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High-School Students' Conceptual Difficulties and Attempts at Conceptual Change: The Case of Basic Quantum Chemical Concepts

This study tested for deep understanding and critical thinking about basic quantum chemical concepts taught at twelfth grade (age 17-18). Our aim was to achieve conceptual change in students. A quantitative study was conducted first (n = 125), and following this 23 selected students took part in semi-structured interviews either individually or in small groups that were allowed to interact under the coordination of the investigators. The planetary Bohr model was strongly favored, while the probabilistic nature of the orbital concept was absent from many students' minds. Other students held a hybrid model. In some cases, students did not accept that the electron cloud provides a picture of the atom. Many students had not understood the fundamental nature of the uncertainty principle. Finally, the mathematical description of the formation of molecular orbitals caused problems in the case of destructive (antibonding) overlap of atomic orbitals. Our approach to conceptual change employed active and co-operative forms of learning, that are consistent with social-cultural constructivism, and to Vygotsky's zone of proximal development. It proved effective in a number of cases, and ineffective in others. The variation in students' approaches was explained on the basis of Ausubel's theory about meaningful and rote learning and of the ability to employ higher-order cognitive skills. Nevertheless, the methodology used can be useful for all students, irrespective of their behavior in traditional written exams.

High-School Students' Conceptual Difficulties and Attempts at Conceptual Change: The Case of Basic Quantum Chemical Concepts

Introduction

Atomic orbitals (AOs), molecular orbitals (MOs) and related concepts derive from quantum mechanical theories of atomic and molecular structure. Because of their conceptual difficulty, these concepts are not taught in introductory school chemistry, but they now form a part of most senior high school curricula at advanced and are also taught at the undergraduate level.

To aid the explanation and understanding of phenomena, science uses a wide variety of *models* and *theories*. Such models play an important role in science education (Gilbert & Boulter, 1998 a, b; Justi & Gilbert, 2003) and can be broadly distinguished into either (i) material or physical or concrete, or (ii) abstract or conceptual or symbolic (Gilbert, Boulter, & Elmer, 2000). Symbolic models include mathematical formulas and equations. We may refer to theories using the term *theoretical models*.

A number of researchers have addressed students' difficulties and misconceptions with current sophisticated models of the atom and the molecule. For a comprehensive review see Taber (2001). Harrison and Treagust (2000) reported that senior high school students *often* confused electron shells and electron clouds. Taber (2002a, 2002b) found that British advanced secondary (A-level) students treated the terms orbital, shell, and orbit, interchangeably, and confused the mathematical modelling (LCAO) of MO formation by referring to 'linear orbitals'. Taber (2005) also proposed a 'typology of learning impediments' that can be used for diagnosing the origins of students' relevant difficulties. Mechanistic thinking ("electrons move around the nucleus in definite orbits", "the electron is always a particle", "electrons move along wavy orbits around the nucleus") was found among first and second year undergraduate physics students in England prior to starting a quantum mechanics course (Ireson, 2001). Senior high school students in Norway were also reported to hold a classical-physics view with respect to wave-particle duality (Olsen, 2001). In the case of hybridization, Zoller (1990) and Nakiboglu (2003) have attributed student difficulties to a poor understanding of the concept of AO and of s, p, d, and f orbitals.

It is noteworthy that even chemistry students who had passed the quantum chemistry course (at the physical-chemistry level) demonstrated many failures in understanding the orbital shapes, the exact definitions for an AO and a MO, Slater determinants and the approximate nature of AOs for many-electron atoms, while a MO was identified only with a linear combination of AOs (Tsaparlis, 1997). Coll and Treagust (2001, 2002) examined advanced (upper secondary, undergraduate, and graduate) students' mental models of chemical bonding, and found that all these learners preferred simple, concrete models, and referred to more abstract models only in the context of tests or examinations. Finally, Kalkanis, Hadzidaki, & Stavrou (2003) suggested that these misconceptions in general arise because of inability of many students to separate the conceptual frameworks of classical and quantum physics, producing epistemological obstacles to the acquisition of the required knowledge.

The Context and Rationale of the Present Study

In Greece, quantum-chemical concepts were only recently introduced (1999-2000) into the upper secondary school (*lykeion*) curriculum, at twelfth grade (final school year, age 17-18). The relevant chemistry course is now compulsory for all students taking the 'positive stream' of studies leading to science, engineering, medicine, and agro-science tertiary education departments. All students study from the same book published by the Greek Ministry of Education, and teachers are required to adhere very closely to the content of the book. In the final national examination, the Ministry of Education sets a common paper. Because achievement in this examination is crucial to a student's chances of obtaining a university place, all students study the course conscientiously during the whole of the twelfth grade. Also, the questions that are included in the examination are of a similar nature each year. The essence of teaching lies of course in the teacher leading the instruction, so we cannot exclude the possibility that some of the teachers may supplement their teaching with additional information. However the contents of the book clearly dominate the teaching programme and it therefore follows that the all students will have a similar background in terms of the taught content.

In a previous quantitative study (Tsaparlis & Papaphotis, 2002), we exposed students to a number of questions that differed from the standard simple recall or application/algorithmic questions set in the examinations, which have been practiced by the students. The questions were intended to test for deep understanding and critical thinking. The findings indicated that many students thought in terms of old quantum theory, assuming that the term ‘orbital’ is another word for an ‘orbit', and that the electrons rotate around the nucleus like the planets around the sun. In addition, a number of them considered that orbitals are unique and represent a well-bound fixed space. Many students failed to realize the probabilistic nature of AOs, subscribing to a deterministic perspective. In addition, students had the misconception that the hydrogenlike orbitals are as exact for many-electron atoms as they are for the one electron case.

In this study, we extend on our previous work by attempting to promote conceptual change in students' thinking. This has been conducted through a qualitative study in which we interviewed selected students individually or in small groups that were allowed to interact under the coordination of the investigators.

Despite the fact that the Bohr atomic model had been abandoned for more than eighty years ago, it still holds a dominant place in chemical education. Considering just the Greek school books, from which the students of our study had been taught, we note that they were taught that “electrons are constantly moving around the atomic nucleus in a strict arrangement on orbits” (Alexopoulos et al., 1996, p. 9) from primary school (in sixth grade), Then in their first chemistry course at lower secondary school (eighth grade) they were informed that:

> “Electrons are moving constantly around the nucleus, in various specific orbits. We say that electrons that have the same (or about the same) orbital radius belong to the same electronic shell.” (Frassaris & Drouka-Liapati, 1989, p. 36)

Ninth-grade physics went along similar lines, but was more elaborate:

> “Electrons carry out two movements at the same time: one around the nucleus (orbiting), and one around their own axis (spinning), in the same manner that earth moves around the sun and its own axis. The orbits of the electrons around the nucleus are elliptic, but for simplicity we consider them as circular. The radii of these orbits are not random, but take certain values that are characteristic for each kind of atom.” (Zenakos, Lekatis, & Schoinas, 1996, p. 91)

Moving on to upper secondary school, in tenth grade, our students studied Bohr’s model of the atom in detail. Although a passing reference was made to the concept of orbitals (Mavropoulos et al., 1990, p. 31), this was unlikely to have much effect on students thinking. Only after nine years of schooling based on Bohr’s ideas had resulted in stable mental models and strong associations in their long-term memory, were students in twelfth grade introduced to the quantum-mechanical model. Note that use of the Bohr model still continued to be widely used. In addition, this model continued to dominate the general-education physics course, for mathematical equations and problems, involving calculation of orbital radii.

Science education research has established that students' scientific concepts are often at odds with accepted scientific views. Such concepts are termed *alternative frameworks* or *alternative conceptions* or *students' misconceptions* (Driver, 1983; Taber, 2002c). The theory of *constructivism* was developed to account for the formation of misconceptions. According to this, knowledge is constructed in the mind of the learner and can never be transferred intact from the mind of the teacher to the mind of the student.

It should be stressed at this point, that the models and concepts of the old quantum theory do not strictly fit into the alternative-conceptions paradigm. They are not misconceptions but rather represent earlier models, which in many ways are still operational and useful today even in actual scientific practice. They constitute deep theoretical constructs to which students have been exposed over a long period of time. Vosniadou et al. (2001) maintain that such constructs (*entrenched presuppositions*) constrain the interpretation of scientific information and are difficult to change. We assume that the Bohr model of the atom and other old quantum-theory concepts constitute such entrenched presuppositions in students. Old quantum theory is the prior knowledge that ideally should serve as a springboard for the learning of new knowledge. On the basis of this knowledge, and depending on various factors, incoming information (the modern quantum models) may be interpreted as right, or wrong, or even a hybrid. In this way, old models very often constitute a learning impediment for the desired deterministic to probabilistic transitions, and, as such, they are operationally equivalent to genuine alternative conceptions.

According to the constructivist paradigm, knowledge "results from a more or less continual process in which it is both built and continually tested. Our knowledge must be viable; it must work … (and) function satisfactorily in the context in which it arises" (Bodner, Klobuchar, & Geelan, 2001). Learning is a matter of actively constructing and reconstructing knowledge in the light of new experiences, and thus involves revising existing knowledge structures (Savinainen, Scott, & Viiri, 2004; Vosniadou et al., 2001). Kelly's theory of *personal constructs* (Kelly, 1955) has two main hypotheses: firstly individuals differ from each other in their construction of events, and secondly that one individual's constructs are similar to another's. The latter hypothesis gives importance to social interaction, combining personal and social constructivism.

Constructivist methods of teaching require that teachers, firstly, recognize their students' alternative conceptions, and, secondly, take them into account in planning and delivering their teaching, so that the aim of *conceptual change* is fulfilled. Successful teaching of the quantum mechanical model needs therefore to incorporate a strategy for conceptual change. Conceptual change consists in the 'replacement' or 'substitution' of misconceptions with the corresponding scientific concepts. Replacement and re-organization of any conceptual framework will only occur when a student encounters cognitive contradictions and conflicts with the exhibiting models (Chi, 1991; Posner et al., 1982).

