Fischler & Lichtfeldt, 1992; Greca & Freire Jr., 2003; McKagan et al. 2008). What are the factors that may have led to this? As previously mentioned, one appears to be the intrinsic mathematical difficulty of quantum mechanics, but there are others. Initially, most physicists used the machinery of quantum mechanics to study the microscopic world, without worrying about conceptual or interpretational questions (Heilbron, 2001). This predominance of quantum theory as a “calculating machine” may have been reinforced particularly in the USA, because of the coexistence in the same departments of theoretical and experimental physicists, emphasizing experiments and applications, and the American inclination towards pragmatism (Schweber, 1986). Kaiser (2007) also indicated another factor, related to pedagogical choices during the Cold War era, when the great enrollment of students on scientific courses required *“accentuating those elements that allowed students to be taught as quickly as possible, while quietly dropping the last vestiges of qualitative, interpretive musings that had occupied so much classroom time before the war. [...] The goal of physics became to train “quantum mechanics”: students were to be less like otherworldly philosophers and more like engineers or mechanics of the atomic domain.”* (Kaiser, 2007). This change has been reflected in the textbooks published since then, with wonderful methods for doing almost any calculus about atoms. However, when it comes to the principles and interpretations of quantum mechanics, they *“are, almost without exception, simplistic and obscure at the same time”* (Barton, 1997). These approaches ultimately worked, because, one lesson from recent history, as we have seen, is that quantum concepts are strictly associated with the quantum mathematical formalism.

Students are more than occasionally encouraged to approach the subject with the idea that it is almost impossible to understand it and that it is so completely different from our classical experience that one’s intuition is of little or no use. As an advanced student said, referring to his experience in quantum physics: “It seems that there’s this dogma among physicists, that you can’t ask that question: What is it doing between point A and point B? ‘You

can't ask that!" (Baily & Finkelstein, 2010, p. 9). It is hardly surprising therefore that students dislike quantum mechanics and non-physics students try to avoid it.

Despite the strength of the traditional methods of teaching quantum physics, it has been challenged over the last two decades. The motivation for studies of its teaching derives from the need to convey quantum concepts not only to physics students, but also to other science and engineering students. These studies attempt to understand how to attract students to study quantum physics rather than make them run away from it. This kind of research has addressed students' difficulties with quantum concepts, using surveys and didactic strategies to introduce quantum physics more effectively in introductory courses at universities – for physics, chemistry and engineering students – and at high school level (for example, McDermott & Redish, 1999; Taber, 2002; Greca & Freire Jr., 2003; Hadzidaki, 2008a & b; Tsaparlis & Papaphotis, 2009; Wutti-prom et al., 2009; Kohnle et al., 2014).

B. New didactics for introductory quantum theory

What do the new proposals for teaching quantum physics which have emerged from research into science education suggest to improve students' understanding of quantum concepts? We have reviewed the literature published in science education from 2000 to 2013 and found 43 articles that tackle new ways to introduce quantum theory topics at various levels. Although only 15 of them discuss the outcome of the implementation in detail, they were in general very well received by the students and with varied conceptual improvements. Many of the papers, amounting to 13, are related to the use of history and philosophy of science, using proper historical reconstruction (Tsaparlis, 2001; Barnes et al., 2004; Niaz, et al., 2010), conceptual discussion of thought experiments (Velentzas et al., 2007; Velentzas & Halkia, 2011), discussion of philosophical, epistemological and/or ontological issues concerning quantum physics, in some cases through historical controversial issues (Pospiech, 2003; Karakostas & Hadzidaki, 2005; Hadzidaki, 2008a & b; Niaz & Fernández, 2008; Garritz, 2013; Levrini & Fantini, 2013), or using quantum mechanics as a tool for improving the views pre-service teachers hold about the nature of science (Kalkanis et al., 2003; Nason et al., 2008). Most research using the historical approach has involved high school students and pre-service teachers. In general, these works try to contextualize quantum physics in an updated historical and epistemological framework – as opposed to the “traditional” historical approach – and in this way help learners to reorganize and enhance their initial knowledge. Kalkanis et al. (2003, p. 270) propose, for example, the juxtaposition of representative models of conceptual systems of quantum and classical physics. Thus, instead of avoiding making reference to classical physics, their strategy reveals the totally different worldview and thinking patterns underlying the interpretation of macroscopic and microscopic phenomena. They used Bohr's atomic model, for example, in order to make the deep conceptual differences between classical and quantum physics concrete. Instead of avoiding dualistic descriptions, they aimed to reveal the inner meaning of the complementarity principle. In particular for chemistry students, Garritz (2013) proposed the use of reconstructed historical episodes, especially those that involve controversies and rivalry between scientists, which are quite important for quantum mechanics and quantum chemistry progress, in order to help students to understand the evolution of quantum concepts and also the complexity that surrounds the development of ideas in science. We can include articles in this category that stress the introduction of quantum physics through unusual interpretations, such as the Bohmian one, as a useful tool to illustrate the relationship between classical and quantum physics (Passon, 2008) or a suspensive perspective on the interpretation of quantum mechanics for the wave-particle duality (Cheong & Song, 2013).

