A developmental research on introducing the quantum mechanics formalism at university level

Koopman, L.

Citation for published version (APA):

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Chapter 2

Literature review

In this chapter we review relevant literature on quantum mechanics education research (Section 2.1) and quantum chemistry education research (Section 2.2). For each subject we discuss the following categories: misconceptions, conditions for prior knowledge, student conceptions and conceptual understanding, assessment tools and new instructional models and methods. For quantum mechanics there is a category on computer assisted instruction, and for quantum chemistry a category on textbooks. These categories are motivated below. Some literature might belong to more than one category, but in such a case it is discussed in the most relevant category.

Research into students’ misconceptions, or alternative conceptions, might be seen as a starting point for research into how students learn a new subject. By revealing alternative conceptions, we can get an impression of the things that students apparently find difficult. Also, the alternative conceptions are an indication of “what goes wrong”, or where teaching has an undesired outcome. However, knowing what misconceptions students have does not necessarily inform us why students have these misconceptions. For example, a misconception might be explained by viewing students as holding on to a different, inappropriate paradigm (Posner, Strike, Hewson, & Gertzog, 1982). Alternatively, the misconception might be explained by viewing it from a language perspective. The misconception can then be explained by assuming that teacher and student speak a different language, or use terms with a different meaning (Klaassen & Lijnse, [1996]).

In part misconceptions, or alternative conceptions, can be seen as resulting from earlier experience, either from every day life or prior education. Using the word misconception focuses on what incorrect conceptions students might have that hinder learning. Conversely, students may need to understand certain concepts prior to learning a new subject, such as quantum theory. This focuses on finding the conditions for prior knowledge, or prerequisites, when learning quantum mechanics. Concepts and knowledge may be tagged as prerequisite if a poor understanding of the prerequisite results in difficulties
learning quantum theory.

Research into students’ misconceptions and alternative conceptions mainly focuses on a current state of students’ understanding of a certain topic. It is interesting to study how these alternative conception develop, and how they are formed as a result of particular teaching. We discuss this under the heading of **student conceptions and conceptual understanding**.

**Assessment tools** are valuable as a research instrument, especially with large groups of students. With the Force Concept Inventory for classical mechanics [Hestenes, Wells, & Swackhamer, 1992] as example, there has also been an effort to develop assessment tools to measure conceptual understanding of quantum mechanics. These tools are particularly valuable to compare different teaching practices and expose common misconceptions. As found by [Johnston, Crawford, and Fletcher, 1998], passing exams is no guarantee for deeper conceptual understanding. Therefore, carefully designed tests may focus on conceptual understanding. Concept tests may also reveal the (conceptual) development of students throughout their academic career.

Some experimental, **new instructional models and methods** for teaching quantum mechanics, and quantum chemistry already have been developed. Some of these methods take into account the available research literature on students’ learning difficulties.

For quantum mechanics we review several instructional approaches that are based on **computer assisted instruction**. We focus only on methods that help students understand the formalism of quantum mechanics and on visualization methods of atomic, or molecular orbitals. The research discussed here is equally relevant for quantum chemistry education.

For quantum chemistry we could find several studies that analyze **textbooks**. A similar analysis on quantum mechanics textbooks was not found.

### 2.1 Quantum mechanics education research

Quantum mechanics education has received some well deserved attention from the physics education research community, especially in the last decade. This section gives an overview of this effort, focusing on literature that was considered relevant for the context of this research (as explained in Chapter 1.3).

#### 2.1.1 Misconceptions

Reports on students’ misconceptions can be found in numerous studies, we here discuss three. [Styer, 1996] provides a detailed list of 15 common quantum misconceptions, mostly regarding the formalism of quantum mechanics. This study is thus relevant to education at the university level. How common these misconceptions are is not clear; the list is the result of observations of the author. However, these misconceptions are a useful starting point for further investigation and an interesting suggestion is made how to address them:
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A very effective strategy is to assign a traditional quantitative/analytical problem that renders the misconception concrete. [...] The best such problems are those that lead to one answer if the misconception is followed and to a different one if the correct path is taken. These problems demonstrate that misconceptions are of operational as well as conceptual importance. (p. 31)

Precisely how effective such a strategy is, is of course not easily answered. Singh, Belloni, and Christian (2006) implement this method in so-called Quantum Interactive Learning Tutorials (QuILTs). The QuILTs give students feedback that may reveal possible misconceptions. This study will be further discussed in Section 2.1.6.

A more systematic, research based analysis of misconceptions related to the formalism of quantum mechanics can be found in Singh (2001) for advanced undergraduates and in Singh (2008b) for beginning graduates. The first study focuses mainly on quantum measurement and time development. An interesting conclusion of the second study is that students tend to inappropriately overgeneralize concepts learned in one context to other contexts. Both studies present a detailed list of misconceptions expressed by students on quantum measurement and time development of quantum states related to the formalism of quantum mechanics.

The misconceptions discussed in the studies mentioned here mostly relate to the formalism of quantum mechanics. On high school level education, the formalism normally gets less emphasis, if it is discussed at all. Ireson (2000) tries to identify what high school students understand of quantum mechanics, before and after a teaching unit on “quantum phenomena”. Students were given 40 statements with a five-point Likert scale from “strongly agree” to “strongly disagree”. The analysis identified different clusters of student thinking. For the post-questionnaire, these clusters are: quantum thinking, conflicting quantum thinking, and conflicting mechanistic thinking. Of course these results are limited by the statements that were given to the students. Nevertheless, they do reveal the discrepancy between what was meant to be taught and what students appear to have understood.

Some of the misconceptions that are reported in the above studies have also been found in this research (see Chapter 4). However, the university level studies focus mainly on the formalism of quantum mechanics. There do not appear to be studies on misconceptions related to the conceptual understanding of quantum mechanics at the university level, for instance to see how students conceptualize the wave function. This will be the main topic of Chapters 7 and 8.