Conceptual change cannot be achieved by traditional didactic methodology, but only through active, constructivist approaches. In particular, *concept addition* and *concept modification* toward the scientific option are proper actions and better terms than 'concept replacement/substitution'. Posner et al. (1982 - see also Strike and Posner, 1985) listed four conditions/elements for bringing about conceptual change: (i) *dissonance* – leading to dissatisfaction with an existing conception; (ii) *intelligibility* - minimal understanding of the new conception (a person must realize how the new conception can restructure experience); (iii) *plausibility* - the new conception must have the capacity to solve problems that the old one could not; (iv) *fruitfulness* - the new conception must be fruitful, opening up new areas of thinking and learning.

Shiland (1997) analyzed secondary school chemistry texts and found that the above four elements were not present in sufficient quantities to promote conceptual change, that is, to have quantum mechanics rationally accepted in preference to simpler atomic models, such as the Bohr model. Stefani (2007) repeated Shiland's analysis with twelfth-grade Greek chemistry texts and her findings were similar: the extensive coverage of the Bohr model reinforced it, contrary to the stated relevant objectives of the official program of studies, according to which "students should be aware of the need for the introduction of the orbital / electron cloud concept" (Pedagogic Institute, 2000, p. 261).

Numerous studies have shown that conceptual change is very hard to accomplish. Concepts deeply rooted in students' mental images are difficult to replace by other models, strongly resisting change, despite the fact that the information presented is logical, and the teaching strategies used are well-thought out and carefully planned and implemented. Further, even if students come close to realizing the limitations of their established thinking, they continue to revert very easily to previous ideas, with which they are more comfortable (Driver, 1983, Eylon & Linn, 1988)

In this study, we employed active learning methods of teaching and learning, with students working together in small groups to accomplish an assigned common learning task under the instructor's observation and guidance. Research evidence suggests that these discursive approaches to learning provide a better learning environment, and contribute to deeper understanding and development of learning skills (Duncan-Hewitt, Mount, & Apple, 1995; Johnson, Johnson, & Smith, 1991; Stamovlasis, Dimos & Tsaparlis, 2006).

Active and cooperative learning methods are consistent with *social-cultural constructivism,* which is linked to Vygotsky. According to Vygotsky (1962), the learner actively constructs his/her knowledge, but this process is greatly assisted by interactions with peers and with the teacher who acts at the students' *zone of proximal development*. Central in

Vygotsky’s approach is the relationship between language and thought, which affects the development of higher mental functions. These functions develop through social interactions (with the teacher and/or peers) but progressively and ultimately are internalized by the individual.

Method

The study was carried out at the beginning of the 2001 academic year, with students from three departments, chemistry (CHE), biotechnologies (BIO), and material science (MAT), at a Greek university. All students had studied the same basic and advanced chemistry courses in upper secondary school, and participated in the same national, university-entrance examination in these subjects. They had just started their university courses that included a general chemistry course, but had not yet received tuition on the topics and concepts related to this study. Hence their knowledge was derived from their education in upper secondary school.

A quantitative study, in which 125 students from the three departments answered a written questionnaire, was conducted first. This was followed by a qualitative study in which 23 of the above students took part in semi-structured interviews.

The written questionnaire, students’ written responses, and all discussions in the interviews were in Greek. Accuracy of translation into English was checked by back translation of the English version into Greek. The two Greek versions (original and back-translated) were then compared, and, after some changes to the English version we arrived at the forms presented in this paper (Brislin, 1970; 1986).

The Written Questionnaire

The Written Questionnaire consisted of 14 questions, of these five (Questions A1-A5) required just the application of known and well-practiced algorithms or simple recall of knowledge. The remaining nine questions (C0-C8) were more demanding, requiring conceptual understanding. One knowledge-only question (A5) and many of the conceptual questions (C2, C4-C8) were also used in the earlier study (Tsaparlis & Papaphotis, 2002), and content validity had been dealt with at this time. Indices of discrimination obtained from this study were taken into account in formulating our questionnaire. In the qualitative study, we dealt only with questions C0, C3, C4, C6 and C7.

Appendix 1 contains all the knowledge-only questions A1-A5, as well as any conceptual questions that are not dealt with in this study; it also provides performance data. Performance was much higher in the recall-algorithmic questions, ranging from 56.8 to 74.4%. Performance in the conceptual questions was generally much lower, ranging from 9.6 to 35.2% with the exception of C3, which was a two-choice question and had a relatively high score of 56.0%.

The Interviews

On the basis of their performance in the written questionnaire, we invited a number of selected students to take part voluntarily in the interviews. We wanted to include students with a range of performances in the written questionnaire: students with an overall satisfactory performance; students with good performance in recall-algorithmic questions but not so good in the conceptual questions; and vice versa. A total of 35 students were invited, of which 23 (12 males and 11 females) accepted.

Appendix 2 includes data for the performances of these 23 students in both the algorithmic/recall of knowledge (ALG) and the conceptual questions (C) on the written questionnaire. The mean mark in ALG was 79.1 (s.d. 19.0), while that in C was only 42.5

(s.d. 16.6). It is noteworthy that two of the three students with the highest marks in C had relatively low marks for the ALC questions. On the other hand, the four students with top mark (100%) on the ALG questions obtained low marks for the C part of the questionnaire. Such discrepancies are well documented in the literature (Nakhleh, 1993; Stamovlasis *et al.*, 2004, 2005).

Interviews were conducted individually or in groups of three or four. There were six individual interviews, with two students from each department; and five group interviews, three with BIO, one with CHE, and one with MAT students. All student names used in this paper are pseudonyms.

Our aim with the group interviews was to bring face to face students, at least some of whom had given different answers to the written questions, to try to get them involved in discussions among themselves, and to observe these interactions. Both of the authors were involved as instructors (I) for the interviews. The interviews ran according to a semi-structured questionnaire.

Questions C0, C3, C4, and C6 referred to the deterministic or probabilistic conceptual interpretation of basic quantum chemical concepts and principles. Question C0 asked students to make a drawing of the hydrogen atom. Question C3 looked for the origin of the uncertainty deriving from the Heisenberg principle. Question C4 concerned the possibility of the electron of the ground-state hydrogen atom being found outside the space that is defined as a 1s orbital. Question C6 was related to Question 4, showing a correct and a faulty diagram of the electron densities deriving from the 1s and the 2p orbitals respectively, and asking students to identify any errors. Finally, question C7, which dealt with MOs as linear combinations of AOs, required good mathematical knowledge.

Note, that while performance in the written question C2 was poor (correct: 22.4%), we will not consider it further here because all students participating in the interviews quickly worked out that the carbon atom configuration entering this question is the ground-state structure, and that there are only two unpaired electrons in it, a fact that is not in agreement with the four equivalent bonds existing in the methane molecule:

> “We have two unpaired (electrons), therefore it is wrong”.
>
> “It is not in agreement because as it appears here carbon can form two bonds, while in essence and in practice it forms four.”

The reference to the bond angle values did not add to understanding. Also, since the hybridization model had not been taught to the students, it is natural that they could not draw inferences based on this model.

Results

Question C0. *Make a drawing depicting the hydrogen atom as you imagine it is in reality.*

At the outset, it must be emphasized that ‘reality’ did not mean the same thing to everyone:

- As it is in nature, not in drawings.
- It is difficult to conceptualize because the atom is very small.
- Giving the right dimensions, that is distance from nucleus (a small nucleus and the electron away from it).
- How the electron moves, the distances from the nucleus, which other orbits it has, to which it can go.
- We could draw the nucleus, and one electron, in fact, anywhere.

- The electron to be on an orbit near the nucleus.

To many, ‘reality’ had simply to do with the fact that the hydrogen atom consists of a (positively charged) nucleus and an electron at some distance away from it (a negatively charged electron to balance the charge):

> “Look, I know that it (the atom) has an electron that moves around the nucleus, it doesn’t have any neutron in the nucleus. So I would have one proton and one electron.”

Figure 1 shows indicative drawings/answers to question C0. Most students had answered in the written questionnaire on the basis of the planetary Bohr model [see Figure 1, (a) and (b)]. As reasons for basing answers on this model, the students said that (i) it was the model taught to them in previous grades, (ii) it was what they most often had encountered in books, and (iii) it was simpler for them. In addition, most students felt it difficult or impossible to draw in static form something that is moving. (To include movement, one student had added a velocity vector on the electron.) It is also worth noting that a mixed/hybrid model is used when a localized electron is included on the “surface” of the electron cloud [Figure 1, (c)].

(FIGURE 1 ABOUT HERE)

In four out of five group discussions, the students accepted or were led by the instructors to accept that the most appropriate description of the hydrogen atom was that of an electron cloud. A decisive role in gaining acceptance of the electron-cloud model was played by the presence in each group of at least one student who had given the relevant answer in the written questionnaire. Take for instance the discussion that took place in the MAT group of students, where two out of the three students (Natalia and Tania) had drawn an electron cloud in their written answers, and where Lampis, who had followed the Bohr model, was easy to persuade to adopt the electron-cloud model:

Lampis: … In essence one cannot see the atom - I drew a proton at the center and the electron moving around it. But the electron is a wave, a wave and a particle, and none could know where it is.

Natalia: .. I showed with dots the space where the electron can move, but certainly (the space) is much larger… the probability is nowhere zero. … I should actually fill in (with dots) all the paper.

…Tania: I should have added more dots.

…Lampis: All these are correct, …there should be more probability for the electron to be found near the nucleus, so there should be more dots, larger the density of dots near the center than outside, at least for the 1s ground state.

In the CHE group of students, only Antonis had drawn an electron-cloud in his written answer, while Manolis and Christina followed the Bohr model. (Manolis actually wrote next to the orbit 'a probable orbit'.) :

Christina: I don't believe that the shell is that way, it is an orbital, a wider space, but I don't know how we should draw it when the electron moves.

I: If you could see it, what would you see?

Christina: I wouldn't see the electron because it moves very fast. … I would see a cloud, a small cloud.

