

The Failure of Reduction and How to Resist Disunity of the Sciences in the Context of Chemical Education

ERIC R. SCERRI

Department of Chemistry, Purdue University, West Lafayette, IN 47907, USA

ABSTRACT. The failure, by philosophers of science, to reduce special sciences such as chemistry to quantum mechanics has produced many responses including the notion of supervenience and that of the disunity of the sciences. This article criticizes these responses and proposes an alternative one, namely the autonomy of chemistry. After examining the history of the atomic orbital model I argue that chemical educators should legitimately continue to view terms such as orbital and configuration in a realistic manner although they are deemed to be strictly non-referring in quantum mechanics. Such a view of autonomous though related levels is opposed in particular to the increasingly prevalent notion of disunified sciences.

INTRODUCTION

It is now generally accepted in philosophy of science that the program for the reduction of the sciences, first elaborated by the Logical Positivists, is untenable for various technical reasons. Since this debate has been well covered elsewhere I will not be adding further arguments in favor of anti-reductionism in general.¹ Instead I shall be concerned, in passing, with one formerly claimed reduction, indeed one which has gone unquestioned for perhaps the longest period of time, that of chemistry to quantum mechanics, as well as the educational implications of the failure of this reduction. It is worth noting from the outset that scientists are less inclined to admit defeat over the question of reduction and broadly speaking the reductive approach, whether entirely successful or not, remains at the heart of modern science.

Before entering into any details of the case of the reduction or otherwise of chemistry, I would like to remain on a general level and consider some responses by philosophers of science to the alleged failure of reduction. I believe that one may identify at least two types of current responses, namely seeking refuge in supervenience and the claim in favor of the disunity of the sciences.² The term supervenience has recently acquired a technical meaning in philosophy which may not agree with what one might find as a dictionary definition. In philosophy it is the view that microscopic identity guarantees macroscopic identity but not vice versa. That is to say, if two systems are constructed microscopically from identical components we expect these systems to behave identically on a macroscopic level. However, the observation of identical features in macroscopic systems, it

is claimed, does not entitle us to infer that the microscopic features or causes governing the identity are themselves identical.

I believe that both responses, namely supervenience and the claim that the sciences are fundamentally disunified both suffer from serious flaws but rather than taking sides with any particular one of these positions or offering a new philosophical solution my task here will be to make a pragmatic suggestion which I hope will be useful to chemical educators. Nevertheless, it is worth considering the philosophical debates which have emerged following the demise of reduction, at least in philosophy, since it may be possible to feed back some conclusions about the present case study, involving the relationship of chemistry to quantum mechanics, into the loftier philosophical discussion.

TWO RESPONSES, SUPERVENIENCE AND DISUNITY OF SCIENCE

The notion of supervenience has been much discussed in recent years throughout the philosophy of science.³ Supervenience has been touted as the way to remedy the void left by the collapse of reduction. Although there is no unanimous agreement on the supervenience relationship, the most popular view is that it is a relationship of asymmetric dependence. Two macroscopic systems which might be constructed from identical microscopic components are assumed to show identical macroscopic properties, whereas the mere observation of identical macroscopic properties in any two systems is not taken to necessarily imply identity at the microscopic level.⁴

In simpler terms, the notion is the seemingly obvious one that phenomena which we study in some secondary science are ontologically dependent upon relationships in the primary or more fundamental science or field. This argument has been widely used throughout the philosophy of science (and the philosophy of mind) as a rescuing maneuver from the failure to establish the epistemological reducibility of any of the special sciences. The claim has thus been that supervenience affords us the virtue of ontological dependence, without the vice of explanatory reduction.

Stated otherwise, the claim is that although reductionism may fail in the traditional sense of there being a breakdown in our efforts to establish a continuity between the special sciences and quantum mechanics, we can still maintain that, 'deep down', chemical, biological or even mental states are governed solely by their physical make-up. In this way materialism may be rescued, even though reduction has been found wanting. Moreover, given this approach there is no need to appeal to "ontological emergence", the "supernatural", or other such questionable notions in order to maintain the autonomy of separate levels.

