Keith S. TABER
University of Cambridge, Faculty of Education

CONCEPTUALIZING QUANTA: ILLUMINATING THE GROUND STATE OF STUDENT UNDERSTANDING OF ATOMIC ORBITALS

ABSTRACT: This paper presents and discusses data relating to student understanding of the orbital concept and related ideas at college level (i.e. between secondary and university level education). The data derives from in-depth research into the thinking of a small sample of U.K. students. Students enter this level of study having been explicitly taught a quantum theory of matter (i.e. the particle model), and implicitly introduced to the quantization of charge. The key principles of quantization of energy and angular momentum are important at the college level when students are taught about orbitals, energy levels and quantum numbers. Interview extracts provide insights into the students' attempts to make sense of these unfamiliar and abstract ideas. It is suggested that this is an area where there is a genuine pedagogic problem: capable and motivated students struggle to learn from experienced and knowledgeable teachers. The present paper describes how students conceptualized these key aspects of the atomic model. A subsequent paper ("Compounding quanta: probing the frontiers of student understanding of molecular orbitals") considers how the same group of students applied their thinking in the more complex context of molecular systems. [*Chem. Educ. Res. Pract. Eur.*: 2002, *3*, 145-158]

INTRODUCTION - THE QUANTUM PRINCIPLE IN SCHOOL AND COLLEGE CHEMISTRY

The essence of a quantum theory is that something that might appear to be continuous in nature (matter, energy, time etc.) is actually composed of discrete 'chunks' or quanta. During school science learners are introduced to a quantum theory of matter: i.e. that matter is *not* continuous, but rather that it consists of many minute discrete particles. This particle theory is sometimes referred to as the *kinetic theory* of matter (especially when discussed in physics classes) or the *molecular model* of matter. It is known that learners commonly have difficulty appreciating the nature of the particle model (see below), and introducing it is often considered to be a key aim of the lower secondary (e.g. 11-14 years) science curriculum.

At the next stage of the science curriculum (e.g. 14-16 years of age) an understanding of the particle model is often assumed, and learners are taught about atomic, ionic and molecular structure in terms of the main 'fundamental' particles: the electron, proton and neutron. In effect this introduces the notion that charge is also quantized: i.e. charge is always found in multiples of e, approximately 1.6×10^{-19}C. (Quarks have fractional electronic charge, but they are not found 'free', and are not discussed at this educational stage.) As the term 'charge' derives from the meaning 'load' (Knight, 1989), the notion of the charge on an electron being a quantum seems appropriate!

The actual *term* 'quanta' is not usually introduced at school level, although the *particle nature* of matter is a key idea in many aspects of secondary science (and especially chemistry). The quantization *of charge* is not usually emphasized as much as the particle nature *of matter* but it is at least implicitly treated at upper secondary level. It is at the next stage of chemistry learning, often at around 16 years or so of age, that quantum theory is *explicitly* discussed, for it is at this level that an appreciation of the effects of the quantization of energy and angular momentum become important, and the concept of the orbital is introduced.

Particles, atoms, molecules and quanticles

In order to discuss the quanta of matter which are assumed by the kinetic theory or molecular model of matter we need a suitable language. The term 'quantum objects' may be used, although this seems clumsy (Polomarev, 1993). Often in lower secondary science (e.g. 11-14 years) the preferred term is simply 'particle': however it is known that pupils commonly confuse these particles with small, but still macroscopic, particles such as grains of sand or salt, or dust particles.

The terms 'atom' and 'molecule' are also commonly used as generic terms at this level, and this may avoid the confusion with macroscopic particles. However, these terms have quite specific meanings. The particles in common substances and materials may be molecules (water, wax), or ions (salt), or cations and electrons (iron, copper), or a mixture of different types (air, brine), although these distinctions are not made when the particle theory is first introduced. The selection of 'atom' or 'molecule' as a generic term at this stage can present difficulties later (e.g. 14-16 years) when more detailed models are introduced and learners are expected to distinguish these terms.

Inappropriate labels can be serious impediments to communicating and learning science (Schmidt, 1991; Watts & Gilbert, 1983) and it is suggested here that an alternative collective term is needed, for these particles. I have here chosen to call such particles (electrons, nuclei, ions, molecules etc.) by the collective label 'quanticles'.

Difficulties with learning about quanticles

Chemists explain the properties of substances largely in terms of quanticle level models. In particular, aspects of the structure of molecules, ions and lattices are key features of chemical explanations. The high melting temperature of diamond, the solubility of salt, the colour and shape of copper sulphate crystals, the relatively high boiling temperature of water, the conductivity of iron, the reactivity of alkenes and the relative stability of benzene are just a sample of the properties of materials that are explained in terms of our structural models at the quanticle level.

Yet it is known that these models used by chemists are not readily accessible to learners (Lijnse et al., 1990). Quanticles are not visible directly, and cannot be shown to students. To a large extent belief in the existence of atoms, molecules, ions and electrons is, initially at least, an article of faith for students. These theoretical entities occur at a scale far removed from everyday experience, and have properties which are *necessarily* at odds with such experience.