I: Then why didn't you draw a small cloud?

Christina: That's how I had thought of then, that was the way I saw it in most books.

… Antonis (reading his written comment): The higher the density of the dots in the figure, the larger the probability of finding the electron in that space.

Manolis: I didn't think it like that. I just wanted to give a static, so to say, form, to show both the electron and the rotation.

Eventually both Christina and Manolis accepted that Antonis' drawing was the 'proper' one. Let us also see the discussion of the three students in the BIO3 group; here Dimitra produced the drawing in Figure 1(d), Isidora the one in 1(b), while Ioanna's was similar to 1(a) with the added comment "s orbital" for the outer circle.

I: Isidora, what does the broken line show?

Isidora: Here is 1s, … if we could say … it is the space where various orbitals, 1s, 2s, 2p, it is all these and these make up the shells, it is what we have learnt in the tenth grade.

I: Is it this that you want to show here, the orbits?

Isidora: Yes, the orbits and the shells.

I: Ioanna, what have you done here?

Ioanna: I was trying to explain that the orbital is not a space that we can determine with precision, … but in the center there is certainly the nucleus, but the larger circle denotes that somewhere inside there, rather inside the larger circle the s orbital is contained and there is probability for the electron to be found.

I: What about you Dimitra?

Dimitra: I have put at the center of the atom one proton that we know that the hydrogen atom has, and with dots that as they go away from the nucleus become sparser, actually I have constructed the probability, rather the possible positions at which the electron can be found.

I: So here we have all these drawings you have made, all of you can see them. …. Which of the three corresponds to reality, the reality we talk about in the question?

Isidora: The one that Dimitra has made, because it has the nucleus and, around it, is the probability to find the electron, to be found in 1s, which does not become zero even at an infinite distance from the nucleus.

I: Ioanna what do you think?

Ioanna: The same.

I: On the contrary, what does your own drawing show?

Ioanna: It reduces the probability and makes it zero at some distance.

Some students' statements show that their views were not clear, mixing in ideas from the planetary model; for instance, the representation of the hydrogen atom using a delineating curve (such as Ioanna's above) represents a hybrid model: during conversations, this curve sometimes was called an 'orbit' and sometimes an 'orbital'. Take for instance the following statements by two students:

"(I drew) a proton at the center and around it the orbits that can … the space where the electron can move." (Tania, MAT group)

"…the hydrogen has a single proton in the nucleus, and the electron rotates on a shell, the first one … I don't believe that it is such [an orbit] this shell, it is a …an orbital, a wider space." (Christina, CHE group)

A hybrid model was also generally used when students replaced their representation of the electron as a dot or small circle with a small electron cloud/packet that again moves on specific orbits. Eleni (BIO1 group), interviewed on her own, was quick to replace the Bohr model with this hybrid model.

Eleni: I made this drawing [Bohr model] because it is the drawing that we very often encounter in books.

I: Would you now make a different drawing?

Eleni (drawing a small packet in the place of the small circle): The electron would not be a small circle, that stands for a (material) body, but it would be some cloud, some frequency, that would move around the nucleus.

I: Could that (cloud) be found here [a point far away from the orbit].

Eleni: It is very far away, I don't think so.

I: So is the probability there zero?

Eleni: Zero no, but it would be very-very small (least).

I: Could that small packet you drew be here, near (the nucleus)?

Eleni: Yes.

I: Could you redraw now to show all these?

Eleni went on to drawing a spread-out orbit, adding dots (see Figure 2).

(FIGURE 2 ABOUT HERE)

In the BIO2 group, the only group for which there was no written answer employing the electron-cloud model, no general change was observed as a result of the discussion. Two students, trying to combine the new ideas with their dominant planetary mental model, were led to accepting spread-out orbits [see Figure 3(b]. This view was also supported by the findings of the individual interviews, where four out of the six students insisted on the planetary model, from which they only moved to accept elliptic orbits in addition to circular or spread-out orbits [Figure 3(a) and (b)]. In two other cases, they arrived at intermediate drawings that combined the two models (hybrid model):

“(the electron) rotates, is found at certain time intervals in different positions around the nucleus, (which however) is not an orbit, simply I have delineated in some way the place where it can be found.” (Haris, MAT)

(FIGURE 3 ABOUT HERE)

Most students accepted that a picture of an electron cloud is just a collection of dots representing probable positions of the electron at various instants in time, but could not accept that such a picture is representative of what we would see if we could see inside the hydrogen atom. So the students, being unable to illustrate motion in a static drawing, ended back with at a planetary model:

> “I would rather not see an electron cloud, I would see the electron at different points … normally I wouldn’t see the electron, I would see a sphere, … an orbital. … an electron cloud is however (made) of dots, I wouldn’t see dots. The dots are the possible positions of the electron.” (Stathis, BIO2 group)

An analogy using the appearance of spokes on a fast rotating bicycle wheel proved effective in helping students to accept, that the probability depiction of an electron cloud was indeed a valid representation for a hydrogen atom.

Note that question C5 (that asked how one could construct the picture of the electron cloud if it were possible to take photos of the electron) again led many students to make various drawings of the atom as shown in Figure 3.

Question C3. *The uncertainty that is predicted by the Heisenberg uncertainty principle is due to:*

(a) The fact that the very process of measurement introduces the errors, so that what we measure does not correspond to the exact values; this causes the uncertainty.

(b) The fact that the particles that we study are so small that there are no available instruments to make the required exact measurements; this causes the uncertainty.

Option (a) expresses one understanding of the uncertainty principle, although we do not claim that it would necessarily cover all understandings. Any discussion of the interviews that follow must keep in mind this limitation. It follows from the interviews that many (probably most) students, irrespective of their answer, attributing the uncertainty to the instruments, the measuring procedures or both, made this selection on the basis of their experiences at the macro level.

Students who were interviewed individually produced a variety of arguments. Petros (BIO) who had not answered the written question, was definite about the cause: “With ideal instruments [in his words: these have zero error], I imagine that there should not be uncertainty”. Marios (CHE), who had chosen option (a), stated that the instrument is part of the process, and even with the proper instruments there will always be a small error:

I: But “what if we suppose that we consider the process independent of the instrument?

Marios: [at the level of molecules]… the error or better the uncertainty, would be due to the measurements and less to the instrument.

Finally, Martha (BIO) used a process of elimination (in her words: ‘reductio ad absurdum’) to support that “option (b) cannot be the case, while option (a) must be at least more valid”. Discussion made her thought shaky for a moment, but she quickly returned to her initial choice.

Martha: I assume that some instruments for the required precise measurements would be there. Therefore, (option) (a) must be valid or at least is closer to the truth.

…I: Is then this uncertainty something that nature requires?

Martha: Maybe, but even in lab always there are errors.

I: Are the lab errors the same with the error of the uncertainty principle or different?”

Martha: They are different.

I: In what are they different?

Martha: By nature, that is, to measure velocity and position simultaneously.

I: For what (material) bodies does the uncertainty principle apply?

Martha: For particles that are very small, maybe because of the size we cannot see them clearly.

I: I ask you to consider it again, is it the process of measurement itself that introduces the errors, or the fact that we don't have the proper instruments, so if we had them there would be no need for the uncertainty principle?

Martha: I am confused now – it might be the second. Because the particles are so small, it may not be due to the process but to the instruments, which must be very specialized.

I: Do we have such instruments?

Martha: We have them – then it is [must be due to] the process.

Martha's momentary confusion could also be attributed, to the limitation of the explanation in option (a) that we discussed above.

Turning to the group interviews, there was only one student (Christina, CHE group) who had chosen option (b) but was then persuaded to change her opinion. In all other cases, it was very difficult, and often impossible, to change the expressed views. Occasionally, even students who had opted for option (a) were doubtful about their choice – but again this could be caused, at least in part, by the problematic nature of the explanation in option (a). The discussion in the BIO1 group is representative. Here Eleni, Leonidas and Themis had chosen option (a), while Irene had opted for (b).

Eleni: I don't know the instruments, simply I assume that with today's technology the instruments to make the required measurements exist.

I: Irene says that we don't have proper instruments to measure.

Irene: That we don't have the instruments, no; that we can't measure velocities or masses or momentums of such small order, yes.

I: Even if we had the instruments?

Irene: Yes.

I: Leonidas, from what you have heard, can you say anything to Sophia?

Leonidas: I believe that the numbers are very small and very large [in the micro and the macro world respectively], so that there is a large difference between the two, the velocity and the mass and all these, and it is not possible that there is something that connects them.

Irene: We can measure separately the mass and the velocity; there is no need to measure both [quantities] with the same instrument; so I am not convinced.

Themis: I agree with [choice] (a), there are the instruments, that is, we can bombard an electron with photons; the coming together of photons and electrons I believe will change the electron's momentum; so when the photon arrives at our eye it will have … it will not have the same momentum and … you know, it will have changed. The momentum will have changed.

I: Irene, has the last argument you heard from Themis convinced you, in any way, to change?

Irene: Yes, he said there are the instruments, but it is just the human agent that makes the error.

I: Supposing that I am going to measure simultaneously the velocity of a car and its position, will the uncertainty principle be valid in that case?

Leonidas: No.

I: What about you Irene, is it valid?

Irene: Even if it is valid, the error will be very minute, that we assume it as zero.

I: Have you, Irene, been convinced – I say this because the others [who have opposite opinion] are three. …

Irene: They don't say anything certain about the instruments, and I don't know; actually I don't understand the process, and I don't know if the instruments exist.

I: So they don't persuade you that they have made the right choice with [option] (a).

Irene: No.

I: Has any one of the others changed opinion after the discussion and changed to [option] (b)?

All (except Irene): No.

In the CHE group, Manolis expressed for the view that one the one hand it is a matter of time for man to achieve precise measurements even in the micro world, but on the other hand the error will always be there both in the micro and the macro world:

Manolis: I assume that both in the micro and the macro world it is (answer) (a), that is, they are just relative, that is, we can later be able to determine both the position and the momentum, that is, to approach the capacities we have in the macro world, but again it will not be so, … it will be due to the fact that … nor in the macro world we have essentially the precise position and the precise determination.