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1Quantum measurement relates quantum states to observables (through operators) and possible measurement outcomes (through eigenvalues of these operators).
2.1.2 Conditions for prior knowledge

Understanding the Schrödinger equation requires students to understand potential energy. A good understanding of the relation between potential energy and the resulting classical movement of an object is thus important (Redish, Lei, & Jolly, 1997; Jolly, Zollman, Rebello, & Dimitrova, 1998). In particular, it is important for students to be able to interpret potential energy diagrams. For a classical system, using such a diagram, we can “read off” the movement of a particle in the potential given. With a total energy given, we can infer what the particle’s kinetic energy is, and thus its speed when subject to the potential given. Quantum mechanically, a similar reasoning is possible, however, we then need to understand what the effect is on the probability. Bao and Redish (2002) argue that in order for students to understand quantum probability, they first should understand how we can describe classical motion using the concept of probability. Thus, potential and kinetic energy determine the “motion” of particles, both classically and quantum mechanically, although differently in each formalism. Part of the approach described by Bao and Redish (2002) is implemented in the teaching design, described in Chapter 6.

For students to understand “wave mechanics”, as quantum mechanics is often named, they should understand the properties of classical waves (Steinberg, Wittmann, Bao, & Redish, 1999; Vokos, Shaffer, Ambrose, & McDermott, 2000). For instance, students were found to think that the amplitude of light is a spatial, instead of an electromagnetic quantity. When discussing photons, students incorporate these “incorrect” ideas in the quantum and for instance think that photons move along a sinusoidal path (Steinberg et al., 1999). The same has been observed for electrons in our research (Chapters 4 and 8). The difficulties students have with the wave nature of light and the interference of waves have been related to understanding diffraction and interference of particles (Vokos et al., 2000). This study also reports on the inability of students to use the de Broglie wave length to reason how electrons interfere and diffract. Students seem to view the de Broglie wave length as a fixed property of quantum particles, instead of varying with the particle’s momentum. This is to be expected, as students are often presented with problems in which they have to calculate the de Broglie wave length of, say, an electron with a certain speed. When introduced to the formalism of quantum mechanics, it is easily forgotten that the wave function (describing an electron) has a varying “de Broglie” wave length. Hence, we cannot say the electron has a certain de Broglie wave length. In the teaching design described in Chapter 6, the de Broglie wave length is first related to a wave function with a fixed wave length. When constructing the Schrödinger equation, this wave function with fixed wave length is chosen as a solution when the potential energy function (potential) is a constant. An inductive step is made allowing potentials that vary as function of the location \( x \). In general, wave functions that are solutions for such cases will have a varying wave length.

As will be argued in Chapter 5 when quantum mechanics is taught using
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A more quantitative approach, as is done in university level courses, proper mathematical skills are an important prerequisite (Koopman, Brouwer, Heck, & Buma, 2008). Transfer from calculus to quantum mechanics does not occur all by itself. Moreover, when students are able to perform the basic calculations with some fluency, more time can be spent on quantum mechanics. Some remedial activities may therefore be needed to help students improve their mathematical skills.

Learning quantum mechanics thus relies on students’ prior knowledge of classical mechanics as well as on their mathematical skills. Although this is a general result of educational psychology (as discussed in Chapter 3), some scholars draw different conclusions. For instance, Fischler and Lichtfeldt (1992) conclude that reference to classical physics should be avoided. This will be further addressed in Section 2.1.5.

2.1.3 Student conceptions and conceptual understanding

In Johnston et al. (1998) third year undergraduate students were interviewed after having followed several courses involving quantum mechanics. The aim was both to determine whether students’ understanding could be considered correct, as well as to give a (phenomenographic) description of their conceptions. It is found that students’ knowledge of quantum mechanics mainly concerns isolated facts, weakly linked to each other. It is concluded that their mental models are fragmented. Furthermore:

...we have found little evidence in this research of a ‘deep’ approach to learning. This is of great concern because these students were about to graduate from the top physics class in a university of world-class standards. These are ‘good’ students on all criteria used by ordinary university physics departments to define ‘goodness’. Clearly, there is need for research into the question of whether our assessment practices do not sufficiently reward deep learning. (p. 442)

The conclusion is disconcerting: students can pass exams with good grades, but nevertheless, their understanding (mental models) remains fragmented. As will be argued in Chapter 9 such a fragmented mental model is likely to result in low retention of learned content and might even be an indication of rote learning.

In Petri and Niedderer (1998) one high school student (Carl) is followed throughout a grade-13 course on (quantum) atomic physics. The course runs for 16 weeks and uses an atomic model based on the Schrödinger equation. The study tries to describe Carl’s learning pathway during the course by identifying his changing conception of the atom. These conceptions are linked to the teaching unit. Four intermediate conceptions of the atom are identified, as well as a final conception. Carl’s initial conception is that of a planetary model. Subsequent conceptions are found to be an incorporation of the
teacher’s explanation in Carl’s existing conception (i.e. the planetary model). For instance, in Carl’s second conception of the atom the wave function’s maxima define the electron’s orbits. The final conception is found to be an “association of co-existing conceptions” (p. 1083). Where an association is “when several conceptions co-exist and are connected to form different layers of the cognitive system, with a metacognitive layer on top” (p. 1083). As the authors report that “Carl was able to reflect on differences, problems and advantages of each conception” (p. 1083), these layers of the cognitive system are presumable connected, enabling a switching between them. This article is in line with the findings of McKagan, Perkins, and Wieman (2008), discussed in Section 2.1.5 and indicates the importance of addressing models explicitly when teaching quantum mechanics. In our design (Chapter 6), students are guided to construct a model of quantum mechanics themselves, involving them in the choices that can be made when constructing this model.

A study on university level quantum mechanics tries to construct students’ conceptions of quantum objects (Mannila, Koponen, & Niskanen, 2002). The study identifies description categories with which student responses can be described. These categories are: (a) quasi-classical, (b) trajectory based, (c) statistical (or probabilistic), and (d) quasi-quantum. Categories (a) and (b) are found to describe most student responses, i.e. students hold on to a classical view of quantum objects. This finding corroborates the results as for example reported in Johnston et al. (1998) and Ireson (2000).

Olsen (2002) reports on how high school students conceptualize the wave-particle duality and, more generally, what conception they have of light and electrons. After instruction, students appear to view light and electrons asymmetrically: electrons are conceptualized primarily as particles and light as having a dual nature. Furthermore, the idea that a particle has wave-like properties is understood to mean that they move in a wave-like manner. This is analogous to what Steinberg et al. (1999) observed for photons and it was also observed in various rounds of this research (Chapters 4 and 8). It may thus be concluded that new information (e.g. about the wave-particle duality) seems to be incorporated in an existing cognitive structure, leaving the meaning of this structure intact, instead of assimilating this cognitive structure. In short, assimilation is the process in which new information is linked to relevant, existing concepts in cognitive structure, where both the new information and the cognitive structure are modified (Ausubel, Novak, & Hanesian, 1978, p. 68, see also Chapter 3).