This last point is particularly pertinent. A question such as 'what does an atom of helium look like' is inherently oxymoronic - in the same way as asking what happened *before* the beginning of time. Since single quanticles are not visible in the normal sense, any image is necessarily a model with arbitrary features. It is now common for school textbooks to include 'pictures' derived from apparatus such as scanning tunneling microscopes,

supposedly showing atoms (von Baeyer, 1993). These images are seen to support the particle model that students are taught, i.e. to give evidence for the existence of atoms. However students may not realise that these are not just 'blown-up' photographs, but images produced by processing completely different types of raw data. The process is not one of *magnification*, but of translation and *re-coding* (more akin to experiencing synaesthesia than wearing spectacles).

This is important because the main significance of the models that chemists use is that they enable us to explain *everyday* properties of substances in terms of the *distinct* properties of the arrangements of quanticles. We might label the scientists' use of particle models as the 'quanticle schemata'. In its most basic form this comprises:

1. an everyday (or macroscopic) property to be explained;
2. a distinct feature of the quanticle level model which maps onto, and explains, (1)

There are very many examples of the use of this explanatory scheme. For example:

1. the high melting temperature of diamond is explained by
2. the extensive lattice of covalent bonds

Clearly this outline lacks detail, and further levels of explanation could be added (such as explaining what a covalent bond was), but it illustrates the principle.

Yet students often find such explanations problematic (Taber, 2001a, 2002a). Where the chemist may explain the high melting temperature of diamond in terms of the strong bonding in the covalent lattice, the student may explain that diamond has a high melting temperature *because* the carbon atoms have a high melting temperature. This type of 'explanation' is easy to apply - e.g. metals expand on heating because atoms expand; they are shiny because the atoms are shiny; they conduct because the atoms conduct, etc. - but of little scientific validity or explanatory value (Taber & Watts, 2000).

Where the thinking of expert chemists may shift effortlessly between macroscopic phenomena and quanticle explanations, these transitions cause difficulties for many learners (Jensen, 1995; Johnstone, 2000). It is therefore important for teachers to be very clear about the level they are referring to at any particular time. Sometimes this may suggest a need for new terminology. For example it is important for students to realise that *substances react*, when their *particles undergo fruitful collisions*. Learners are likely to refer to the particles themselves 'reacting', and the term 'interact' is too general (as most interactions at this level are elastic collisions) and so it has been suggested that a new term is needed. The term 'quantaction' has been suggested (Taber, 2001b): e.g., the *substances* hydrogen and fluorine *react* when *their molecules quantact* .

Often, then, it is the very way that quanticles behave *differently* from everyday particles that makes their study important. The human scale world that we experience directly is only the way it is because:

a) matter behaves differently at the scale of molecules, ions and electrons;
b) the change in scale is so vast that the everyday properties of materials can 'emerge' from the vast conglomerations of quanticles.

Students tend to mis-apply the quanticle schemata even when the properties concerned are not alien to their experience. For example, electrostatic charges and their effects can be (and are) demonstrated on the macroscopic scale in school science. However, students do not readily accept the importance of electrical forces in determining atomic,

molecular and lattice structures and their properties (and so indirectly determining many macroscopic properties). These learning difficulties have been reported in some depth, and reviewed in this journal (Taber 2001a).

Many of the important features of the behaviour of matter at the scale of molecules, ions and electrons are *not* familiar from experience of the macroscopic world. These features might be considered as 'quantum properties'. If students find application of the quanticle schemata difficult when explanations involve the electrical attractions between charged particles (something with examples within common experience), then it is not surprising that the 'weirdness' of quantum behaviour - which even Bohr recognised required "a conscious resignation of our usual demands for visualization and causality" (Petrucciolo, 1993, p.19) - proves to be a greater barrier to applying the quanticle schemata. The quantization of energy, angular momentum etc., and the wave-particle nature of entities such as electrons, are alien to students.

In everyday experience, substances appear continuous, and may apparently be sub-divided indefinitely. Also, in everyday experience, clumps of matter - salt grains, metal coins, vehicles - behave unambiguously like particles rather than waves. Although it is quite possible to calculate, for example, a de Broglie wavelength for a motor car or an ocean liner, these macroscopic objects behave in ways such that their quantum properties are swamped, and are both difficult to detect and practically irrelevant. Quantum-mechanical tunneling may be significant on an atomic scale, but we have to look elsewhere for an explanation if a camel passes through the eye of a needle.

This paper is concerned with learning about the properties of matter at scales where these quantum effects *do* become significant. The quanticle nature of these systems is of utmost importance in the most basic areas of the chemistry curriculum. For example, a simple model of atomic structure is usually taught at secondary school level, so that students will learn about electron 'shells'. On this model an atom of sodium has eleven electrons arranged in three concentric shells: 2, 8, 1. The very existence of such electronic configurations is tied to the sub-atomic particles being quanticles: particles where the quantum restrictions significantly effect behaviour. Yet this is usually just passed over when teaching at this level. It becomes very significant for those learners who select to study chemistry at college (i.e. post-16) level.

Atomic structure and the orbital concept

The electrons in atomic (and molecular) systems are considered to be located in orbitals. Key principles that are introduced into the chemistry curriculum at College level (Taber, 1997) are:

- orbitals: atomic orbitals, hybridised atomic orbitals, LCAO (linear combination of atomic orbitals), molecular orbitals;
- p, d, f nomenclature for labelling orbitals;
- energy levels;
- electron (quantum-mechanical) spin;
- quantum numbers and associated rules (the exclusion principle, Aufbau principle, Hund's rules).