Christina: But the errors [in the macro world] haven't very large difference, compared with the micro world.

Manolis: OK they don't have because they are smaller, but it isn't something that is prohibited to man to measure something like this (in the micro world). Some time (in the past) it was prohibited to man to make measurements also in the macro world. This is something that will be just there, … the error will exist always.

Finally, Stathis (BIO2 group), who got the highest mark in the conceptual written questionnaire, expressed an interesting view; apparently, he based his thinking on the mathematical equation that expresses the uncertainty principle:

"When we talk about the process, we don't mean only the instruments, we may also mean the mathematical process that we will follow; that's why I selected [the option] (a), that is, we know that from the equation we used to find one of the two, when we determine with a great precision the one, precision is wiped out for the other."

Question C4. *Is it possible for the electron of the ground-state hydrogen atom to be found outside the space that is defined as 1s orbital? Explain.*

Students who held a probabilistic model of the orbital (thinking of the orbital as a probability envelope) were consistent in accepting that there was a probability of the electron being found outside the orbital:

> "It is possible. The orbital is the space inside which there is a large probability for the electron to be found; hence, in some special case it is possible [that the electron] is not found in that space." (Manolis, CHE group)

> "I answered in accordance with what we learnt in school. I am not certain if the number I have put is right, but … the probability for the electron to be found in the space that is defined as the 1s orbital in the ground state is 95%; hence, there is a 5% probability for the electron to be also found outside the space of the 1s orbital (in the ground state), even if this probability is small, but it is there." (Isidora, BIO3 group)

> "Certainly, because the electron can be found anywhere. Nowhere is the probability zero. It has just near the nucleus more probabilities, around 90 to 97%." (Natalia, MAT group)

On the other hand, many students identified the orbital only with the space enclosed (or possibly only its surface), that is, they believed that the fixed shape of the orbital corresponded to a certain probability:

> "It is not possible (to be found outside the 1s space), because as an orbital is defined the space where the electron can be found – it is basically the space where the electron can be found, that is, the positions where the electron is found delineate (chart) the 1s orbital."

Stathis (BIO2 group) who had a probabilistic approach, was critical of the question itself.

He also emphasized the distinction between the orbital in terms of probability and the electron cloud (while the concepts of electron probability and electron density are essentially equivalent):

> "I believe that you set a trap in examining the students, that is, if they have confused the concept of the orbital with the concept of the electron cloud. The orbital is the probability, I think 95 or 99%, for the electron to be found, while the electron cloud is all the possible positions which the electron can take. Hence, from what I've said, it [the electron] can also be found outside the orbital."

It is important to note that in pictures of the electron cloud, dots that were drawn outside the circle that was used to "define the orbital" were assumed by several of the students to belong to other orbitals, "They are in other, … they are other orbitals." The difficulty of conceptualization of this question became very apparent in the case of Pavlos (CHE) who was interviewed individually (and who had performed poorly on the conceptual written questionnaire). In his case, the instructors went through questions A6 and C6, according to which "the precise size of the orbitals cannot be shown, since the probability of finding the electron does not become zero even at large distances from the nucleus. This is shown in the orbital shapes, with a dense electron cloud near the nucleus which becomes sparser as we move away from the nucleus." While this student accepted that the sparse dots meant that the probability for the electron to be found there is smaller, but not zero, he refused to accept that the electron was still in the 1s orbital: "Outside the sphere, no, it will not be, or it will be in another orbital."

In the BIO3 group interview, Isidora appeared to hold a probabilistic approach (see above), but was not very much involved in the group discussion. On the other hand, Dimitra answered in terms of excited states and Ioanna in terms of energies. Remarkably here Dimitra was led on her own to the acceptable view by invoking her answer to question C0; also she made a correct intervention in connection with energies and distances from the nucleus.

Dimitra: … for the electron to be found outside the space defined as the 1s orbital it must be in an excited state, because we know that every such region of an orbital is characterized by a certain energy.

I: When it is excited, is it 1s or something else?

Dimitra: Something else, who knows, [can] be 2s, 3s.

I: But the question here asks about the 1s.

Dimitra: Of course, on the basis of what I have … drawn at the back [question C0], probably the space defined by the 1s orbital might be also these one-two dots at infinity, which essentially I have drawn [for question C0].

I: That is, you mean that the space of the 1s orbital is the whole space.

Dimitra: Not really, I just believe that, yes it is a space, it is like a closed sphere that defines a certain space, but also the orbital is also these remaining possible points where the electron can be found.

I: Therefore, your answer to questions C0 and C4 are in conflict to each other.

… Dimitra: Now I assume that they are about the same thing, so if I had to answer it [question C4] again, I would say that yes, the electron of [the] hydrogen [atom] can be found outside the 1s orbital.

… I: On what does the energy of an electron depend?

Ioanna: On the distance I think.

… I: Is it possible for an electron in the 1s orbital to be farther from the nucleus than an electron in the 2s?

Ioanna: According to the definition of the orbital I think that, yes, it can.

… I: Is it possible for a 2s electron at some moment to be closer to the nucleus than the 1s electron, is this possible at some moment?

Dimitra: Momentarily yes. According to the definition of the orbital we have stated, the more we move toward the nucleus the higher is the probability for the electron to be found there, but this does not exclude that we can find it somewhere "outside".

The CHE group interview is representative of the various approaches taken. Manolis, as stated at the beginning of this section, held the acceptable probabilistic approach. Antonis, on the other hand, had rubbed out his initially written probabilisitc answer. Finally, Christina had answered in terms of excited states; but she quickly changed her view. We would like to emphasize the effectiveness of relating orbital size to the probability of encountering the electron as an approach to promoting conceptual change.

Christina: It is not possible because the ground state exists in the subshell with the smallest energy, and the 1s has the minimum, therefore in anyone else it would not be in the ground state.

… Christina: Yes, the hydrogen is in the ground state, well, and it tells us that it is outside the space that is defined as the 1s orbital, and since it is in the ground state, it has there the smallest energy, in which case it cannot go to another orbital, therefore …

I: To be found outside that space it must go to another orbital – do you agree, Manolis, with this?

Manolis: No, because the space also includes, let us say, the 2s orbital, even the p or the d orbital.

Christina: It will not then be in the ground state.

Manolis: Yes, it will not be in the ground state, but the electron moves in a region around the nucleus … that is, the issue of how the electron moves is relevant …

... Manolis: When we say space of the orbital, we can say it is something very large, the space that the 1s orbital occupies, some part of the space occupies also the 2s orbital, … or even the p or the d orbital.

Christina: But it will not be in the ground state then.

… I: What about you Antonis, what are your comments?

Antonis: The 1s is a small sphere, and the 2s is a larger sphere, and the 2s contains the 1s, hence *in the 2s the probability must be higher because it occupies larger space*. [*This is a misconception*.]

I: Let’s return to your answer.

Antonis: In the ground state, how far the electron is from the nucleus, if it is in the ground state we say it is in the 1s orbital.

I: Which has a specific distance, specific shape, hasn’t it? Hence, it cannot be found outside that [space]?

Antonis: No.

I: Could you repeat your definition of the orbital?

Antonis: It is the space where the electron can be found.

I: What about you Manolis? It is the space …

Manolis: Where there is large probability to be found…

I: How much probability? Let’s set a number … let’s quantify it.

… Christina: It is 95%.

I: So we can even set it at 98%, can’t we? If I set 90 it goes up to a point, if I set 95% it reaches another point. … If I set 100% how far will it reach?

Christina: To infinity.

I: That is, all space … that’s why we don’t set 100%.

I: Antonis, may be what you wrote and then rubbed off was more correct? Please try to read what you have rubbed off.

Antonis: “The orbital is defined as the space with the largest probability of finding an electron; hence there is always a least probability of finding it outside that space.”… It depends how we will define the orbital; if we define it to have a certain size, to stop somewhere, then there is a very small probability.

I: Therefore, we must set the probability at a lower value, of necessity, so we give it [the orbital] some shape. … If we set it, say, at 90%, we leave a 10% to be outside, so this answer is more correct.

Antonis: This is what Manolis said.

I: Let us see what Christina has to say.

I: That is, when we say that there is 90% probability of finding it [the electron], this gives it [the orbital] some shape, spherical – there is also a 10% to be outside. Do you agree?

Christina: Yes.

I: And it still is the 1s orbital.

Christina: It still is.

I: Then in what way does the 2s differ from the 1s?

Manolis: In the 2s the electron can be found at larger distance from the nucleus with larger probability.

I: With larger probability, do you agree Antonis?

Antonis: Yes.

… Antonis: If we had defined the orbital differently, there would be different probability of finding it [the electron] outside the orbital.

I: … So if I defined the 1s it at 95%, what would change from 90%, in relation to the space, what would change?

Antonis: The size would be a bit larger.

I: A larger space, do you understand this Christina?

Christina: Yes, because when we set 95% probability of finding the electron versus 90%, *it means that we would have 5% more space* [*This is a misconception*.]

Consideration of ion formation when the electron is found at an infinite distance from the nucleus provides another interesting conceptualization perspective. The MAT group interview provides an example. In the written questions, only Natalia appeared to hold a probabilistic approach, while Tania and Lampis gave answers in terms of a fixed orbital. Concerning the formation of ions, Lampis initially thought that when the electron is at infinity, we have formation of an ion, but then he added a prerequisite to this: the presence of another atom to take the electron would be necessary.

Lampis: … as long as it [the electron] is in the 1s orbital, it can be found even at infinity, but still it will be in the 1s orbital, neither in the 2s nor …

… I: …We draw a sphere and we call this sphere [a] 1s orbital. … Can [the electron] be found outside this sphere, and still be in the 1s?

Lampis: The electron? No, after that it [the atom] would be an ion.

I: But it can, can't it be even at infinity?