Quantum tunneling is a conceptually difficult topic when learning quantum theory. Morgan, Wittmann, and Thompson (2004) have found that students think that energy is lost in the tunneling process. This can be linked to the use of combined energy-wave function diagrams, where there are actually two vertical axes: one for the (potential) energy and one for the wave function. Because of the decaying form of the wave function in the potential barrier, students might incorrectly think that energy is lost in the barrier. The research also reveals that students seem to reason with an analogy of a mountain through
which the quantum particle (literally) tunnels: only the width of the mountain, not its height, influences the energy that is lost during the passage. In a follow-up study, the development of thinking about tunneling is studied by following one student during three years of education (Morgan & Wittmann, 2006).

Many of the studies here discussed seem to have in common that they view learning quantum mechanics as the transformation of students’ conceptions from a classical to a quantum viewpoint. Experimental instructional models exist that try to accomplish such a “conceptual change”. These will be discussed in Section 2.1.5.

### 2.1.4 Assessment tools

Cataloglu and Robinett (2002) developed the Quantum Mechanics Visualization Instrument (QMVI) to identify conceptual and visualization understanding of students during the undergraduate career. The test contains 25 multiple-choice questions, each presenting the student with a graphical representation of the wave function, sometimes in combination with the potential energy function. The questions thus focus on students’ conceptual understanding, as the questions do not require students to perform any complicated calculation. The development and validation of the test are described in Cataloglu (2002). Parts of this test have been used in this research (Ch. 8 and Ch. 9).

In McKagan and Wieman (2006) work on the Quantum Mechanics Conceptual Survey (QMCS) is announced. The QMCS is a multiple-choice test to measure basic concepts in quantum mechanics. It is in part based on other tests, such as the QMVI, mentioned above. The test can be retrieved online, by requesting access from one of the authors (http://per.colorado.edu/QMCS). A more recent use of the QMCS can be found in Carr and McKagan (2009).

A more recently developed test by Wuttiprom, Sharma, Johnston, Chitaree, and Soankwan (2009) is the Quantum Physics Conceptual Survey (QPCS), aimed at students’ understanding of introductory quantum physics concepts. The test covers five themes: the photoelectric effect, waves and particles, de Broglie wavelength, double-slit interference, and the uncertainty principle. A distinction is made between non-interpretive and interpretive questions. The latter being questions whose answer can be argued about, depending on the interpretation used. The study suggests a special relation between these two types of questions. Students can perform well on the non-interpretive questions, without necessarily doing well on the interpretive questions. Conversely, good results on the interpretative questions correlates with good results on the non-interpretive questions. We can interpret this result in two ways. Firstly, non-interpretive questions may be seen as prerequisite to questions of an interpretive kind. If this is the case, this might be an argument to first focus on the formalism of quantum mechanics and address its interpretation later. Secondly, the non-interpretive questions might be answerable following recipe-like rules, without having to worry too much about their meaning. In Chapter 3...
we consider how the interpretation of quantum mechanics might be related to understanding. We will also see that interpretation plays a role in our teaching design, as explained in Chapter 7.

2.1.5 New instructional models and methods

An early and influential contribution to the literature on quantum mechanics teaching design is given by Fischler and Lichtfeldt (1992). This study is aimed at high school instruction. The authors identify two problematic topics, traditionally discussed in high school instruction that hinders students in adopting a quantum view: the Bohr model and the wave-particle duality. They state that:

An approach which prevent students from attempting to understand the phenomena of quantum physics in terms of the conceptions of classical physics will have to proceed from the following basic premises:

(a) Reference to classical physics should be avoided.
(b) The teaching should begin with electrons (not with photons when introducing the photoelectric effect).
(c) The statistical interpretation of observed phenomena should be used and dualistic descriptions should be avoided.
(d) The uncertainty relation of Heisenberg should be introduced at an early stage (formulated for ensembles of quantum objects).
(e) In the treatment of the hydrogen, the model of Bohr should be avoided. (pp. 183-184)

These premises formed the basis of an experimental teaching design, which was compared to a conventional teaching approach. From evaluations, the authors conclude that after instruction more students from the experimental group show a conceptual change towards quantum thinking. However, the premises seem to be stronger than need to be. Several (experimental) teaching approaches exist, discussed in some detail below, that deviate from the premises and nevertheless report good results. Müller and Wiesner (2002) drop (b) and the second part of (c). Kalkanis, Hadzidaki, and Stavrou (2003) strongly oppose premises (a), the second part of (c), and (e). McKagan and Wieman (2006) explicitly discusses the Bohr model, thus “violating” premises (a) and (e). However, again, all of these studies, including Fischler and Lichtfeld’s, report good results. This might be an indication that detailed lists of do’s and dont’s are not helpful. This might be expected as there are so many variables involved. This is an argument for research based information on how to use a certain approach successfully. More specifically, in the above case, it is more informative how (and why) the Bohr model can be taught effectively, instead
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Müller and Wiesner (2002) report on an introductory course divided in two parts. The first part is addressed mainly to non-physicists with emphasis on qualitative reasoning. Photons and electrons are discussed to let students develop a conceptual understanding of the main characteristics of quantum mechanics: wave-particle duality, Born’s probability interpretation and quantum observables. The authors have chosen the statistical ensemble interpretation of quantum mechanics (Ballentine 1970), because it “provides a clear and comprehensive way of talking about quantum phenomena” (p. 202). To let students explore the quantum phenomena, use is made of computer based, “virtual laboratories”. The qualitative introduction is followed by a second part, aimed at students with a special interest in physics. Based on the qualitative discussion from the first part, the second part introduces the formalism of quantum mechanics. This sequence has been evaluated using a pre-/post-test with statements to determine the degree to which students think “classically”, or “quantum mechanically”. Results show that after the course, students thinking can be characterized mainly as “quantum”.