The second most proposed strategy, with 10 papers, is the use of simulations, computer animations or games to improve the intuitive understanding of abstract quantum concepts, especially for students with a limited science and mathematics background or for advanced students with knowledge of traditional or purely mathematical quantum concepts (for example, Zollman et al., 2002; Goff, 2006; McKagan et al., 2008; Singh, 2008; Magalhães & Vasconcelos, 2006; Kohnle et al., 2014). For example, Kohnle et al. (2014) have created a collection of freely available interactive animations and visualizations for teaching quantum mechanics, at all levels of the undergraduate curriculum, each of which includes a step-by-step exploration that explains the key points and specifically targets student misconceptions and areas of difficulty in quantum mechanics. In general, the simulations presented in this group of papers, some of which integrate hands-on activities, attempt to build intuition for the abstract principles of quantum mechanics through visualization in introductory physics, with precursors in the quantum physics series of the Lawrence Berkeley Lab (Gottfried, 1978) and the programs Eisberg (1976) designed for visualizing wave functions with the early programmable calculators. This “wavy” tendency can be seen in the names of some of the typical simulations; quantum tunneling and wave packets, quantum wave interference, matter waves, probabilities and wave functions, wave functions and energies in atoms. However, wave interpretations without reference to complementarity have not endured in the history of the research on the foundations of quantum physics, and none of these papers mentioned the complementary principle. Finally, it is worth stressing that several of the proposals not included in this group also make use of certain computer simulations.

In third place, with eight papers, there are different “technical” approaches (deformation quantization, evolution operator method, field theory, computer algebra systems), most of which for advanced courses in physics (for example, Hirshfeld & Henselder, 2002; García Quijás & Arévalo Aguilar, 2007) that we will leave untouched here, as we are dealing with introductory quantum physics courses.

Finally, in fourth place, there are seven papers with proposals that share an emphasis on conceptual discussions of quantum features of the systems, using in general real-world applications or recent experimental advances (for example, Holbrow et al., 2002; Carr & McKagan, 2009; Deslauriers & Wieman, 2011; de Souza & Iyengar, 2013). As an example of these proposals for chemistry students, we would suggest the work of de Souza & Iyengar (2013, p. 717), who describe a first-year undergraduate course that introduces quantum mechanics for chemistry students through a conceptually detailed approach. The first idea tackled in the course is quantization as arising from the confinement of a particle, the use of which introduces the reasons behind resonance, molecular orbital theory, degeneracy of electronic states, quantum mechanical tunneling, and band structure in solids and quantum dots. Other papers of this group (for example, Müller & Wiesner, 2002; Greca & Freire Jr., 2003) explicitly state the need to stop searching for classical or semi-classical analogies in introductory quantum courses. From the experimental results on the foundations of QM obtained over the last twenty years, they tend in general to use very simple systems that show clear quantum behavior, leaving aside non-physics fictions such as the Heisenberg microscope. These works are in consonance with researchers linked to the area of quantum optics (for example, Schenzle, 1996; Barton, 1997; Zeilinger, 1999; Jacques et al, 2005), who have stressed the relevance of introducing quantum concepts from the very beginning.

Hence, science education researchers, although unanimous in rejecting the traditional “quasi-historical” introduction or the formal one, have hitherto given quite different answers to our questions about how to introduce quantum concepts. It is worth mentioning that we do not have any strong evidence for advocating one way or another, because few of the proposals have been tested. Thus some of our arguments from now on derive from the recent history of

the research on the foundations of quantum mechanics as well as from empirical evidence in science education research.

C. Quantum theory interpretations and research in science education

It is striking that although all the papers emphasize the need to improve the conceptual understanding of quantum concepts, few of them clearly state the interpretation of quantum mechanics that is adopted. It appears that the intense debate about the different interpretations, which is a conceptual debate, has yet to inform our research into the most effective ways of teaching quantum mechanics.