Previous research acknowledges that learning about these topics is problematic (Cervellati & Perugini, 1981; Cros et al. 1986, 1988; Jones, 1991; Mashhadi, 1994; Shiland, 1997). In view of research findings that students do not readily apply familiar principles (e.g. electrostatic interactions) in the context of atomic structure (Taber, 1998), it is not surprising

that the less familiar ideas deriving from quantum theory also prove difficult. Students may be introduced to these key ideas in their pre-university courses, but this does not imply they have a sound understanding of them when they enter university (Cervellati & Perugini, 1981)! Students often conceptualize atomic structure in terms of electrons in planetary-type orbits even after being taught about more sophisticated models. This has been found in pre-university (Mashhadi, 1994; Petri & Niedderer, 1998) and university courses (Cros et al. 1986, 1988), and may lead to students making sense of quantum ideas by trying to graft them onto incongruent anachronistic models (Jones, 1991). Tsaparlis (1997) refers to how university students develop misconceptions due to "previous elementary, imprecise, incomplete and mostly pictorial instructions" (p. 279).

THE CONTEXT OF THE PRESENT STUDY

The data reported in this paper derive from an interview-based research project with UK college students (c. 16-18 years of age), designed to explore their developing understanding of ideas related to the chemical bond. The purpose of the present study is to describe how the students made sense of the atomic orbital concept and related ideas (energy levels, electron spin). These students were enrolled on two-year 'A level' courses (i.e. the General Certificate of Education Advanced Level), including the study of chemistry as one of their chosen subjects. The teaching team were chemistry graduates and experienced at teaching at this level. Typically, students taking this course were intending to proceed to university, and the A-level course was the standard means of bridging between school and university level study. Orbital ideas were presented during the students' first chemistry lesson at their college, and were regularly used in the teaching throughout the course.

The interviews were all undertaken by the author, who was one of the lecturers on the course, and therefore knew the students as a teacher as well as a researcher. The data presented are from a selection of in-depth interviews with a sample of students, who volunteered to be interviewed. Fifteen students were interviewed for the study (Taber, 1997, pp. 395-400). The students are referred to by assumed names. The material forms part of the larger research project where grounded theory approaches were used to move from detailed exploration of the ideas of individual learners to the development of general models of wider application (Taber, 1997, 2000a). This approach led to the reporting of a model of student progression in understanding aspects of chemistry which involved a shift from a common alternative conceptual framework (the octet framework) to an increasing reliance on electrostatic *and orbital* ideas (Taber, 1999). The extent to which orbital ideas were used by the colearners in the interviews varied, and specific data from twelve of the fifteen students are presented in this paper and its sequel (Taber, 2002b).

It is important to emphasize that the learning difficulties considered here are largely discussed in terms of the comments of a small number of learners in one college in one country. Clearly the findings can not be *assumed* to be generalized to all students studying chemistry at this level. Such accounts may be considered to be *illustrative* of the types of thinking, and sorts of learning difficulties, that students at this level may present; but should not be taken to be representative of the extent or specifics of such thinking in the wider population of college level students.

The theoretical approach used in this research, grounded theory, is primarily a qualitative approach. Grounded theory can produce models which are suitable for forming the basis of quantitative surveys (Taber, 2000a), and the categories of student difficulties presented in this study *could* be used in this way. However, in the present papers no attempt is made to quantify the frequency with which the particular difficulties were observed, as the

methodology (i.e. the nature of the sampling and data collection) would not justify such an approach.

Verbatim comments from individual learners may seen idiosyncratic when they can not be claimed to be representative of the wider population, but this approach is part of a developing research programme of exploring aspects of science learning by detailed case studies (e.g. Harrison & Treagust, 2000; Johnson, 1998; Petri & Niedderer, 1998; Scott, 1992; Taber, 1995a, 2000b, 2001c). The value of the data discussed is in providing authentic cases of how students *make sense* of these scientific ideas. These cases should be seen as *examples* which *indicate* the nature and range of both the learning problems in a topic, and the student responses in terms of the conceptualizations formed. Each reader needs to consider the extent to which conclusions could be transferred to her own teaching context - a process labeled reader generalization (Kvale, 1996).

FINDINGS FROM THE STUDY

The interviews with the college students suggested that they were mentally 'groping' to make sense of new concepts such as orbital, energy level, quantum number, and so forth. The research suggested that students (1) did not appreciate why quantization was introduced into the atomic model; (2) had difficulty forming an adequate concept of orbitals; (3) confused related concepts such as shells, sub-shells, orbitals, energy levels; (4) did not appreciate what was meant by electronic spin; (5) found the designations of orbitals confusing; (6) did not clearly distinguish molecular orbitals from atomic orbitals; and (7) held limited notions of what resonance structures were meant to represent. The present paper considers the first five of these points: the latter two are considered separately in a second paper (Taber, 2002b).

The need for the quantum hypothesis: why don't atoms collapse?

A key issue in the history of the atomic model of matter is why atoms should be stable, when classical electrodynamics suggested they should radiate energy and collapse. The quantum hypothesis (of energy) 'saved the phenomena', so that an atom in its ground state could not decay to any lower energy state (Petruccioli, 1993). To appreciate this key aspect of quantum theory one has to see the planetary model of the atom as flawed, as - within it - electron orbits 'should' decay. The interviews reported here suggest that even though students may accept the quantum model of the atom, they may not appreciate this flaw of earlier atomic models.