Zollman, Rebello, and Hogg (2002) developed a “hands-on” approach in learning quantum mechanics, initially intended for high school and non-science majors, but later expanded and adopted for undergraduate physics majors. With the hands-on approach, students work on experiments or computer visualizations. The credo is: do experiments first, then let students think and explain. As such, this approach is also qualitative and focuses on conceptual understanding:

Sometimes students learn the mathematics of quantum mechanics and not its conceptual basis or applications. We do not want this situation, so we introduce devices whose operation can be understood conceptually and can be explained only with quantum mechanics. (p. 253)

Kalkanis et al. (2003) signal physics education’s need for a qualitative approach to the quantum mechanics world view, which warrants a reform of science education. They argue that this reform requires appropriate teaching to in- and preservice teachers. On epistemological grounds, they argue that classical and quantum mechanics should be viewed as two totally independent conceptual systems. For learners to adopt the quantum mechanical world view, a paradigm shift is needed. This places their approach in the tradition of Posner et al. (1982). The best way to achieve this paradigm shift is to contrast quantum mechanics to classical mechanics, and thus force learners to “radically” change their views, as opposed to a more gradual change. This radical change is achieved by contrasting Bohr’s semiclassical atomic model to the modern physics model of the atom.

Related to the design of Kalkanis et al. (2003) is McKagan, Perkins, and Wieman (2008), whose goal it is to design a teaching sequence that successfully teaches the Bohr model. The question they want to answer is whether
teaching the Bohr model is an obstacle to learning the Schrödinger model of the atom. In other words, they want to test premise (e) from Fischler and Lichtfeldt (1992). The study reports on a teaching design in which several models of the atom are compared and contrasted. There is thus an explicit focus on models’ limitations. The models discussed are: Democritus’ billiard ball, Thomson’s plum pudding, Rutherford’s solar system, Bohr’s, de Broglie’s, and Schrödinger’s model. In the final exam special questions were asked that forced students to use a specific model of the atom. From the results it becomes clear that a majority uses Schrödinger’s model. Furthermore, many students use multiple models, by either blending models, or by comparing and contrasting models. Although the Bohr model has been taught, this did not appear to hinder students in adopting Schrödinger’s model of the atom. The findings of this article are supported by Frederiksen and White (2002), who focus on linkage between models.

Carr and McKagan (2009) report on a complete curriculum reform for university, graduate level quantum mechanics: course content, textbook, teaching methods, and assessment tools have been reviewed and modified, based on (physics) education research. The goal of the graduate reform was to cover not only the foundational period of quantum mechanics (shortly after the formulation of the Schrödinger equation), but also subsequent periods, up to modern applications of quantum mechanics in quantum information processing and quantum encryption. This effort is interesting because it involves multiple years, with many teachers, and tries to address the teaching as a whole. The reform was evaluated using two concept tests: the QMCS, as introduced in Section 2.1.4, and the Graduate QMCS (GQMCS), which was developed to better test the material covered in graduate quantum mechanics. Basic conceptual understanding of quantum mechanics did not progress during the three years of graduate instruction. Furthermore, the QMCS did not correlate with the final exam score. From these findings, the authors conclude that basic conceptual understanding is not improved by and does not improve students performance on advanced graduate courses. On the other hand, the results to the GQMCS show a strong correlation with the final exam score. Because 75% of the final exam consisted of calculations, the authors conclude that “this result reinforces other research demonstrating that conceptual knowledge can improve the student’s ability to perform calculations” (p. 314). In Chapter 8 we focus on the interplay between conceptual understanding of the wave function and applying the wave function in calculations (procedural fluency).

2.1.6 Computer assisted instruction

Because of the abstract nature of quantum theory, some have focused on computer assisted instruction. However, the pedagogical background varies. For instance, computer visualization may be used to augment the traditional textbook treatment of “simple” quantum models, as for instance the infinite square potential well and the harmonic oscillator (Thaller 2000, 2004). In this case
the computer is used to visualize the mathematical expressions that result from the quantum mechanical treatment. In line with this, a computer can also be used to visualize the hydrogen wave functions to study their properties in depth \cite{Broklová & Koupil, 2006}. In these cases we might say that we “only” add visualization to what we already know (i.e. the mathematical solutions to quantum systems).

Computer assisted instruction can also focus on simulating quantum phenomena, or experiments \cite{Rebello, Sushenko, & Zollman, 1997; Zollman et al., 2002; McKagan, Perkins, Dubson, et al., 2008}. A simulation in this context is a model of reality enabling the student to investigate and discover the properties of quantum phenomena. One example used in this research is the simulation of the photoelectric effect (Chapter \ref{ch6}). Another method to “capture reality”, is to digitize a real experiment \cite{Bronner, Strunz, Silberhorn, & Meyn, 2009}. Here a real experiment is set up and it’s settings and outcomes are recorded and implemented in interactive software. This way, the student can “repeat” the experiment and change it’s settings. Somewhat related to this category are \cite{Jolly et al., 1998} and \cite{Bao & Redish, 2002}, where the computer is used to let students develop an understanding of classical prerequisites to quantum theory, respectively: potential wells and probability. The latter is implemented in the teaching approach described in Chapter \ref{ch6}.

Another focus for computer assisted instruction is to give instant feedback to students when learning quantum mechanics. For instance, \cite{Singh, 2008a} has developed quantum interactive learning tutorials, so-called QuILTs, where students have to first express what they expect will happen in specific situations and next, compare their expectations to the outcome on the computer screen. This is particularly useful to accommodate the observed fact that students tend to inappropriately overgeneralize what they have learned earlier \cite{Singh et al., 2006}. The QuILTs give students the opportunity to revise their ideas, or possible misconceptions, by making these generalizations explicit and checking them using a visualization. In Chapter \ref{ch10} we propose to use QuILTs after students have been introduced to the formalism of quantum mechanics.

2.1.7 Conclusions

What conclusions can we draw from this review of literature on quantum mechanics education? We might identify the following two main perspectives.

First, learning quantum mechanics is viewed as a conceptual change process. New cognitive structures are needed to understand quantum phenomena. Old cognitive structures, either stemming from prior education in classical mechanics or everyday experience, need to be adjusted. Opinions on how this process should take place vary from a gradual adjustment, to radical change. There is also no general agreement on how classical and quantum physics should be represented in cognitive structure. Although quantum theory is radically new compared to classical mechanics, the conceptual change focus does not seem to be unique to learning quantum mechanics, it is also applied...
to learning classical mechanics for instance.

Second, there is much research that identifies a tension between working with the quantum formalism on the one hand, and conceptual understanding of quantum theory on the other. There are various reports that a focus on the former does not necessarily benefit the latter. Singh (2001) neatly formulates this as:

Although students in advanced quantum mechanics courses may have learned to solve the Schrödinger equation with complicated potentials and boundary conditions, many have difficulties with conceptual understanding of quantum measurements and time development. (p. 892)

Again, this tension does not only seem to be relevant for learning quantum theory. It has been reported in the teaching of other areas of physics as well. Paul Hewitt’s Conceptual Physics in fact has a goal to “fix” this focus to “plug and chug” (Hewitt, 2009).