From the 43 papers identified over the 14-year period from 2000–2013, only 15 explicitly mention the existence of different possible interpretations and use them in some way in their teaching proposals. We have Bohr's realist interpretation (Karakostas & Hadzidaki, 2005; Hadzidaki, 2008a; 2008b; Levrini & Fantini, 2013); the statistical ensemble interpretation (Muller & Weisner, 2002); the Copenhagen interpretation (Kalkanis et al., 2003; Barnes et al., 2004; Tsapalis & Papaphotis, 2009); an orthodox but realist interpretation (Greca & Freire, 2003); the Bohmian dualistic interpretation (Passon, 2004; Niaz & Fernández, 2008); the interpretation of the quantum states as potentialities (Pospiech, 2003); and the stochastic interpretations (Garritz, 2013).

It is interesting to note that all but two of them can be included in the spectrum of realistic interpretation; moving away from the epistemological position of the Copenhagen interpretation and giving an objective character to the concept of the state of a quantum system and therefore less dependent on the measurement process. It seems that realistic interpretations are seen by science education researchers as the best interpretational option for introducing quantum mechanics to students. For example, we have argued (Greca & Freire, 2003) that our aim to help students to develop mental models whose results – predictions and explanations – coincide with those accepted by the physics community has led us to seek a realist interpretation of quantum physics.

An insensitivity towards the philosophical choices seen in the papers we have analyzed may have biased some of the research results. For example, McKagan et al. (2010) reported that in the construction a conceptual survey of quantum mechanics, they were unable to find any version of a question trying to address the wave-particle duality in which the faculty agreed upon a "correct" answer. It is also evident that the didactic strategies will be different depending on the interpretational choices, and that the uncritical adoption of one of them – which occurs when it is not clearly stated – may have undesirable consequences. For example, the proposals that attempt to represent some quantum concepts in a "more displayable" way using simulations tend implicitly towards a wavy interpretation that, by its nature, may reinforce links with classical physics. Such proposals may reinforce the classic ideas that students may already have formed, preventing them from gaining a better understanding of quantum concepts. This happens, for example, in the difficulties students have with replacing the idea of an electromagnetic wave with a probability wave (Greca & Freire, 2003): many students consider the probability density representation to be a movement representation. Similar results were found among chemistry students introduced to the wavy model of the atom, who understood the concept of orbital as a "space" and not as a mathematical function (Tsapalis & Papaphotis, 2009).

Related to the example of the need for images to think about quantum physics, a need that is shared by many researchers, Clauser (2002, p. 6) while recognizing the use of images for interpreting physics concepts is aware of the pitfalls that images associated with the wavy model may have:

“In quantum mechanics, the books all make this seem like simple wave mechanics, i.e. what you would see – a direct analogy with waves on the surface of a pond. And they show pictures. [...] And then even worse, they say, “Okay. A particle, we can represent kind of as a wave packet,” whatever that means. [...] propagating in real space. [...] Which means this whole idea of wave packets that all of the books put in there is to try and make you feel comfortable with it, all of those chapters, you might as well rip up and throw them away because they are wrong because that’s not the correct conceptual model.”

We are not saying that the use of images or materials that may make quantum concepts more visible do not have a place in teaching. In fact, by applying cognitive psychology to research in science education, it is possible to find evidence that many college students use imagistic mental models to make sense of physics concepts (Greca & Moreira, 1997, 2002); that is, they need to “visualize” what is happening in order to understand. Furthermore, the need for visualization may be a way of working in a subject, such as in chemistry (Gavroglu & Simões, 2012). As emerges from the history of science and as indicated in Aspect’s explanation, the use of images appears to require references to ideas of complementarity, to guide students away from “classical” images, which eventually prevent them from understanding the core quantum concepts that may not in principle be displayed. As the results from the research of Greca & Freire (2003) and Tsapalis & Papaphotis (2009) appear to show, the images that students form are very difficult to modify, even when the teaching strategy is specially designed. Therefore, we consider that a thoughtful introduction of the complementary principle will help students overcome this obstacle, when illustrating the world of quantum physics with images. By a thoughtful introduction we mean not reduce complementarity to the pair wave-particle features. In Bohr’s own terms, wave-particle duality is just the particular case of a wider view:

Information regarding the behaviour of an atomic object obtained under definite experimental conditions may [...] be adequately characterized as complementary to any information about the same object obtained by some other experimental arrangement excluding the fulfillment of the first conditions. Although such kinds of information cannot be combined into a single picture by means of ordinary concepts, they represent indeed equally essential aspects of any knowledge of the object in question which can be obtained in this domain (Bohr, 1987, p. 26).