So Edward knew that there would an attraction "between the negatively charged electrons and the positively charged protons", and demonstrated that he appreciated the idea of atomic energy levels, and of the 'quantum jumps' possible if the correct quantum of energy was provided,

> "you could put energy into it, [of] the correct frequency, which a particular electron would absorb, it would absorb a photon of energy and be promoted to another vacant orbital...energy equals Planck's constant times the frequency of the radiation".

However, Edward did not relate these two sets of ideas. Rather, he explained the failure of electrons to be attracted into the nucleus purely with the initial state of the atom,

> "it's something to do with, like the planetary motion, they had some initial kinetic energy, that's why they don't - well attract each other [i.e. move together due to attraction]. Perhaps in

creation they were given some initial kinetic energy, and some rotational energy, and that's why they rotate"

Edward's explanation was not satisfactory from the scientific perspective, as he was clearly unaware of the historical expectation that oscillating electrons should radiate energy. For Edward there was no problem here for the quantum hypothesis to address.

Another student, Jagdish, had a different approach. She believed that there were "the attractions from the nucleus, pulling in the electrons" but the electrons did not fall into the nucleus, as although "they're being attracted, the attraction isn't that strong", and that "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." Here we see confused physics used to interpret the chemistry.

Adopting the orbital concept

The research suggested that learners might acquire the term 'orbital' without having an appropriate conceptualization for what the term represents. So Annie referred to "the quantum shell, on what the electrons sit" and to electrons that "go round, like in orbitals, or in spherical things". Another student, Debra's uses the term 'orbital', although her meaning seems closer to the notion of 'orbit', describing how "the orbital closest to the nucleus ... [is] the *path* the electron takes around the nucleus" as the electron "*circles* the nucleus in a sphere".

Edward described a picture of a sodium atom with the electrons in three concentric shells as a "representation of an atom, with its electron *orbitals*, in different shells, around the nucleus". He went on to explain that there were three *orbitals* containing two, eight and one electron respectively,
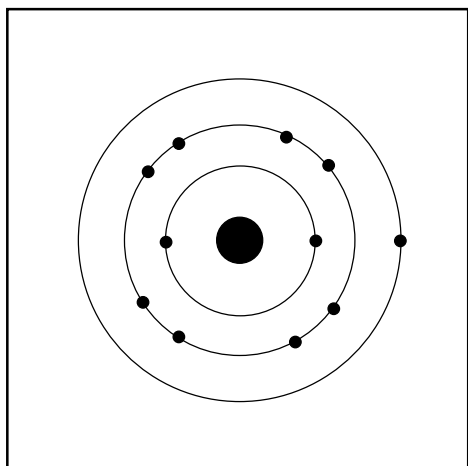
> "there's three electron *orbitals*. In the first one there's two electrons, in the second, there's eight, and in the third one there's one electron."

Tajinder was another student who used the term orbital to label electron shells shown on diagrams of atoms. He thought that "each orbital is like a sphere". In a subsequent interview Tajinder had developed his ideas so that he was able to describe "an orbital is just an area around ... the nucleus of an atom, where electrons are likely to appear, or be held". The confusion between orbitals and shells was still present, so that he suggested that a sodium atom would have three orbitals. Tajinder recognised that his existing knowledge from school science, where "they draw the sodium nucleus, and they have three rings about it [cf. Figure 1], and that's where they like place the electrons", was interfering with this new learning.

Relating orbitals, sub-shells and shells

We have seen, then, that when students are first introduced to the idea of an orbital they may have difficulty distinguishing the meaning of the new concept from the more familiar notion of an electron shell. At the level at which quantum ideas are first explicitly met there are also other *closely related, and yet distinct*, ideas that students are also expected to master: *sub-shell* and *energy level*. The students were expected to appreciate the significance of the *designations* of orbitals, and to appreciate that atomic orbitals may be grouped into sub-shells, which are in turn grouped into shells

Some students find this conceptual scheme difficult to master. In the case of Carol

this confusion was still evident shortly before her end-of-course examination, when she knew that there could be eight electrons in the second shell of an atom, but thought that this would only require *two* orbitals (i.e. she had confused orbitals for sub-shells). Another student, Kabul, made a different error of confusing shells for sub-shells,
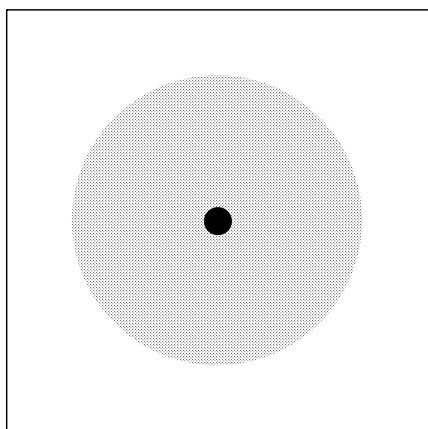
> "a sub-shell consists of orbitals. Like you know L is a sub-shell consisting of 2p and 2s orbitals"

> "if all the p-orbitals are all full of electrons, if you work out where they are most likely to be, then it will show like a sphere shape of electrons smeared out, so then that is represented by *the shell* in the diagram that we learnt for G.C.S.E. [i.e. the school leaving examination]".