Both these perspectives are relevant for the current research, and have played a role in our teaching design. The first, when introducing this new subject to students, the second when students advance to the formalism of quantum mechanics. These perspectives also show an apparent dichotomy in the research literature. One either takes as starting-point the quantum formalism, and students need to work with it (e.g. Singh 2008a). Or one focuses on quantum phenomena from which students are expected to learn how nature behaves (e.g. Zollman et al., 2002). It would be interesting for students to study how the phenomena lead to the formalism of quantum mechanics. This is in part implemented in the teaching design, described in Chapter 6.

Apart from these two main perspectives, we can also draw some more general applicable conclusions. First of all, several studies report on how what is taught differs from what is learned. This warrants the need for accurate and practical assessment tools. Also, it shows the need for feedback during instruction. Feedback not only informs the teacher of the conceptions students form, but also informs students whether their conceptions are accurate or not. Also, students’ prior conceptions influence the learning of quantum mechanics.

2.2 Quantum chemistry education research

A large part of this research has been carried out in a course on quantum chemistry. For chemists the main motivation to study quantum theory is to understand chemical bonding. From a physicist’s perspective, quantum chemistry is “just” quantum theory applied to a chemistry context. In other words quantum chemistry might be “simply” reduced to quantum physics. Then quantum chemistry education might be expected to include the same issues as quantum mechanics education. However, both statements do not seem to hold. First, quantum chemistry is not reduced to quantum theory (Scerri
Second, teaching quantum chemistry in general and bonding in particular has its own learning and teaching difficulties, as we shall see in the current section. For example, it seems that in chemistry education, when explaining bonding, more use is made of models than in physics education, when teaching quantum mechanics. This section briefly discusses some of the issues around the teaching of chemical bonding as found in the literature. We use the same categories as in the literature review on quantum mechanics education, except for “computer assisted instruction”. There is an additional section on chemistry textbooks.

2.2.1 Misconceptions

A literature review on students’ misconceptions on chemical bonding for different levels of education is given by Özmen (2004). Three of the studies reviewed are discussed here in more detail. They play a role in Chapter 8 when we consider how quantum mechanics is used to explain bonding.

Taber (1998) reports on a study in which 15 A-level (high-school) students were interviewed on their understanding of chemical bonding. Alternative conceptions might be logically connected forming a coherent alternative conceptual framework. Using a grounded research approach, it is found that the basis of this alternative conceptual framework is formed by the octet rule. Perhaps not surprising, as the octet rule plays a prominent role in teaching chemistry at high school. However, “[t]his framework includes notions that are incorrect, but also perceptions that would better be described as partial perspectives or limited understandings” (p 601). For example, students view electrons in a covalent bond as belonging to either of the bonded atoms (p. 602). Related to this is that students consider electrons to have a personal history, as students talk about electrons returning to their own atoms (p. 604). Both conceptions might imply that students think that electrons can be distinguished from each other. In quantum mechanics, the Pauli exclusion principle relies on the notion that this is not possible. As another example, students consider atoms instable when their outer shell is not full. This idea is so strong that students were found to consider the sodium-seven-minus ion (Na\(^{7-}\)), with an electronic configuration of 2.8.8., more stable than a sodium atom (p. 603). The octet rule framework and its full shells principle explains many of the observed alternative conceptions students have. It appears to be a very strong and persistent conception in students. Understanding this may be useful when designing education on this subject. Furthermore, it might be expected that this will play a role when learning quantum mechanics. It is expected that students will only appreciate quantum chemistry, when they see that this theory is more successful than the octet rule framework. This condition is also expressed by Posner et al. (1982) in their theory to accommodate conceptual change (see Section 2.2.6).

Nicoll (2001) interviewed 56 students from a university chemistry class on chemical bonding and the octet rule framework. The interview also focused on
how students conceptualized molecules, orbitals, bonding and electron motion at the microscopic level. The interviews were analyzed to identify categories of student misconceptions. We here discuss some of the misconceptions that are related to chemical bonding and which are relevant when learning quantum chemistry.

Students appear to have difficulties with several concepts describing bonding. For instance, students are unable to explain polarity in terms of electronegativity, or see polarity as a property of atoms, not molecules. Furthermore, definitions of ionic and covalent bonding are mixed-up. Finally, a valence bond is conceptualized as electrons being strictly shared between two atoms, instead of belonging to the entire molecule (p. 718). This misconception might be explained by two facts. First, the use of Lewis structure diagrams (octet rule framework), where bonds are drawn between two atoms, each of which is counted as two (valence) electrons. Second, it is explained by the finding of Taber (1998) that students tend to think that electrons “belong” to a certain atom and are thus distinguishable.

Some misconceptions were found that appear to relate to earlier discussion of Bohr’s model of the atom. For instance, students were found to view the atom as solar system: they conceptualize orbitals by electrons placed at a fixed distance from the nucleus. Related to this is that the bonding electrons in a molecule are visualized as orbiting the two nuclei at a fixed distance, describing a figure of eight pattern (p. 720). Although not mentioned in the article, this observation might also be related to the fact that $\pi$-bonds are often drawn as a figure eight in a 2D representation.

Most of these misconceptions are found to appear throughout the academic career and are thus resistant over time. However, this was not a longitudinal study and it is not clear how these misconceptions develop.

In a larger study, Birk and Kurtz (1999) administered a test to over 800 people, ranging from high school students to faculty members. The test measured both knowledge and understanding in the following six conceptual areas: bond polarity, molecular shape, polarity of molecules, lattices, intermolecular forces, and the octet rule. The results show that misconceptions occur on all levels, but decrease with years of experience (i.e. increasing level of education). The authors conclude:

Significant changes in numbers of misconceptions seem to occur after the first year of college chemistry and during the first year of graduate school. This observation supports long-term anecdotal evidence that general chemistry topics are not thoroughly understood until an individual has to teach those topics to others. (p. 128)

Furthermore, the results show that students perform better on items testing knowledge, than on items testing understanding. This might be expected, as understanding often implies, or requires knowledge. Being a cross-sectional study, this study shows that misconceptions occur at all levels. To really conclude whether a given misconception is truly persistent, a longitudinal study
would be needed. Such a study might also better reveal whether misconcep-
tion form during education, while others are resolved. After all, this might
also explain the above results.