Lampis: Yes, but if over there … would be no other electrons, other neighboring atoms to exert forces …

I: You said an 'ion', it is considered an ion when it [the electron] goes to infinity, but to go to infinity for a moment or for ever?

Lampis: For ever if it is to leave…

I: Do we consider that it will go to infinity for ever or it will go for a moment and [then] come back? … If it goes forever, I have an ion, if it comes back, I don't have an ion.

… Lampis: Yes but this electron must go somewhere, there must be another neighboring atom that needs this electron.

Question C6. *Observe the pictures (a) and (b) that show the electron clouds in the 1s and a 2p orbital respectively* (see Figure 4). *While in (a) there are sparse dots far away from the nucleus, in (b) such dots do not exist. Do you think there is an error in either or in both of the pictures?*

PLACE Figure 4 ABOUT HERE

Students who had given acceptable written answers, offered explanations such as the following in the interviews:

- “I believe picture (b) is wrong because, as we had said, the probability of finding the electron is never zero, even if it is very minute; therefore there should exist more dots more sparse.” (Martha, BIO)
- “Picture (b) is wrong. The probability of finding the electron in an orbital is not confined to a certain space but it extends to infinity, without ever becoming zero.” (Ioannna, BIO3 group)
- “We know from the previous question that the exact size of the orbital is impossible to be interpreted, since as we have said the probability of finding the electron doesn’t become zero even at large distances from the nucleus. Therefore in picture (b) too it should be shown that the electron could be also found far from the nucleus.” (Dimitra, BIO3 group)

In the interviews, we observed ad hoc attempts to explain the differences between the two pictures, based on a belief that both are correct:

- “The first is an s orbital, representation, the other is a p. … It must be correct because probably for energy reasons this, in some way, must be like that, I am not quite sure.” (Pavlos, CHE)
- “…Picture (a) shows the electron cloud, while picture (b) shows the orbital”. (Stathis, BIO2 group)
- “The existence of electrons in the 2p orbital assumes a large nucleus that increases the attraction, so they (the electrons) won’t be able to get away from the nucleus. … But because the picture shows that [the cloud] stops somewhere abruptly, there is no probability of finding [the electrons] outside.” (Antonis, CHE group)

Also, we encounter behavior and ideas that were observed in previous questions. Thus, the dots that are far from the nucleus may belong to another orbital “the electron there might have been excited”. It is encouraging however other students who had used the probabilistic model stuck to their view, as the following excerpt from the MAT group interview shows:

Tania: Where there is larger density of dots, it is there that there is a larger probability.

I: … But when the dots are far away, does (the electron) continue to be in the 2p or is it excited?

Tania: It might be excited.

I: The same could happen with the 1s couldn't it?

Tania: Yes.

I: You, Natalia, what do you think, would it be excited or would it still be in the 2p (… or the 1s) … when it is far?

Natalia: I think that … it can still be in the 1s, only the probabilities are more when it is closer.

Lampis: I agree with Natalia.

Antonis (CHE group), who spoke of larger attraction to the electron by the larger nucleus, extended the same argument providing the correct concept about the electron cloud size of the same orbital for different atoms. "When we have many protons together in the nucleus, the increased positive charge will attract the negative charge of the electron with a larger force, so it is more probable that [the electron] will be found closer to the nucleus than if it was in a hydrogen.atom". This concept helped the investigator to lead Antonis to the answer that is consistent with the probabilistic model:

I: If I asked you to draw the 1s orbital boundaries when we set the probability say at 90%, where would you place them?

Antonis: [draws a circle on the paper]

I: And where if the probability was 80%?

Antonis: A smaller circle.

… I: If we consider the 2p orbital and the probability was 100%?

Antonis: 100%, according to the picture, because it stops abruptly, we could say that it would be where the dots stop, but again we could consider it would be the whole space.

I: So you see here that it stops abruptly, while it should not stop?

Antonis: Yes.

I: So, is it correct that it stops abruptly or is it wrong?

Antonis: It is wrong.

Finally, Marios (CHE) (who had given the acceptable answer in the written question) had also an interesting view about the size of the 1s orbital. Asked to draw a sphere representing the orbital, he encircled all dots shown in picture (a).

I: So you haven't left any dots outside.

Marios: No, I haven't.

I: What then do these dots mean for you?

Marios: That somewhere inside these dots there is probability that the electron is.

I: Therefore, since there are no dots [left] outside, it must be ruled out that [the electron] is [outside].

Marios: It is not ruled out, possibly it is inside here.

I: Shouldn't we then have left some dots outside?

Marios: However, how far, it seems to me …

I: Let's say, just a little outside.

Marios: We should have an error in the orbital, that's why, possibly, it is not certain that it will be inside.

I: If we had left several dots outside, you wouldn't accept that as an orbital?

Marios: I would accept it.

I; What then would be the difference from the one you drew?

Marios: That we leave more dots outside, that is, the probability of finding it [the electron] inside here would be smaller than inside here. Maybe, we could draw it [the orbital] larger.

… I: Therefore, we could enlarge the distance [the radius], and it will still be 1s orbital, without the need to excite it?

Marios: Up to its ionization energy.

It appears that Marios felt more secure with a fixed shape for an orbital that includes all shown dots but accepted that there is still a possibility for the electron to be outside this fixed orbital.

Question C7. *A molecular orbital is formed by the combination-overlap of two atomic orbitals. Mathematically, this combination is equivalent to addition of the two atomic orbitals. In your opinion, would it also be possible to subtract one atomic orbital from an other? If yes, what would be the consequences of that subtraction for the electron density in the space between the two nuclei as well as for the chemical bond?*

There were a considerable number of students (20.8%) who gave acceptable answers to the written question: “The electron density in the space (between the two nuclei) would decrease and the bond would break.” In the interviews, these students did not change their views, but often developed them:

> “ From the moment that we wouldn’t have full electron density on each orbital, the bond of the MO would break, hence the two AOs would form again.” (Stathis, BIO2 group)

In the case of the group interviews despite the fact that students with acceptable written answers and views were present in each group, great difficulty was encountered in understanding and accepting the subtraction of AOs. In fact, even in the cases where students arrived logically at the correct answer, they were not sure if that could happen in practice, that is, if there exist MOs that derive from subtraction of AOs or if that has simply to do with a theoretical-mathematical artifact:

"Here I mean that we can create this mathematically only, while chemically, in practice, we can't create it." (Antonis, CHE group)

The instructor found it hard to lead students into accepting the possibility and the consequences of subtraction, as the following excerpt from the CHE group interview shows:

I: If I tell you that the result of subtraction would be fewer dots, you can accept this, but you have difficulty in understanding how subtraction can occur.

Manolis: The rationale would be that when they come close (to each other) the rule would be that with the addition of the orbitals a bond should form, but I can't understand how with subtraction there would be no possibility of finding the electron.

I: Subtraction leads to the conclusion that now the probability of finding electrons becomes less, therefore the result is no bond. How do you see this?

Christina: Reasonable.

Antonis: If it could happen, it might be reasonable, but it seems very improbable that it could occur.

Manolis: I cannot picture in my head how this could happen.

The main obstacle to accepting subtraction appears to be the way they think of an orbital,, seeing it as a 'space' and not as a mathematical function. For instance, Eleni (BIO1 group), while accepting the possibility of adding or subtracting probabilities, would not accept that orbitals might be subtracted because they are spaces: "… spaces where the electron can be found, not just numbers that can be subtracted." Despite having a student (Irene) who both in her written answer and in the interview held the acceptable view, in the group, the others could not be convinced:

Irene: … because mathematically we say that the combination of the orbitals is addition (of orbitals), therefore mathematically it can also be subtraction, … why not. … When I am doing subtraction, it must be the part of the orbitals in the figure where they do not overlap. (We have) reduction of the density.

I: And what would be the consequences for the chemical bond? Since the electron could not be inside there, would a chemical bond exist?

Irene: No, a chemical bond would not exist.

I: In the final analysis, what is the meaning of overlap? When I have positive overlap, the probability of finding the electron there increases, when I have negative (overlap) it reduces.

Irene: There would be less probability that a bond would be formed.

I: So the bond would be more … ?

Irene: Weaker..

I: Are you convinced by that Eleni?

Eleni: No, I insist that subtraction of two orbitals cannot take place. Because they are spaces, we cannot subtract two spaces.

Themis: I completely agree - we cannot do it.

Using the analogy of waves, starting from the quantum-mechanical wave model of the electron (a model that students accepted that they had heard of) did not help either. The discussion resulted in deadlock.

There were also objections to subtraction, on the grounds that addition and hence bond formation, should be preferred by nature:

"The thought therefore is that they [the AOs] always come close to each other, but while, let us say, the rule should dictate that a bond should form by means of addition of the orbitals, I can't understand how subtraction could mean that there is no possibility of finding the electron, therefore it would not happen. I can't understand it." (Manolis, CHE group)

> "Why, however, should nature favor weakening of bonds instead of stabilization of bonds?" (Themis, BIO1 group)

Another misconception was that of the two nuclei moving apart from each other as a result of subtraction of the AOs. Also, where the overlapping orbitals were identical (e.g. both 1s) bond breaking would result, but if the orbitals were different (e.g. 1s and 2s) the result would merely be bond weakening.

Using pictures of electron clouds seemed to facilitate understanding of the addition of orbitals, that is understanding of the thickening of the electron cloud at the regions where addition occurred. But the same approach did not appear to promote understanding of the process of subtraction of orbitals: "No, because we would not be able to distinguish the 'points' (the dots) of the one orbital from the other."