FIGURE   Σφάλμα!   Άγνωστη παράμετρος αλλαγής.**:** *Representing an atom in*
 terms of shells.

Relating orbitals and probability envelopes

Representations of quanticles might show electrons arranged in shells, or in orbitals, or might illustrate overall electron density. Students are expected to distinguish between the orbitals themselves, and diagrams which reflect the 'envelope' of electron density - with its arbitrary cut-off (see Figure 2). An electron occupying an orbital will always be 'in' that orbital, but will only be 'probably found' within the area represented by *diagrams* of orbitals.

This is an inevitable consequence of drawing a meaningful representation of a technically infinite orbital! Students, however, may confuse the orbital itself, and the common diagrammatic convention of representing the geometry of the orbital in terms of a probability envelope.

Near the end of his two year course, Umar described an orbital as the "space *most likely* to contain the electrons". Tajinder also confused the orbital with the diagrammatic representation of a probability envelope when he suggested that the electron is sometimes *outside the orbital*. He thought the orbital was

> "a probability of finding the electron in that certain area, so that's where the electrons will mainly be found...an orbital just distinguishes a sort of barrier around where you're most likely to find that electron, so it doesn't mean that it just sticks in that one place"

FIGURE Σφάλμα! Άγνωστη παράμετρος αλλαγής.**:** *Representing an atom in*

terms of an electron density envelope.

Another student, Jagdish, referred to *shells* being "just something like arbitrary", before changing this to "*orbitals* were arbitrary",

"they [orbitals] were just regions of space that had the highest probability of finding the electron".

Relating orbitals to energy levels

The energy level associated with an electron would be primarily determined by shell, and then (except in the single electron case) sub-shell, but could also depend upon orientation (e.g. 'd-level splitting'), and occupancy (thus Hund's rules). The notion of energy levels provides a further concept to be confused with shells, sub-shells and orbitals. So, for example, near the end of her two year course, Annie's explanation of why electrons do not fall into the atomic nucleus invoked *quantum shells*, *energy levels*, *orbitals* and even *hybrids*, without suggesting that she had a clear idea of the distinction between these concepts,

"The electrons are held in sort of levels, so it's to do with sort of bonding, like you can only get two electrons in the first quantum shell. So that they are held in these shells. ... so they're all held in quantum shells which are different energy levels, and you can sort of promote electrons should you need to in bonding, so if for example you need a bond to have - I don't know - an extra electron in a p orbital, you can donate an s electron across, to give you hybrids."

Another student, Jagdish, thought that electron shells "show you the energy levels". Carol was another student who learnt the term 'energy level' without clearly distinguishing this from her existing notion of electron shells. She described the circles showing shells in an atom (see Figure 1) as the "*energy levels* around an atom" of sodium, but she also used the same term to refer to the 'boundary' of electron density in a figure showing a molecule with an electron cloud (like Figure 2) as "an energy level". Near the end of her first year of study at this level she also referred to how the electrons shown in a simple representation of the oxygen molecule "all look as though they're on the same energy level".

Relating orbitals to electronic transitions

Students need a clear appreciation of the difference (and relationship between) the concepts of shells, sub-shells and orbitals if they are to understand the nature of electronic transitions. After one year of the course Debra knew that after a molecule had absorbed light "it's got more energy" and "it's excited" which she thought meant that the electrons were "vibrating, and moving more". However Debra did not relate this to ideas about orbitals (or shells) and did not think the electrons would move into a different 'orbit'. Rather, Debra thought that *all* of the electrons which normally "move round the nucleus" would "probably move faster". Although by the end of her two year course Debra could explain that an atom was excited when "you promote an electron to a higher energy level", she was only able to bring this to mind when she was specifically reminded of an experiment she had performed in her *physics* course.

In Tajinder's fifth interview he discussed how an electron could be promoted to an excited state, but he was not sure whether he should refer to the electron moving *between shells*, or *between orbitals*,

"when you put it into a Bunsen burner, a Bunsen burner's like a lot of heat, and that heat is like energy to the outermost electrons, and when we were drawing the lines, like going up in stages, across the board, we were just showing how when you give the outermost electron of sodium energy, it rises up to a certain amount,...then it gains energy, and when it falls back down, the

energy it gives out is in the form of light, and that is the light it gives out so that's why that sodium has the colour when it gives it out, when it's like heated. So it's just the movement of the outermost electron, out of the shells, out of shells? Shells or orbitals, I'm not sure, but it might be like shells...but then there's only a certain amount of energy that's given in, and when that energy is released back it's given out in the form of light"

Only after he sketched out his recollection of the diagram he had seen on the board during a class did Tajinder conclude that the transitions were between energy levels.

Another student, Kabul, managed to confuse the emission *of electrons* in thermionic emission with the emission *of photons* from a luminous body,

"when we heat the metal, the electrons will rise from a lower energy level to a higher energy level, as it's vacuum the electrons will just jump off there, I mean the metal, if you heat it quite sufficiently, the electrons will rise from a lower energy to a higher level and, just be emitted outside...[for] example if you take iron, if you heat it you will see it turns red, it turns red because it starts emitting electrons, but once it cools down the electrons go back to the electron shells and it regains its shiny colour. While you're heating the electrons are being emitted, so it gives off colours of different wavelength when you cool down the electrons go back to their original energy levels."