2.2.2 Conditions for prior knowledge

Table (2005) provides a generic framework (called a topology) to describe
learning impediments explaining learning difficulties (see Figure 2.1). The
framework is more general than the heading of this section might suspect. It
not only incorporates conditions for prior knowledge, but also conditions for
current teaching practice. Impediments are either “null” (not enough link-
age with existing conceptual framework), or “substantive” (new material is
misinterpreted due to inappropriate existing conceptual framework). The null
learning impediments might be identified as our category “conditions for prior
knowledge”, whereas the substantial learning impediments roughly concern
misconceptions or alternative conceptions. The null learning impediments are
further subdivided in two categories. Relevant material might simply be miss-
ing from cognitive structure (deficiency impediment), or the cognitive structure
might be too fragmented (fragmentation impediment), resulting in poor (or
no) priming of relevant knowledge when students are confronted with new ma-
terial. The substantive impediments are subdivided in categories depending
on where the alternative conception originate from: either intuitive ideas from
every day experience (ontological impediment), or from earlier education. The
distinction is made, because a teacher might prevent impediments from the
latter category, whereas the first category is beyond his influence.

To show its validity, the framework is applied to learning the orbital model
of atomic and molecular structure. The data for this survey are taken from
an interview study among college students in the UK (aged 16–18) enrolled
in two-year “A level” courses. We summarize the null learning impediments,
as the substantive impediments have already been discussed to some extent in
Section 2.2.1

In learning about atomic structure, two learning deficiencies are discussed. The
first is the classical result that an electron orbiting a nucleus is an elec-
tronic oscillator, and electronic oscillators emit electromagnetic radiation, and thus energy. This is the problem that gave rise to the quantum postulates of Bohr. Taber argues that students who are not aware of this, do not see the need for the quantization of energy levels and will still consider the electron as a classical particle with some (continuous) energy. This learning deficiency also plays a role in our teaching design, when discussing the existence of energy levels (Chapter 6). Another deficiency has to do with the (classical) description of circular motion, which requires a central force which provides a centripetal acceleration. One student was found to explain why electrons will not fall into the nucleus even though there are “attractions from the nucleus, pulling in the electrons” as “the attraction isn’t that strong,” whereas “if you could actually physically make those electrons get closer to the nucleus then they would fall in because the attraction would be so strong.” This student is considered to have both learning deficiencies described here.

Taber (2005) gives several examples of “fragmentation learning impediments”. We summarize two here. The first example is from an interview in which the interviewer asks a student (Debra) whether it would be “possible to have an excited hydrogen atom? In electrical terms, can you excite a hydrogen atom?” (p. 101). Debra answers no. Then the interviewer asks a different question: “Have you done an experiment, in physics, not in chemistry, but in physics, where you have to work out spectral wavelengths? […] With a spectrometer, and you … measure angles, and work out the wavelengths of colors of light?” (p. 101). Debra remembers doing this experiment. The interviewer then repeats his initial question and now Debra is able to give a detailed answer. This shows that the knowledge was available in cognitive structure, but initially not connected to the question that was asked.

Another example is given by a student (Carol) describing the structure of the benzene molecule, where there was,

kind of like a ring [with] like electron thing underneath it, and electron thing on the top … the electron density below and above it … because they’re–bonds … and then you’ve got delocalized electrons in the middle, but I don’t know what they look like. (p. 101, original emphasis)

Taber explains why this is an example of a fragmentation learning impediment:

At this point, in her studies Carol had learned about the pi-bonding in benzene as two areas of electron density forming rings above and below the framework of carbon – carbon sigma bonds: however, she has not reconciled this with the circle sometimes used to represent the electrons that are not involved in the sigma bond framework. (p. 102)

For our context, these examples show the importance of relating to what students have learned during earlier education (either high school, or other university level courses). In Chapter 5 we describe our effort to refresh this prior knowledge.
2.2. Quantum chemistry education research

2.2.3 Student conceptions and conceptual understanding

Taber (2000) describes a case study in which one students’ explanation of chemical bonding is analyzed during a two year pre-university chemistry college course. When explaining bonding, this student was found to use three distinct explanatory principles, paraphrased in the article as:

- so that atoms could obtain full shells;
- to give a lower energy level;
- because of the attractions between charged particles. (p. 404)

The first principle was found at the start of the two year course and is also discussed under the heading of “Misconceptions” above as the full shells explanatory principle (see also Taber, 1998). The latter two principles were developed throughout the two year course. All principles are found to be stable alternative conceptions, because they extend over a period of months, are used as explanation in a range of chemical bonding contexts, and are often used alongside each other as explanation for the same specific example (i.e. they are alternative). Concerning the “correctness” of these explanatory principles, Taber concludes:

> From the perspective of orthodox chemistry, the octet rule explanatory principle is deeply flawed [. . .] and the minimum energy principle would not be considered to be independent of the Coulombic forces principle; but to [the student] himself, the three conceptions were viewed as alternative narratives that could be employed to make sense of chemistry.

Nevertheless, all explanatory principles are at some point in education considered valid. As Taber (1998) concludes that the octet rule principle is very stable in cognitive structure, advanced education in quantum chemistry should address how and why this principle is “deeply flawed” and how quantum chemistry is more successful and complete. Such an approach is described by Nahum, Mamlok-Naaman, Hofstein, and Kronik (2008), discussed in Section 2.2.5 below.

Stefani and Tsaparlis (2009) report on a phenomenographic study on students’ levels of explanations and conception of models in basic quantum chemistry. This article is interesting because it gives some insight into the connection between students’ idea of “model”, and their level of understanding. Nineteen second-year students were interviewed on the following topics: atomic orbitals, the Schrödinger equation, molecular orbitals, hybridization, and chemical bonding. The study classifies students reasoning using two dimensions: their view of models and their level of explanations. The latter indicating whether students’ understanding can be labeled as rote or meaningful (cf. Ausubel et al. 1978 discussed in Chapter 3). The following four levels of explanation are defined:
Level a “answers that consist of verbatim reproduction of words, terms and mnemonic rules” (p. 524);

Level b “answers that show evidence of verbatim reproduction of definitions or explanations from textbooks” (p. 525);

Level c “answers that consist of textbook knowledge, which, although directly reproduced, imply causality” (p. 525);

Level d “statements that imply causality and are not direct reproductions from textbooks” (p. 526).