Changes in students' ideas

The aim of our intervention was to try to change students' simplistic ideas into modern (probabilistic, quantum-mechanical) views. In Tables 1-3 we provide data for changes in student ideas concerning the uncertainty principle, the nature of orbitals and the atomic model. Employing a chi-squared statistical test, changes for the last two concepts were found to be statistically significant

(Tables 1, 2, 3 here)

Discussion, Conclusions, and Implications

Research has shown that students at all levels prefer concrete or simple abstract models, for example: space-filling models of atoms and molecules (Harrison & Treagust, 1996); the Bohr model of the atom (Fishler & Lichtfeldt, 1992; Nicoll, 2001; Petri & Niedderer, 1998); or the octet rule (Coll & Taylor, 2002). These preliminary models are very stable. Although students at a higher educational level may have been exposed to abstract models with higher explanatory power, such as the quantum mechanical model of the atom or the concept of MO, they find it difficult to replace the earlier models. What is frequently observed is that learners accommodate new knowledge into their preexisting knowledge, constructing personal meanings and alternative mental models that contain elements from these earlier models (hybrid models) (Vosniadou & Brewer, 1992). The findings of this study are in agreement with these earlier observations.

The Findings

The planetary Bohr model remains prominent in the minds of many students. This is because it is simpler, it is the model taught in earlier education, and is most often encountered in books. Some of our students insisted on the planetary model, but were prepared to accepted elliptic orbits in addition to circular or spread-out orbits. Other students were mixing ideas from the planetary model, representing the hydrogen atom with a delineating curve, thus mixing orbitals and orbits. Even if many students knew the concept of the electron cloud, they did not accept that it provides a picture of the atom. The analogy of an electron's movement with the appearance of the spokes on a fast rotating bicycle wheel proved effective. A hybrid model was also the common replacement for the representation of the electron as a dot or small circle with a small electron cloud/packet that moves again on specific orbits.

A large number of students had not understood the fundamental nature of the Heisenberg principle. Based on experience at the macro level, they considered instruments or the measurement procedures or both as responsible for the uncertainty deriving from the Heisenberg principle. Consequently, "it is a matter of time for man to achieve precise measurements in the micro world". In general it was very difficult and often impossible to change students' views, while even students who had opted for the (assumed as) correct answer were doubtful about their choice. These findings suggest that the uncertainty principle does not fall within Vygotsky's 'zone of proximal development'. There were, however, students who considered correctly that the instrument is part of the process, and even with the proper instruments there would always be some error. We must point out, however, that the issue dealt with in the relevant question is a non-consensus topic in science, so the 'correct' explanation offered to the students [option (a)] might not be consistent with all explanations acceptable to physicists, and might not help students in their own interpretation of the uncertainty principle. The assumption that there is a fundamental limit to measurement because of the nature of the phenomena themselves, regardless of the measurement, provides an alternative approach that is consistent with the Copenhagen interpretation of quantum mechanics.

Many students found it difficult to understand the probabilistic nature of the orbital concept. In addition, they identified the orbital only with the fixed space enclosed by the orbital shape used (or sometimes only with its surface), that is, the shape of the orbital refers to a certain probability. It is useful to emphasize that the particular envelope that is 'fixing the orbital' and we are interested in is the one which includes this probability distribution in a minimum volume. In pictures of the electron cloud, those dots that were outside the circle that was drawn to "define the orbital", were assumed by several students to belong to other (excited) orbitals. An effective approach to promoting conceptual change (bringing the relevant concept within the 'zone of proximal development') was through relating change of orbital size with the value of the probability of encountering the electron.

Energy considerations might also contribute to distinguishing between a dot 'belonging' to a lower- or to a higher-energy orbital; thus, a lower-energy electron spends most time closer to the nucleus than a higher-energy electron. Also the distinction made between an atom where an electron is momentarily at infinity but still technically part of the atom, and the ion with its separated electron is an interesting one. Again this distinction can be linked to the energy of the state: in the former case the energy is the respective orbital energy, while addition of the ionization energy is required for ion formation.

The mathematical description of the formation of MOs by means of linear combinations of AOs caused no problems in the case of constructive (bonding) addition, but was very problematic in the case of destructive (antibonding) subtraction. While there were several students who appeared to be comfortable with this process, many students encountered great difficulty with understanding and accepting the subtraction of AOs. Even in cases of logically correct answers, they were uncertain if that could happen in practice, or if it had simply resulted as the consequence of a mathematical artifact. The main obstacle to accepting the idea of subtraction appears to be the way in which students have built their concept of an orbital, seeing it as 'space' and not as a mathematical function. The analogy of waves, starting from the quantum-mechanical wave model of the electron, did not appear to be helpful. Some students believed that addition and hence bond formation, would be preferred by nature. Another misconception was that of the two nuclei moving apart from each other (separating) as a direct result of AO subtraction. Also it was often believed that where overlapping orbitals are identical (e.g. both 1s) *bond breaking* will occur, but if they are different (e.g. 1s and 2s) subtraction will result in *bond weakening*. Finally, the use of pictures of electron clouds seemed to facilitate understanding of the addition but not of the subtraction of orbitals.

It is worth noting that Question C7 is considered within the LCAO model that uses mathematical expressions for orbitals. There was then a shift in the meaning of orbital from that of space that the students of this study held into one of mathematical function.[*] Thus, while subtraction may be possible in terms of LCAO, it becomes hard to be accepted if orbitals are approached from their probability/density perspective, and even harder if they are assumed simply as spaces. The students' attempts to answer Question C7 should be seen in these terms.

Our study uncovered three main problems for the learning of basic quantum chemistry concepts by high-school and freshmen university students: (a) the reliance on deterministic models of the atom derived from old quantum theory; (b) the misinterpretation of models and theories, and the poor understanding of modern quantum concepts, including their mathematical features; (c) the formation of misunderstandings and misconceptions.

With regard to question C4, Martha (BIO) interviewed individually, revealed many of the relevant deterministic views, misunderstandings and misconceptions, as well as difficulty with and a reluctance to accept the probabilistic model of the atom. The interview started with the instructor asking her to show the actual 1s orbital. She responded by encircling the darkest area in figure (a) of question C6, assuming that the 1s electron could move only on the corresponding fixed spherical surface, but not inside or outside this boundary.

Martha: The electron … I think … on the surface because it is an orbital.

I: What is an orbital?

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[*] In a study with students who had passed the quantum-chemistry course (Tsaparlis, 1997), the definition of an AO as a one-electron, well-behaved mathematical function was found to be unfamiliar to the majority of the students, who understood or connected an AO with a region in space.

Martha: It is these three quantum numbers, *n*, *l*, m_l, that … is in a three-dimensional space, in which case it cannot, I think, be found inside this space.

I: Then it [the electron] moves in specified orbits.

Martha: That has specified size, orientation, and shape.

I: So it moves only on the surface, hence it has a certain distance from the nucleus.

Martha: Yes.

I: Is this in agreement with the Heisenberg uncertainty principle?

… Martha: The uncertainty principle says that it is impossible to determine the electron's position, that is, we go according to probabilities.

… I: Let's then talk in terms of probabilities – is there [a] probability of finding it inside the sphere you have drawn?

Martha: Depending on the density of the electron cloud, … the more dense the dots are ….

I: What does each dot stand for? … Does the dot relate to the electron?

Martha: No. – it relates more generally to the space, that is, …

I: So, somewhere where I have many dots, what does this mean?

Martha: There is [a] probability of finding the electron there. … It helps us, when we see lots of dots, a large density there, may be there is high probability…

I: So what does each dot stand for?

… Martha: An electron? … a possible position [for the electron].

After a lengthy further discourse, Martha accepted that there is a probability of finding the electron inside and a small possibility of finding it outside the sphere. But then a new complication arose:

I: When it [the electron] is outside the sphere, will it still be in the 1s?

Martha: I think that it leaves the 1s.

I: But all this time we talked about the 1s.

Martha: I don't know, it can be it can also can … be somewhere in between.

Eventually we arrived at a deadlock, with Martha concluding that the electron will be excited. (The view that the electron can be found outside the space that is defined as the 1s orbital only when it is excited was very common.) Note that according to her performance on the written questionnaire, Martha would be categorized as algorithmic high and conceptual low (see also below).

Meaningful and Rote Learning

The concepts and processes of quantum chemistry are abstract and complex, so learning is difficult without a thorough understanding of the subject. Otherwise, students have to resort to rote learning of definitions, formulas, and processes.

Ausubel (2000) has distinguished between meaningful and rote learning, while Novak (2002) has shown how meaningful learning and the transfer of knowledge relate. Both rote/meaningful and reception/discovery dimensions of learning exist on a continuum rather than being dichotomous in nature. According to Novak (2002), "meaningful learning at one edge of the continuum requires well organized relevant knowledge structure and high commitment to seek relationships between new and existing knowledge. Rote learning at the other edge results from little relevant knowledge poorly organized and little or no commitment to integrate new with existing relevant knowledge." Evidence of meaningful learning occurs when tests of comprehension are presented in a somewhat different context to that originally encountered. The questions used in this study clearly have this feature.

Pavlos (CHE) provides an example of a student who according to his performance in the written questionnaire could be categorized as a rote-learner (algorithmic high and conceptual low). For instance, in his answer to question C3, he appeared to stick to and reproduce verbatim what is written in the books:

> "…in school we had not learnt exactly what it is … I don't remember precisely now, but in any case, we had said that the more [precisely] we can measure the position, the more we lose in measuring velocity or momentum. Therefore, I don't believe that even with very good instruments, we would be able to measure precisely."

The Role of Mathematics and of Higher-Order Cognitive Skills

In this study, we discussed with students their views on abstract quantum concepts. We focused on the ideas they expressed about the theoretical descriptions of non-observable entities and the connections they made between non-observables and reality. Quantum theory enables us to describe matter (as a rule, approximately) by means of mathematical functions and expressions that derive from Schrödinger's wave mechanics. Although the Schrödinger equation can be derived using only classical arguments (Fong, 1962; see also Tsaparlis, 2001) (with Planck's constant *h* serving as the bridge between classical and quantum mechanics), it has to be admitted that quantum mechanics can bring about a new way of thinking about the physical world at the submicroscopic level. It has even been suggested that thinking abilities beyond Piagetian formal operations may be required for an adequate understanding of quantum mechanics and relativistic issues (Castro & Fernandez, 1987). These *post-formal operations* include what Borkhoff and von Neumann (1936) have described as *quantum logic*.