Labelling orbitals

The labelling of atomic orbitals is closely tied to the relevant quantum numbers (q.n.), with numbers for the principle q.n., letters (s, p, d, f...) for the azimuthal q. n., and subscript letters (from Cartesian axes) for the magnetic q.n. Students are expected to master this labelling system, and to learn the order in which orbitals are filled in the first rows of the periodic table. Orbital *occupancy* is commonly represented by an additional superscript after the orbital label. For learners who find the *orbital* concept abstract, and confuse it with *shells*, *sub-shells* and *energy levels*, the designations given to orbitals must seem puzzling. Near the *end* of her course, Carol described an s-orbital as an "x, y, z, type of thing" and thought the next orbital to be occupied after 2s was "3p".

Tajinder seemed confused when he tried to make sense of the recently introduced orbital concept,

"first lesson here, we learnt about 1sp, 2sp, $2p_x^1$, $2p_y^2$, was it 2? I'm not sure, I can't remember, but ... this is like an orbital, which [is a] sphere sort of shape, and - it's hard to describe - if this is a sphere, and has a nucleus in the middle, but one electron would be here, and one would be on the opposite side of the orbital.... there's x, y and z axes. Like if you put it on the axes then - it would become clear. So it's hard, it's hard for me."

Tajinder had remembered the flavour (if not the details) of orbital labeling, in terms of letters and numbers, with references to Cartesian axes. In a subsequent interview Tajinder corrected a suggestion of his own that a sodium atom would have *three orbitals*: but still seemed mystified by the way orbitals were labelled,

"no wouldn't have three orbitals, it'd have more than three orbitals, like you have the s orbital, p orbital, d and the f. Is it the f? I'm not sure. There's four different types of orbitals. And on the p orbitals there's p_x^1 p_x, p_y^1 and p_z^1. So I was wrong when I said there were three orbitals ... I think there's more...I don't know"

During one interview Tajinder referred to orbitals with designations $1s^1$, 1p, $1p_x$, $1p_y$, $1p_z$, $3s^1$ and 1d. When he attempted to recall the order of occupancy of orbitals (i.e. the Aufbau order) he suggested 1s, 2s, 2p, 3p, 3s, 1d, 4p, 4s, 2d:

"I think it goes 1s, 2s, 2p, no you don't have a 1p orbital do you? No you don't, done that wrong actually. 2p, 3p, 3. Then you have 3s, then you have 1d, then you have 4p, 4s, 2d."

Tajinder found this scheme confusing, and did not clearly distinguish orbital labels and indicators of occupancy (i.e. the superscripts). Edward also confused the labels for orbitals and configurations, referring to the atomic hydrogen *orbital* as "1s[1]".

Electron spin

The notion of electron spin is abstract, but has important consequences at this level. The term quantum-mechanical spin is sometimes used to stress how this 'spin' is "an intrinsic angular momentum independent of any orbital angular momentum" (Beiser, 1973, p.205). The everyday meaning of 'spin' implies movement, but "the idea that electrons are spinning charged spheres is hardly in accord with quantum mechanics" (ibid.) Edward had read that electrons were "spinning on their axes", but said that he did not "know what that means". He referred to electron spin direction, which he 'assumed' meant,

"that an electron moves about this volume of space that's called an orbital in *one particular direction*, whereas the other moves in *the opposite direction*".

Quorat explained spin as a *consequence* of electrical repulsion,

"because they're all going to be repelling each other and circling, always trying to get as far apart, 'cause that's why they're always spinning"

Even when a student, Umar, seemed to conceptualize 'spin' in terms of the exclusion principle, he was still tempted to relate the notion to a 'direction'. He explained that to be spin-paired meant that,

"The electrons can be in the same orbital. It doesn't actually spin, it's not really spinning itself, but it just means they're allowed to be together, I think, and they're in the same orbital, so they might be in opposite directions."

Clearly students associate the term 'spin' with the macroscopic phenomenon of that name, of which a key feature is *movement*, rather than "the intrinsic angular momentum of a subatomic particle, nucleus, atom, or molecule, which continues to exist even when the particle comes to rest" (Lafferty and Rowe, 1994, p. 556).

DISCUSSION

This paper has shown that students may have considerable difficulties constructing the scientific models of the quantized atom in terms of orbitals and related concepts.

A central theme was that *learners were failing to adequately distinguish between concepts that needed to be seen as distinct* - but were rather conflating the new ideas - both among themselves, and with their existing toolbox of relevant concepts (Taber, 1995b). These students began their college course holding a model of the atom as having electrons in shells with planetary orbits. Although they readily adopt the new terms 'quantum' and 'orbital', they initially used these *new labels* to apply to their existing understanding of atomic structure. So orbitals became confused with shells, sub-shells, energy levels and visual representations of probability envelopes. The terms were acquired, but the distinct meanings did not readily follow.

Without such clear demarcation between related concepts it was difficult for students to appreciate what was meant to be happening when (for example) electronic transitions occurred. Such understanding was also impeded by a failure to make sense of the labeling of orbitals - something that must seem arbitrary in the absence of any clear appreciation of how orbitals have the different attributes (roughly size, geometry and orientation) which determine how they are conceptualized in terms of sub-shells and shells.