The views of models are classified using the following three levels:

Level 1 At this level, models are seen as replica’s of reality;

Level 2 “Students do not adopt a full correspondence of models and physical entities. However, they do ascribe macroscopic properties to what is happening in the submicroscopic world. They consider models as useful scientific constructions, but the emphasis is still on reality.” (p. 527)

Level 3 “Students consider models as scientific constructions that possess the properties predicted and/or verified through scientific experimentation.” (p. 527)

The interview results were analyzed using the above two level systems, resulting in four categories of explanations. Table 2.1 lists the results. Both levels seem to correlate: the higher the level of explanation, the higher the level of models. Categories A and B are qualified as variations of rote-learning, while categories C and D are qualified as meaningful-learning. This finding shows the need to also address the nature of the models used in chemistry to explain bonding. Often these models are discussed isolated from each other, and are presented as fact. However, they are related and, being models, they are limited in their applicability. Again, this is addressed in the teaching approach described by [Nahum et al., 2008], discussed below in Section 2.2.5. In Chapter 10 we propose to use this approach after students have been introduced to the formalism of quantum mechanics.

2.2.4 Assessment tools

Many of the studies discussed in this section use diagnostic tests that might prove their use outside the context for which they were developed. We briefly mention three such tests that are relevant for our focus of quantum chemistry. All three tests consist of multiple choice, two-tier items: the first tier tests knowledge, and the second tier asks for an explanation of the first tier. [Birk and Kurtz, 1999], mentioned in Section 2.2.1 used a 15 item test on the following six conceptual areas: bond polarity, molecular shape, polarity of
2.2. Quantum chemistry education research

Table 2.1: Combined categories of explanations and models. 2(3) indicates a borderline state between level 2 and 3, with emphasis on level 2.

<table>
<thead>
<tr>
<th>category</th>
<th>level of explanations</th>
<th>level of models</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>a(b), b, or b(c)</td>
<td>1</td>
</tr>
<tr>
<td>B</td>
<td>b or b(c)</td>
<td>2</td>
</tr>
<tr>
<td>C</td>
<td>b(c), c or c(d)</td>
<td>2, 2(3), or (2)3</td>
</tr>
<tr>
<td>D</td>
<td>c(d), d</td>
<td>2(3), or 3</td>
</tr>
</tbody>
</table>

molecules, lattices, intermolecular forces, and the octet rule. The test was administered amongst 800 students ranging from high school to graduate school. Shusterman and Shusterman (1997) describe a method of teaching electronic structure and its relevance to chemical phenomena, based on computer-generated three-dimensional models of electron density distributions. The models used are common in chemical research and the authors thus conclude that there is no need for students to “unlearn” anything when moving to more advanced topics. The method described requires students to understand two basic facts about quantum mechanics. The first is that “electron positions cannot be defined precisely”, the second is “an understanding of what is meant by the phrase electron density” (p. 771). There is no need to understand and use the formalism of quantum mechanics. Arguments are given how these two points can be addressed in teaching. However, these arguments are somewhat imprecise concerning their implied interpretation. For example, the first property of quantum mechanics students should understand might be argued by starting “with the Heisenberg uncertainty principle as a fundamental postulate of what can be measured, and conclude from this that electron positions can never be known” (p. 771). We do, however, measure electron positions. What might be meant here is that with the same preparation, repeated measurements will yield different positions, depending on the state in which the electron was
The models of electron density distributions are visualized by looking at different representations (i.e. mappings) of electronic states. For example, one might plot the density on a plane (slice) through the lithium atom, or, alternatively, map an isodensity surface, connecting all points with the same electron density. These electron density models are used to study atomic and molecular structure. For example, they can be used to compare Li and Li\(^+\), showing how the latter is smaller, but the core of both is more or less the same. Several of such examples are given for atoms and molecules. The models are also used to distinguish between “ionic, covalent, and polar covalent bonding, identify covalent bonds of different bond orders, and distinguish localized and delocalized bonds and charges” (p. 773).

The described method is the effort of two lecturers on this topic. It has been tried out multiple years and adapted based on experiences. As such it is an interesting contribution. However, there is no link with literature on (quantum) chemistry education, as for example described in this section. It would be interesting to know whether the method used is able to remedy some of the learning difficulties observed. Furthermore, not all concepts from quantum mechanics and quantum chemistry are addressed that nevertheless may be considered important for students to understand. Also, the origin of the density models remains unclear to students.

Nahum et al. (2008) describe a new framework for teaching chemical bonding that is a result of a cooperation between chemistry teachers, educators, and researchers. The article also discusses some of the literature that is reviewed in this chapter. The authors describe current practice in teaching chemical bonding as a framework that is the result of the historical development of chemistry. The traditional framework can be described as a top-down framework, that classifies different types of bonds, each of which is described by different, sometimes heuristic models. Because newer models were simply added to this framework, we are now left with multiple models describing, with increasing accuracy, the same phenomenon. These multiple, concurrent models have been found to be one of the origins of learning difficulties when studying chemical bonding. Furthermore, the different categories of bonds are limited, as “we now know that many important groups of modern materials simply cannot be forced into one of the rigid categories” (p. 1681).

The new framework that is described in this work is “bottom-up”, based on fundamental principles. Such a bottom-up approach is also advocated by Frederiksen and White (2002) in the case of electricity. The framework described by Nahum et al. (2008) is divided in five stages, starting with the properties of atoms (stage 1), general principles of chemical bonding between two atoms (stage 2). In stage 3 the traditional categories of chemical bonding are explained using the general principles established thus far as “extreme cases of various continuum scales” (p. 1682). Stage 4 explains how the underlying stages result in molecular structures, ranging from localized bonds, to delocalized electrons in metallic lattices. Finally, stage 5 treats the macroscopic level
2.2. Quantum chemistry education research

at which chemical properties are explained.

One clear advantage of this approach is that it acknowledges the fact that, for example, the “octet rule” is no law, but a guideline. Furthermore, these known concepts (the octet rule) are linked to the new framework. However, it seems that this approach is largely based on (advanced) quantum chemistry, including all its difficulties. From the underlying quantum principles, up to the conceptual and theoretical difficulties of the LCAO-MO approach. Although the authors claim the benefits of the new framework, it remains unclear what new difficulties are introduced. An important question that remains unanswered is what prior knowledge is necessary for the described bottom-up approach. Before students can appreciate such an approach, they must already have learned (some) of the historical models (e.g. octet rule principle).