However, there is an obstacle: complementarity has virtually disappeared from teaching and research in science teaching. For example, only 13 of the papers we sampled cited the existence of the complementarity view, two of them without considering its potential usefulness (Greca & Freire, 2003 ; Passon, 2004). This strange finding, however, comes as no surprise to those who know the history of quantum mechanics teaching. At the end of 1927 the complementarity view was clearly held by the most influential of the founding fathers of quantum mechanics. The period from the creation of quantum theory until the 1950s was called the time of the unchallenged monocracy of the Copenhagen school (Jammer, 1974). However, adhesion to this monocracy was weaker than this term may suggest. Its diffusion outside Germany and Denmark was not without its difficulties (Schweber, 1986; Heilbron, 2001). As a matter of fact, the complementarity view was absent from the one of the most powerful tools in the training of physicists: textbooks. Kragh (1999, p. 211) remarked that only 8 out of the 43 quantum physics textbooks published between 1928 and 1937 mentioned the complementarity principle, while 40 cited the uncertainty principle. Despite how central complementarity was to Bohr’s interpretation of quantum physics, “most textbook authors, even if sympathetic to Bohr’s ideas, found it difficult to include and justify a section on complementarity”. Kragh noted that Dirac, the author of one of the most influential textbooks

ever written (Dirac, 1930), while closely connected to the supporters of the Copenhagen interpretation and having great respect for Bohr, “did not see any point in all the talk about complementarity. It did not result in new equations and could not be used for the calculations that Dirac tended to identify with physics” (Kragh, 1999, p. 211). Indeed, even in most current textbooks, when some reference to complementarity is made, it is restricted to the mutual exclusion of wave and particle representations. Also, as noticed above, complementarity appears to have played no role in the development of quantum chemistry, nor is it mentioned in any of the papers on quantum mechanics for chemistry students.

IV. CONCLUSIONS: LESSONS FROM HISTORY AND PHILOSOPHY FOR THE TEACHING OF QUANTUM MECHANICS

In the same way as there is no privileged interpretation for quantum mechanics, there is no ideal way for its introductory teaching at undergraduate level. There is however, a spectrum of options available. In our analysis, we prioritize the following at times complementary possibilities, which in our opinion are grounded in the history and philosophy of science and teaching experience:

- The inclusion of philosophical interpretations and their defense: the first thing that follows from our argumentation is that conceptual and interpretational issues are indissoluble in quantum mechanics and any research into quantum mechanics in science education must declare its interpretational choice, which has to be justified and defended. Not to do so may not only reduce the scope of the research results, but also the possibilities of the teaching strategies, as the introduction of elements not explicitly explained to students may confuse them. An excellent example of this is the research on quantum numbers in general chemistry textbooks by Niaz & Fernández (2008). There are many books and articles with differing interpretations for discussion in the chemistry university classroom, such as the last chapter of Blinder (2004) and Bell (1992).
- The emphasis on strictly quantum features of the systems under study: the discussion of quantum features appears to be important for all students that embark on the study of quantum mechanics, in order to prevent them from establishing undesirable links with classical concepts. The by now conventional images that chemistry students receive when exposed to the Bohr model of an atom may only be surmounted with great difficulty. Hence, the initial strategy appears to be the use of very simple, dual-level systems, which show clear quantum behavior and from which it is possible to discuss the most important quantum properties. Teaching along these lines should stress quantum features such as the superposition principle and the measurement problem, as well as such effects as quantum entanglement, quantum beatings, and decoherence, etc., in addition to the description of the current research in these topics which may be grasped at a qualitative level. In the case of chemistry courses, these initial subjects should emphasize the probabilistic aspect of quantum mechanics, in particular in order to prevent students from attributing physical reality to core chemistry concepts, such as orbitals, rather than mathematical constructs, as appears to happen (Tsaparlis & Papaphotis, 2009; Niaz & Fernández, 2008). Moreover, we should explicitly state the fruitful results of quantum mechanics in the solution of chemistry problems, in opposition to the Bohr model.
- The introduction of historical cases following old quantum physics should be avoided: as a direct consequence from last point, the inclusion of historical elements that incorporate cases from old quantum physics (black-body problem, photoelectric effect, atomic model) should be avoided, as has been shown in our analysis. This is partly because the most important steps in the early construction of quantum theory do not show the specific

quantum features in a clear cut manner and some of which are very complex for students on introductory courses to understand. In contrast, new experiments are conceptually more accessible and can also be reproduced in undergraduate laboratories (see, for example, Dehlinger & Mitchell, 2002; Thorn et al., 2004; Galvez et al., 2005). It is worth stressing that a similar strategy is often employed in the teaching of classical mechanics: astronomical calculus that led to the classic (and unintuitive) form of seeing the world is not present in the introductory teaching of classic mechanics. We begin with very simple examples and models, in order to help students understand the basic concepts.