This paper has presented some data collected from students at the stage of chemical education when they are first introduced to the notion of the atomic orbital, and related concepts (viz. 16-18 years of age in the U.K. system). The data derives from students in a single institution, and such a case study does not claim to be representative of a wider population in any statistical sense. Qualitative studies of this nature increase the burden on the reader in terms of judging the extent to which the case made for the *particular* group discussed may also be relevant to other educational settings. Of course, such judgment is always required when interpreting any form of educational research, but it is more onerous when the work reported is from a single, specific context.

Yet there are also significant advantages to such an approach. Notwithstanding considerations about generalization, the use of an in-depth approach allows the *authentic* voices of the students to be represented in the research. The author believes that by presenting many verbatim quotes, including a number of extended extracts, it is possible for the reader to appreciate some key features of the students' learning about orbital ideas. This is important because I wish to suggest that the evidence supports two key conclusions.

The first is that *the group of students discussed had real difficulties conceptualizing quanta and making sense of orbital ideas*. By itself, such a conclusion is not very surprising in view of the literature cited above, and could perhaps have been better demonstrated in the context of a survey of a larger and more representative sample of students. However, the second point suggested by the evidence presented (and which would not have been clear from a survey approach) is that *these learning difficulties do not seem to derive from omissions in teaching or from any lack of ability or commitment from the students*.

A close reading of the comments of the students shows that they had been introduced to the key concepts and that they were strongly motivated to make sense of them. This is significant, as it means that this paper is not just reporting a simple failure of the teachers to cover the content, or of the learners to fail to take responsibility for their role in learning. Rather, this is an example of keen teachers failing to explain key ideas to eager learners. This paper reports a genuine pedagogic problem, i.e. that teaching about orbital ideas at this level needs to be informed by specific theory about how students learn science.

Previous research has suggested that college level students have difficulty in developing their ideas beyond a planetary model of the atom (Mashhadi, 1994; Petri & Niedderer, 1998), and that such a conceptualization often predominates when students start university courses (Cros et al., 1986, 1988; Tsaparlis, 1997). The present research supports such findings, and fills in some of the details of how college level students struggle to make sense of the atom as a quantum system. It is also suggested that if students are to be expected to have a more scientific understanding of these ideas on entrance to university (cf. Cros et al, 1986; Tsaparlis, 1997), then the way that these concepts are taught at college level may require attention.

However, this present paper does not exhaust the extent of student difficulties making sense of orbital ideas at this level. It has explored student understanding of the orbital context within the context of *isolated* atoms, which are seldom important in either the composition of useful materials or as reacting species in important chemical processes (Taber, 1996). Chemists are interested in the more realistic context of larger 'quanticles'. At the level of study being considered this would normally be represented in terms of relatively simple

molecules. In this context students will be expected to appreciate basic notions of the structure of molecules in terms of orbitals. Clearly this knowledge needs to be developed from a solid foundation of understanding the mono-nuclear case (i.e. atoms and simple ions), which this present paper suggests students may not have. A companion paper (Taber, 2002b) considers how the group of students discussed here attempted to make sense of the more complex case of molecular orbitals.

Clearly, identifying a problem is only one step in the process of using research to inform practice. These two papers will provide a 'rich description' of student conceptualizations that can act as a platform for exploring *why* student learning about orbitals ideas is so problematic, and *what* educational theory suggests needs to be done to improve our teaching in this area.

The problem highlighted in this paper is a serious one that, in view of the importance of the topic, needs urgent research attention. One promising sign is that - despite the abstract nature of the concepts, and the clear difficulties faced - the students seldom gave up on the topic. Learners are clearly interested in understanding the quantum model of the atom, and are motivated to make sense of orbitals, electron spin, hybridization, energy levels and the rest. As teachers, we need to find ways to scaffold their learning to help them avoid the overload of new, subtly distinct, ideas they meet at this stage of their chemical education.

CORRESPONDENCE: *Keith S. TABER, University of Cambridge Faculty of Education, Homerton Site, Hills Road, Cambridge, CB2 2PH, U.K.; kst24@cam.ac.uk, keith.taber@physics.org http://www.educ.cam.ac.uk/staff/taber.html*

REFERENCES

Beiser, A. (1973). Concepts of Modern Physics (2nd ed.) Tokyo: McGraw-Hill Kogakusha

Cervellati, R. & Perugini, D. (1981). The understanding of the atomic orbital concept by Italian high school students. *Journal of Chemical Education*, *58*, 568-569.

Cros, D., Amouroux, R., Chastrette, M., Fayol, M., Leber, J. and Maurin, M. (1986). Conceptions of first year university students of the constitution of matter and the notions of acids and bases, *European Journal of Science Education*, *8*, 305-313.

Cros, D., Chastrette, M. and Fayol, M. (1988). Conceptions of second year university students of some fundamental notions in chemistry. *International Journal of Science Education*, *10*, 331-336.

Harrison, A.G. & Treagust, D.F. (2000). Learning about atoms, molecules, and chemical bonds: A case study of multiple-model use in grade 11 chemistry. *Science Education*, *84*, 352-381.

Jensen, W. B. (1995). *Logic, history and the teaching of chemistry*. Text of the keynote lectures, given at the 57th Annual Summer Conference of the New England Association of Chemistry Teachers, Sacred Heart University, Fairfield, Connecticut.