2.2.6 Textbooks

Two studies on the role of quantum mechanics in chemistry textbooks are worth mentioning. The first is an analysis of high school textbooks, the second on freshman/college level introductory chemistry textbooks. Although both studies concern chemistry textbooks their analysis is relevant more generally for quantum mechanics education.

Shiland (1997) has analyzed eight high school chemistry textbooks, using a model of conceptual change, to determine whether the textbooks “contain the elements required for the rational replacement of an existing belief, the Bohr model of the atom, with a new theory, the quantum mechanical model” (p. 537). The analysis uses the four factors that accommodate conceptual change, according to Posner et al. (1982):

- **dissatisfaction** learners must be exposed to phenomena that their current conceptions cannot explain;
- **intelligibility** learners must be capable of making an internal representation of the new conception;
- **plausibility** the new conception must appear to solve problems the old concepts could not; and
- **fruitfulness** the new conception must lead to the possibility of additional applications. (p. 537)

The analysis thus focuses on the textbook, not on how students work with these materials. However, it might be expected that a textbook that poorly incorporates the four factors accommodating conceptual change, also gives poor learning results. The converse, however, will not necessarily hold.

The results show that **dissatisfaction** with the Bohr model is addressed poorly in most textbooks. **Intelligibility** of quantum mechanics was estimated by the number of pages needed to explain the theory. Based on this observable, in contrast with concurrent theories (Bohr’s theory, Dalton’s theory),

\[^2\text{LCAO-MO stands for Linear Combination of Atomic Orbitals-Molecular Orbital.}\]
the intelligibility of quantum mechanics is considered low. The plausibility of the quantum mechanical model is poorly established, as none of the analyzed textbooks show how quantum mechanics is able to explain atomic spectra, which the Bohr model could not explain. Finally, the fruitfulness of quantum mechanics might have been demonstrated by showing problems that can successfully be explained with quantum mechanics. However, such problems were sparse, and two textbooks only discussed applications that actually did not require quantum mechanics, but could be explained by use of a simpler model. Shiland concludes that “none of the conditions of dissatisfaction, intelligibility, plausibility, and fruitfulness were met” (p. 542). It must be noted that this study is somewhat dated and new textbooks might have emerged that do meet the conditions for conceptual change. If this is the case, it would be interesting to know whether such textbooks are more successful in eliciting the expected conceptual change.

Niaz and Fernández (2008) have evaluated 55 freshman college-level general chemistry textbooks with a focus on quantum numbers and electron density. The textbooks were classified to the extent to which the following five topics (criteria) were discussed: (1) Origin of the quantum hypothesis, (2) Alternative interpretations of quantum mechanics, (3) Differentiation between an orbital and electron density, (4) Differentiation and comparison between classical and quantum mechanics, and (5) Introduction of quantum numbers based on electron density. These criteria are in part based on the four criteria to accommodate conceptual change (Posner et al., 1982, see discussion above) and on the three levels on which a scientific theory can function (Cushing, 1994, discussed in Chapter 3). The authors motivate these criteria with the claim that “improvement in the conceptual framework of the textbooks could facilitate students’ conceptual understanding” (p. 872).

Each of the 55 textbooks was evaluated by classifying the aforementioned five criteria as either “satisfactory”, “mention”, or “no mention”. The result of this analysis is summarized in Table 2.2. The findings are in line with Shiland (1997). Most textbooks are found to focus on providing a “formula or an algorithm that is capable of reproducing experimental data”, which Cushing defines as empirical adequacy (p. 895). There is thus little focus on understanding. The textbooks also score poorly on the four criteria of conceptual change. Again, this study is only concerned with textbooks, not with how students work with this material.

2.2.7 Conclusions

Regarding the topic of quantum theory, models seem to play a different role in chemistry education when compared to physics education. In chemistry education it is clear that models exist alongside each other. On the other hand, in physics education, models are either historical (e.g. the Bohr model of the atom), or appear in analogies. In chemistry education, to explain bonding, there are different models available with increasing theoretical abstraction.
2.2. Quantum chemistry education research

Table 2.2: Distribution of chemistry textbooks according to criteria and classification. Table reproduced from Niaz and Fernández (2008).

<table>
<thead>
<tr>
<th>Classification</th>
<th>No Mention</th>
<th>Mention</th>
<th>Satisfactory</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>54</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>49</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>51</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>27</td>
<td>28</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>49</td>
<td>5</td>
<td>1</td>
</tr>
</tbody>
</table>

The Lewis structure and octet rule might even be called a heuristic. VSEPR theory\footnote{VSEPR theory stands for: Valence Shell Electron Pair Repulsion theory.} extends this model, with the concept of electronic structure to explain molecular geometry. In part the existence of these models can be explained historically; they reflect a scientific development. However, these historical models can exist alongside each other, because they enable inferences without too difficult calculations. Furthermore, no one would consider it wise to discard the historical models and teach quantum chemistry in high school instead. Similarly, in physics education Newtonian mechanics is still taught, although we know special and general relativity is a more accurate description of nature.

Both the literature review on quantum mechanics and quantum chemistry education research showed the importance to address the nature of models (e.g. having limitations), and the relation between them (Section 2.1.5, Section 2.2.5, and Section 2.2.3). This seems especially relevant for chemistry education on bonding, including quantum chemistry. First of all, students tend to prefer earlier learned, more simple models over the later, more complicated ones (Taber, 2005, discussed in Chapter 8). Related to this, when viewed from a conceptual change perspective, textbooks do not seem to motivate students to use more advanced, more complicated theories. Furthermore, several of the reported misconceptions show that students conceptualize several elements of quantum chemistry as real objects (i.e. the electron orbitals), indicating the poor understanding of students of the theoretical status of quantum theory.

The approach described by Nahum et al. (2008) seems promising to address the learning difficulties related to models for bonding in chemistry (Section 2.2.5). However, this bottom-up approach must somehow require that students are already familiar with the models that need to be placed in this larger framework. More importantly, it is questionable whether this approach takes into account the principles needed for conceptual change. This seems to come down to a question of when a bottom-up (i.e. deductive, theoretical) approach is to be preferred over a top-down (i.e. inductive, empirical) approach.
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