- An emphasis on formalism, without worrying about the ultimate ontological status of mathematics: the teaching of quantum mechanics may emphasize formalism, without worrying about the ultimate ontological status of mathematical terms. Of course, introductory courses have to be pitched at an acceptable mathematical level. This may be illustrated by the case of two-level systems, which strike a balance between rigor and assistance and can be treated with matrices and vectors (see, for example, the recent proposal of Kohnle et al. 2014). As we have seen, quantum formalism is self-sufficient and there is a new generation of scientists, working in advanced quantum research areas, who appear to have no need for the classical counterpart to manipulate quantum mechanics with proficiency (Zeilinger, 1999; Aspect, 2007). We think that although for chemistry students, it is necessary to use more complicated mathematics in order to solve quantum chemistry problems, their first approach with quantum concepts should be with simpler two-level systems.
- The incorporation of quantum mechanics applications to real problems: the inclusion of applications of quantum mechanics to real (although simplified) problems is not only important for the understanding of quantum mechanics, but will also motivate students to continue their studies in this subject. Attention paid only to mathematical complexities makes both teachers and students “lose the physics (the actual world, the forest)” (Tsaparis & Papaphotis, 2002). In the literature review, a potentially useful example for chemistry teachers is provided by de Souza & Iyengar (2013). Their work begins with the confinement of a particle as a basis for the discussion of real problems in physics and chemistry, focusing on the physical rather than the mathematical situation. It is worth stressing that this way of introducing quantum mechanics, as we have seen, may be compatible with either realism or instrumentalism in terms of epistemological views. The contradictions between instrumentalism and realism has accompanied the history of science – perhaps the best known example is Galileo’s struggle to describe the solar system – and the teaching of quantum mechanics is not the place for settling such a philosophical issue. However, students on introductory courses should be introduced to the pervasive dilemma and quantum physics courses may be a space in which to prioritize them.
- The use of images to assist with conceptual understanding: a further option of interest could be the use of images (in the form of simulations or other), in order to make quantum concepts more understandable. As we have seen, both from the reports of top-ranking physicists and from the research in science education informed by cognitive psychology, many students may need concrete models or some way of visualizing the abstract mathematical structure to grasp quantum concepts. Students who are perhaps more numerous outside physics courses (for example, engineering, chemistry and biology students) may profit from this approach. However, if this approach is used, we are convinced of the need to introduce complementarity in a serious and explicit way in our explanations of the right quantum use of these images. Finally, it is possible to combine the formal approach with the introduction of the complementarity view, as we have seen in Aspect’s explanation of his experiment on the dual nature of single photons.

- The controversy over its foundations and interpretations can serve as the basis for the teaching of historical and philosophical aspects of science. Finally, we would like to stress that the teaching of quantum mechanics, perhaps more than any other subject in physics, must be informed by the history and philosophy of science. The controversy over its foundations and interpretations has been one of the longest-running controversies in the history of science, being a lively example of science as a human and social product and students should not be deprived of the presentation of histories that humanize science. In the case of chemistry, students should be aware of the historical evolution of the concept of chemical bonding, from which the lively discussion concerning the reduction of chemistry into physics, a fundamental debate for understanding the specificity of chemistry as a scientific discipline, that took place after the success of quantum mechanics in explaining the bonding in the hydrogen molecule, as illustrated by Garritz (2013). For this, can be used Gavroglu & Simões (2012) history of quantum chemistry and Scerri (2007) history of the periodic table. Of course, the generalization of teaching strategies using philosophy and history of science is not a simple task, due in part to a lack of knowledge among university teachers of these issues and also, because they considered that these topics are really quite complicated for students, as the research by Padilla and Van Driel (2011) has shown for quantum chemistry professors.

Of course, all these possibilities directly imply that the teaching of, as least, introductory quantum mechanics for any science undergraduate student and in particular for chemistry students, should be mainly conceptual, if we do not wish them to run away from areas that use quantum mechanics concepts, as may appear to happen today. Moreover, conceptual teaching in quantum mechanics not only appears to improve understanding and motivation related to quantum concepts, but also the extent of its retention, as recently shown by Deslauriers & Wieman (2011).

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