Johnson, P. (1998). Progression in children's understanding of a 'basic' particle theory: A longitudinal study. *International Journal of Science Education*, *20*, 393-412.

Johnstone, A. H. (2000). Teaching of chemistry - Logical or psychological? *Chemistry Education: Research and Practice in Europe*, *1*, 9-15. [Available at http://www.uoi.gr/conf_sem/cerapie]

Jones, D. G. C. (1991). Teaching modern physics - Misconceptions of the photon that can damage understanding, *Physics Education*, *26* (2) 92-98.

Knight, David (1989). *A Companion to the physical sciences*. London: Routledge.

Kvale, S. (1996). *InterViews: An introduction to qualitative research interviewing*, Thousand Oaks, California: SAGE Publications.

Lafferty, P. & Rowe, J. (eds.) (1994). *The Hutchinson dictionary of science* (revised edition). Oxford: Helicon Publishing.

Lijnse, P. L., Licht, P., de Vos, W., & Waarlo, A. J. (1990). *Relating macroscopic phenomena to microscopic particles: A central problem in secondary science education*. Utrecht: Centre for Science and Mathematics Education, University of Utrecht: CD-β Press.

Mashhadi, A. (1994). Advanced level physics students' understanding of quantum physics. Paper presented to the *British Educational Research Association* Annual Conference, Oxford, September 1994.

Petri, J. & Niedderer, H. (1998). A learning pathway in high-school level quantum atomic physics, *International Journal of Science Education*, *20*, 1075-1088.

Petruccioli, S. (1993). *Atoms, metaphors and paradoxes: Neils Bohr and the construction of a new physics*. Cambridge: Cambridge University Press.

Polomarev, L. I. (1993) *The quantum dice*. London: Institute of Physics.

Schmidt, H-J. (1991). A label as a hidden persuader: chemists' neutralization concept. *International Journal of Science Education*, *13*, 459-471.

Scott, P. H. (1992). Pathways in learning science: a case study of the development of one student's ideas relating to the structure of matter. In Duit, R., Goldberg, F. & Niedderer, H., (eds.) *Research in physics learning: Theoretical issues and empirical studies*, pp.203-224. Kiel: I.P.N. (Institut für die Pädagogik der Naturwissenschraften).

Shiland, T. W. (1997). Quantum mechanics and conceptual change in high school chemistry textbooks. *Journal of Research in Science Education*, *34*, 535-545.

Taber, K. S. (1995a). Development of student understanding: A case study of stability and lability in cognitive structure, *Research in Science & Technological Education*, *13*, 87-97.

Taber, K. S. (1995b). An analogy for discussing progression in learning chemistry. *School Science Review*, *76* (276) 91-95.

Taber, K. S. (1996). Do atoms exist? *Education in Chemistry*, *33* (1) 28.

Taber, K. S. (1997). Understanding chemical bonding - the development of A level students' understanding of the concept of chemical bonding, Ph.D. thesis, University of Surrey.

Taber, K. S. (1998). The sharing-out of nuclear attraction: Or I can't think about Physics in Chemistry. *International Journal of Science Education*, *20*, 1001-1014.

Taber, K. S. (1999). An explanatory model for conceptual development during A-level chemistry. Paper presented at the annual meeting of the *British Educational Research Association*, September 1999, University of Sussex.
[Available via Educati*on-line*, at http://www.leeds.ac.uk/educol]

Taber, K. S. (2000a). Case studies and generalisability - Grounded theory and research in science education. *International Journal of Science Education*, *22*, 469-487.

Taber, K. S. (2000b). Multiple frameworks?: Evidence of manifold conceptions in individual cognitive structure. *International Journal of Science Education*, *22*, 399-417.

Taber, K. S. (2001a). Building the structural concepts of chemistry: Some considerations from educational research. *Chemistry Education: Research and Practice in Europe, 2*, 123-158. [Available at http://www.uoi.gr/conf_sem/cerapie]

Taber, K. S. (2001b). The campaign to stop molecules reacting. *Education in Chemistry*, *38* (1), 28.

Taber, K. S. (2001c). Shifting sands: A case study of conceptual development as competition between alternative conceptions. *International Journal of Science Education*, *23*, 731-753.

Taber, K. S. (2002a). *Chemical misconceptions: Prevention, diagnosis and cure*, London: Royal Society of Chemistry.

Taber, K. S. (2002b). Compounding quanta: Probing the frontiers of student understanding of molecular orbitals. *Chemistry Education: Research and Practice in Europe, 3*, 159-173. [Available at http://www.uoi.gr/conf_sem/cerapie]

Taber, K. S. & Watts, M. (2000). Learners' explanations for chemical phenomena. *Chemistry Education: Research and Practice in Europe*, *1*, 329-353.
[Available at http://www.uoi.gr/conf_sem/cerapie]

Tsaparlis, G. (1997). Atomic orbitals, molecular orbitals and related concepts: conceptual difficulties among chemistry students. *Research in Science Education, 27,* 271-287.

von Baeyer, H. C. (1993). *Taming the Atom: The emergence of the visible microworld*, London: Viking (First published by Random House Inc., 1992).

Watts, D. M. & Gilbert, J. (1983). Enigmas in school science: Students' conceptions for scientifically associated words. *Research in Science and Technological Education*, *1*, 161-171.