According to Pauling and Wilson (1935, p. iii), "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." As a result, "mathematics is now so central, so much inside, that without it we cannot hope to understand our chemistry … These [quantum-chemical] concepts have their origin in the bringing together of mathematics and chemistry" (Coulson, 1974, p. 17). The mathematical complexity has led even many practicing chemistry researchers to adopt a quasi-quantum character to the quantum chemistry tools they employ in their practice (Sánchez Gómez & Martín, 2004).

In any case, the issues that are discussed in this work are highly conceptual, requiring what has been termed as higher-order cognitive skills (HOCS). According to Zoller and Tsaparlis (1997, p. 118), HOCS items include "quantitative problems or conceptual questions unfamiliar to the student, that require more than knowledge and application of known algorithms for their solution; they require analysis and synthesis, and problem solving capabilities, the making of connections, and critical evaluative thinking (Zoller et al. 1995)". HOCS should be contrasted with lower-order cognitive skills (LOCS), "that require simple recall of information or a simple application of known theory or knowledge to familiar situations and contexts; they can also be problems (mostly computational exercises) solvable by means of algorithms, already familiar to the learner through previous specific directives or practice or both."

The Role of Interactive and Dialogic Communication

The method we have employed can be considered within the analytical framework developed by Mortimer and Scott (2003). It focuses on the teacher's role in making science concepts and issues available to the students and in helping them to make sense of them. At the heart of Mortimer and Scott's analysis lies the communicative approach, which describes the different ways a teacher can work with students to address the different ideas that are under discussion. One can consider two dimensions of communicative approach: (i) interactive and non-interactive - in terms of participation of more than one person or just one person respectively; (ii) dialogic and authoritative discourse. In a dialogic communicative approach attention is paid to more than one point of view - different perspectives and different ideas are explored. In authoritative communicative approaches attention is paid to just one point of view, that of the teacher. Scott, Mortimer and Aguiar (2006) see these two forms of discourse not in terms of a dichotomy but as a continuum, with one form of discourse merging with the other in supporting meaningful learning. By combining the above two dimensions, we arrive at four classes of teacher-student classroom communication: (i) interactive and dialogic, (ii) non-interactive and dialogic, (iii) interactive and authoritative, and (iv) non-interactive and authoritative.

Our study confirmed that the interactive and dialogic method of teaching and learning employed provided a better learning environment and contributed to deeper understanding and development of learning skills. In particular, very positive proved the dialogues and interactions that took place among the students within groups.

As expected, students who performed well (Stathis, Leonidas, Ioanna) or satisfactorily (Isidora, Danae, and Antonis) on the conceptual questions of the written questionnaire gave 'good' answers during the interviews, although they often encountered conceptual difficulties. Also, students with moderate or low performance on these questions often made useful, constructive, and interesting contributions. Our net conclusion is that the methodology used can be useful for all students, irrespective of their behavior on traditional written exams.

Implications for Instruction and Curricula

The ideas and concepts of the old quantum theory can be so dominant in shaping students' thinking that their introduction in early school chemistry is questionable. They deserve of course a distinguished place in the history of science, but this could be visited at a later mature stage. Even at the elementary level, alternative approaches exist that while avoiding consideration of orbitals, do not use models such as the Bohr atom and the octet rule.

Johnstone, Morrison and Reid (1981) provide an example of this by considering bonding in terms of the concept of electrons trying to keep as far apart as possible. Gillespie contends that more emphasis should be placed on electron density rather than on orbitals; further, Lewis structures and VSEPR are all that is required at secondary school level, while the electron-domain model is sufficient for most general chemistry courses (Gillespie & Matta, 2001).

Staying with the orbital ideas, in our opinion, the following represents a minimal list of theoretical facts that (as a rule) are related to the findings of this study, and should form the basis for leading our students to better conceptual understanding and more meaningful learning:

- Quantum mechanics has a probabilistic (in contrast to a deterministic) nature.
- A physical meaning is attributed to the AOs by relating them to electron probabilities or equivalently to electron densities.
- The representations of AOs as various shapes are just graphical forms of mathematical functions; particular emphasis needs to be placed on sections of contours with equal probability.
- MO theory, which is based on linear combinations of AOs, is also a mathematical model, while constructing MO shapes by combining AO shapes is again a graphical representation of mathematical functions.

Despite the mathematical character of quantum chemistry and the necessity for a mathematical approach, it could be argued that the quantum chemistry concepts can be understood at an acceptable level with only a minimal mathematical treatment, using mathematical equations and functions but without the need to solve differential equations or performing other complicated mathematical operations. It is also advisable to reconsider the depth of the mathematical coverage of quantum chemistry even at the physical chemistry level. In any case, the underlying physical picture and its connections with mathematics should be emphasized. Conceptual meaningful learning should always be the main instructional target.

The problem of misconceptions, arising partly from textbooks and instruction and partly from the very nature of quantum theory (Bodner, 1991; Fishler & Lichtfeldt, 1992; Kalkanis, Hadzidaki, & Stavrou, 2003; Tsaparlis & Papaphotis, 2002) is very serious. Misconceptions form *epistemological obstacles* to the acquisition of quantum mechanics knowledge *(*Kalkanis, Hadzidaki, & Stavrou, 2003). It is difficult to overcome these problems using traditional didactic teaching methods. It seems unlikely that more and better content, taught in the old didactic way will improve the situation (Stofflett & Stoddart, 1994).

Despite limitations arising from the nature of learning, a constructivist pedagogy that employs active and cooperative forms of learning, and aims at *conceptual conflict* and *conceptual change*, holds the promise of being more effective in diminishing or indeed overcoming misunderstandings and misconceptions. To this end, special techniques, such as *integration* (which attempts to link concepts, for example AOs, hybrid orbitals, and MOs) and *differentiation* (which aims at identifying differences between related concepts, for example between hydrogenlike and non-hydrogenlike orbitals or between AOs and MOs) (Hewson & Hewson, 1984) can be effective.

Last but not least, let us acknowledge that any improved instruction that takes into account the findings from this and similar studies, does not imply that the only reasonable outcome from instruction should be no lingering misconceptions (zero error tolerance). Needless to add our best current theories are only approximately true. “Orbital concepts are merely aspects of the best presently available model; they are not ‘real’ in the same sense that experimental observations are" (Simons, 1991, p. 132). AOs, MOs, and related concepts derive from Schrödinger's wave mechanics, which is itself an approximation to nature (a model). Suffice it to add that Dirac's relativistic quantum mechanics (which takes the theory of relativity into account), is a better model that explains experimental observations which the Schrödinger model does not - such as the correct prediction of the entire hydrogen-atom spectrum, the electron spin and the Pauli principle, and various chemical properties (McKelvey 1983). It is noteworthy that the AOs and related concepts (quantum numbers, orbital shapes, physical meaning of the electron spin) which arise from the treatment of the hydrogen atom with relativistic quantum mechanics neither coincide nor are in a one-to-one correspondence with the 'picture' that emerges from Schrödinger's wave mechanics (McKelvey, 1983).

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Appendix 1. *The Questions of the Written Questionnaire that Are Not Dealt With in this Study*

A1. Arrange sub-shells 3d, 2p, 5s, 4p, 5f, 3p, 4d, 4s, and 2s in order of ascending energy for any atom, except hydrogen. [*Acceptable answers:* 74.4%; *no answer:* 1.6%; *unacceptable answers:* 24.0%]

A2. Find the electron configuration for the chromium atom (Z = 24). How many unpaired electrons exist in the atom of this element? [*Acceptable answers*: 56.8%; *acceptable answers to one part only:* 27.2%; *no answer:* 1.6%; *unacceptable answers:* 14.4%]

A3. State the Heisenberg uncertainty principle. [*Acceptable answers:* 61.6%; *no answer:* 18.4%; *unacceptable answers:* 20.0%]

A4. What is the physical meaning of each of the four quantum numbers? [*Acceptable answers:* 59.2%; *no answer:* 4.0%**;** *unacceptable answers:* 36.8.0%]

A5. The Schrödinger equation can be solved exactly for the hydrogen atom, but only approximately for all other atoms. Do you know for what reason the equation cannot be solved in the case of the other atoms? [*Acceptable answers:* 35.2%; *no answer:* 41.6%**;** *unacceptable answers:* 23.2%]

A6. In one school chemistry text for twelfth grade it is stated that "The exact size of the orbitals is impossible to show, since we have said the probability of finding the electron does not become zero even at long distances from the nucleus." How is this shown or should be shown in the shapes of the orbitals? [*Acceptable answers:* 64.8%; *no answer:* 18.4%**;** *unacceptable answers:* 16.8%]

C1. The order you wrote in answering question **A1** is different in the case of the hydrogen atom. Which is the order now? Do you know for what reason hydrogen is differentiated? [*Acceptable answers:* 9.6%; *no answer:* 45.6%; *partially acceptable answers:* 4.0%;

unacceptable answers: 40.8%]

C2. Is the ground-state configuration $2s^2\ 2p_x^1\ 2\ p_y^1$ for the valence shell of the carbon atom in agreement with the fact that carbon forms four covalent bonds, e.g. in CH_4, as well as with the tetrahedral arrangement of these bonds, with all angles HČH equal to 109^o? Explain. [*Acceptable answers:* 22.4%; *no answer:* 46.4%**;** *unacceptable answers:* 31.2%]

C5. Supposing that one could take a photo of the electron as it moves around the nucleus, how could you construct the picture of the electron cloud? (HINT 1: The picture of the cloud is stable - still. –HINT 2: A camera takes still pictures. HINT 3: Photos can be either prints or transparencies.)

[*Acceptable answers ("I would take many photos of the electron printed on transparent paper, and then I would superimpose all these photos."):* 12.8%; *no answer:* 28.0%; *irrelevant answers (electron cloud drawn):* 41.6%; *irrelevant answers (Bohr or hybrid model drawn):* 13.6; *unacceptable answers:* 4.0%]

Appendix 2. *The 23 Students of our Study and their Performance in the Written Questionnaire*

The following table lists the 23 students who participated in the interviews and their percent performance in the algorithmic/recall of knowledge and in the conceptual questions. Two percent marks are given for each student: the first mark is for the average for the five algorithmic/knowledge recall questions; and the second mark is the average for the nine conceptual questions.

Group Interviews							
CHE group	Antonis	100	55.6	BIO2 group	Stathis	60	77.8
	Manolis	100	44.4		Alexia	100	44.4
	Christina	80	22.2		Danae	60	55.6
MAT group	Tania	80	44.4		Stavros	100	11.1
	Lampis	70	33.3	BIO3 group	Isidora	80	55.6
	Natalia	40	50.0		Ioanna	60	66.7
BIO1 group	Leonidas	90	66.7		Dimitra	80	44.4
	Eleni	100	44.4	*Individual Interviews*			
	Themis	100	33.3	CHE	Pavlos	90	22.2
	Irene	70	50.0		Marios	60	33.3
				MAT	Lazaros	80	22.2
					Haris	80	22.2
				BIO	Martha	100	33.3
					Petros	40	44.4

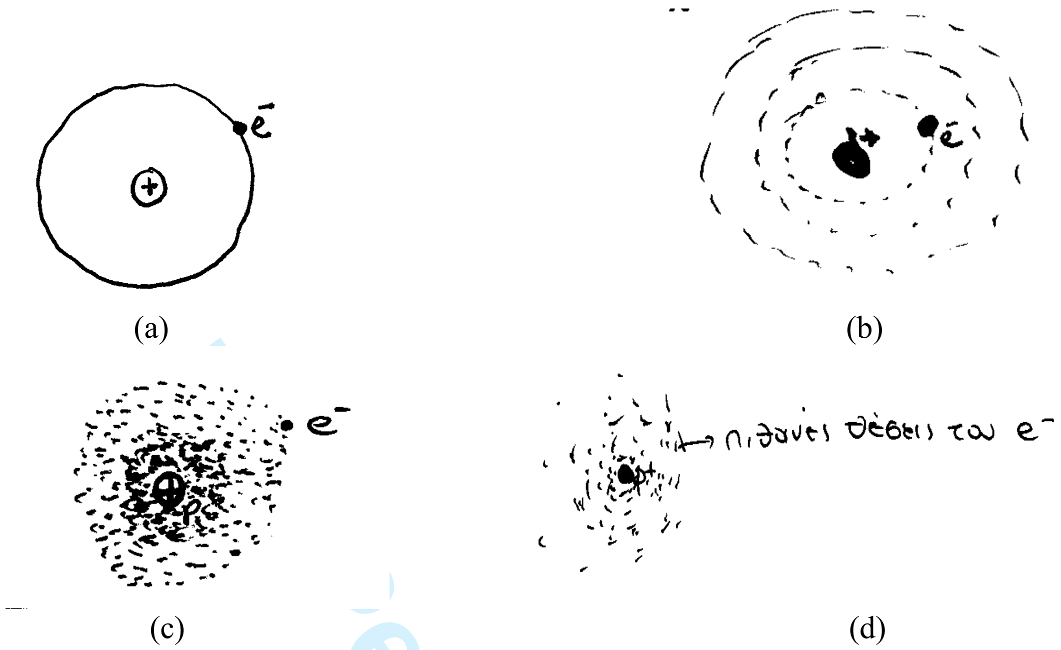
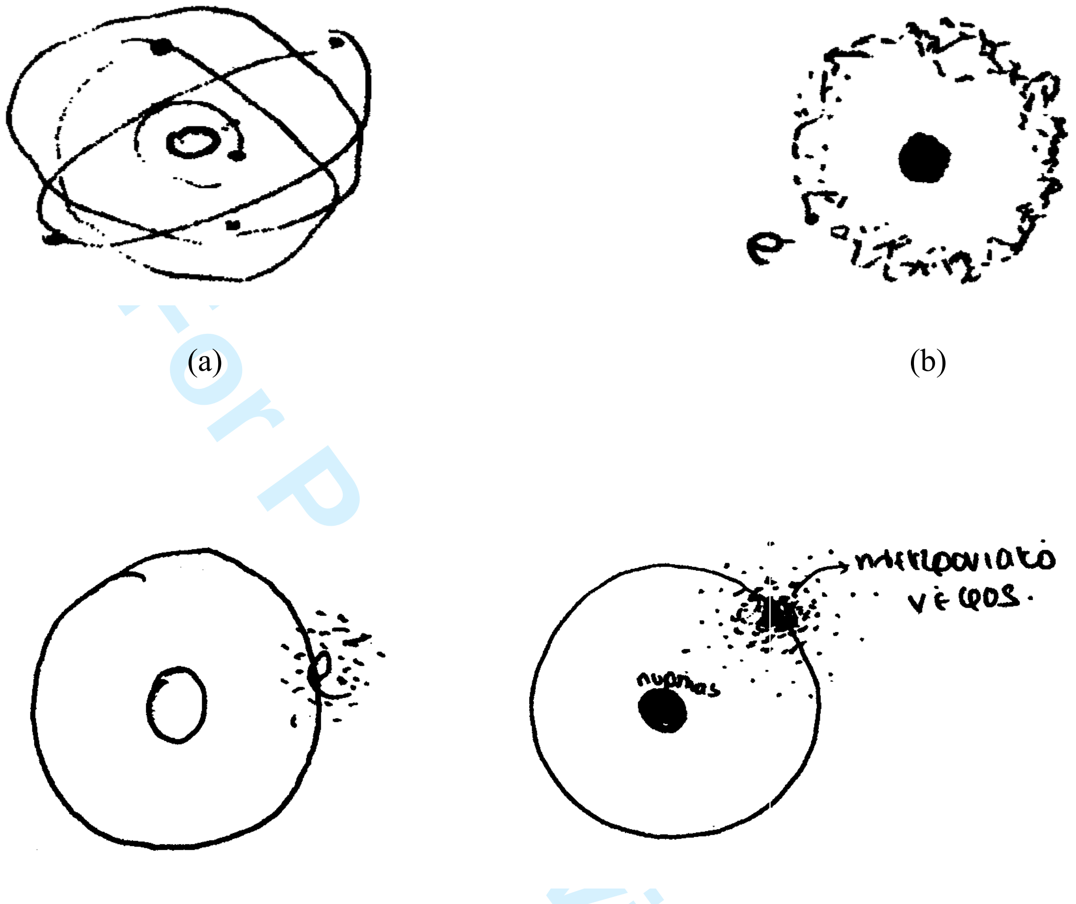


Figure 1. Indicative drawings/answers to question C0 (“Make a drawing depicting the hydrogen atom as you imagine it is in reality”). Drawings (a) and (b) are according to the planetary model. Drawings (c) and (d) show the electron cloud, with (c) showing also the elecron localized. The comment “probable positions of the electron” is added in (d)

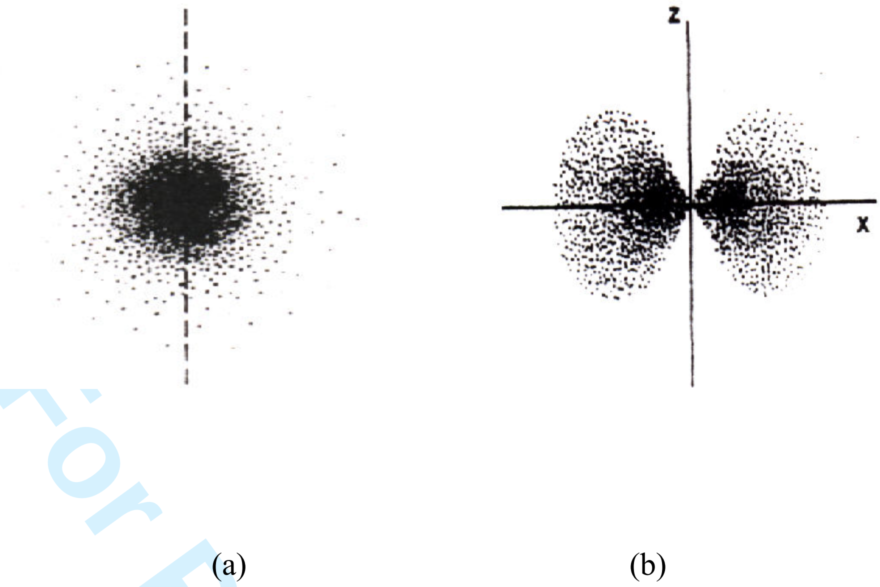
Figure 2. Consecutive representations of the hydrogen atom by Constantinia (BIO1 group) during the interview. (The first drawing was her answer in the written questionnaire.)



(a) (b)

(c) (d)

Figure 3. Indicative drawings/answers to question C5 (“Supposing one could take a photo of the electron … How could you construct the picture of the electron cloud?”). [The comment “electron cloud” is added in (d)]



(a) (b)

Figure 4. The two pictures of Question 6, showing the electron clouds in the 1s and a 2p orbital respectively [taken from the students' textbook (Mavromoustakos et al., 1999, pp. 7 & 8)].

Table 1: Change in student ideas for the uncertainty principle

Option (a)		Option (b)		χ^2
Before	After	Before	After	
9	11	8	6	0.486*

* $\chi_{0.95}^2 = 3.84$ (d.f. = 1)

Table 2: Change in student ideas for the nature of orbitals

Deterministic interpretation		Intermediate interpretation		Probabilistic interpretation		χ^2
Before	After	Before		Before	After	
7	0	4	2	6	15	11.52*

* $\chi_{0.995}{}^2 = 10.6$ (d.f. = 2)

Table 3: Change in student ideas for the atomic model

Planetary model		Intermediate model		Quantum mechanical model		χ^2
Before	After	Before	After	Before	After	
12	0	0	6	5	11	20.25*

* $\chi_{0.995}^2 = 10.6$ (d.f. = 2)