Several authors, myself included, believe that this approach may be largely wishful thinking.⁵ The way that supervenience is meant to rescue us from the failure of reduction may be put in yet another way. Epistemo-

logical reduction, that is the reduction of the axioms or laws of one science to the axioms or laws of a putative deeper science, cannot be carried out in the required fashion. However, we seem to be loath to give up the belief in the ontological dependence of the macroscopic on the microscopic. For example, we find it difficult to consider that chemical substances are anything 'more' than collections of fundamental particles, and so even though reduction cannot be shown in detail we trust that chemistry supervenes over physics. We assume that two chemical systems constructed in an identical fashion from exactly the same fundamental particles ought to behave identically in a chemical fashion. But are we justified in holding such a view?

Conversely it is claimed that it is reasonable to maintain that two systems showing the same chemical behavior can differ microscopically. This represents a view of multiple realization of macroscopic behavior but of unique realization from the fundamental level upwards, so to speak, to the macroscopic. Once again this would seem to be something more akin to a hope than a view which must necessarily be accepted by everyone. Moreover the above asymmetrical supervenience argument is not so compelling to all philosophers, and for example Dupré writes,

But supervenience is not *self-evidently* true. It is surely imaginable, for instance, that people with identical physical states, including states of the brain, might be thinking different things. This possibility is defended by those who believe that the content of thought typically depends on facts external to the thinker. *Evidence* for supervenience, it seems, would have to be the kind of evidence necessary for reductionism. It would be evidence that higher level phenomena are indeed determined by lower-level phenomena, or that identical (or sufficiently similar) lower level phenomena do indeed produce the same higher-level phenomena. As in the case with evidence for reductionism generally, the problem is that where such evidence exists at all, it is in a narrow range of quite specialized cases, and the legitimacy of extrapolation to a general philosophical thesis is, to say the least, questionable. [original italics] (Dupré 1993, p. 97)

To caricature the situation, one might say that the supervenience thesis consists of the view that although repeated attempts have shown that reduction does not operate between any two special sciences we should nevertheless go on believing that it holds essentially or ontologically.

The second response, which appears to be gaining popularity for a variety of reasons, is to maintain the disunity of the sciences, as has been proposed by the likes of Dupré, Galison, Cartwright and others.⁶ In spite of the initial shock with which many working scientists and educators might respond to this disunity thesis it must be said that it has some features to commend it. The thesis seems to play on an interesting form of blurring of the epistemological–ontological distinction, as I believe does the supervenience thesis. In the case of disunity, we are urged to make an ontological conclusion on the basis of the failure of epistemological reduction. The conclusion urged by Dupré, one of the members of the 'Stanford Disunity Mafia',⁷ is not just that theories of the special sciences cannot be reduced to the theory of fundamental particles, but moreover

that this failure should be interpreted to mean that the sciences are ontologically disunified. Dupré makes no secret of wanting to draw such a conclusion when he says on the first page of his book,

The disunity of science is not merely an unfortunate consequence of our limited computational or other cognitive capacities but rather reflects accurately the underlying ontological complexity of the world, the disorder of things. (Dupré 1993, p. 7)

One attractive feature in the disunity thesis is that it forces us to recognize the contextualization of philosophical views about any particular science in question. Rather than making bold pronouncements across the board, concerning all the sciences, regarding realism or anti-realism for example the disunity, and related contextualist view espoused in part by Fine, Cartwright, Dupré and Rouse suggest that different interpretations to philosophical questions can be maintained in different areas of science. This lies in contrast to the work of authors like Laudan and Boyd who despite being on opposite sides of the realism–antirealism debate appear to take it for granted that one should be either a realist or anti realist about all theoretical terms or all theoretical entities, regardless of the science in question (Laudan 1981; Boyd 1983). My own view on these matters is that one can be a contextualist and maintain that such philosophical questions as realism might demand different responses in different areas of science but without needing to admit the more radical disunity of science thesis espoused by authors such as Dupré.

But it is far from clear that all aspects of the disunity of science movement can be considered in a positive light. In a recent book entirely devoted to disunity in science the first page of the editorial introduction by Peter Galison begins with,

Unity. The very term has always evoked emotions. As a political call to arms it rises countries to civil strife, revolutions, and international war. (Galison 1996, p. 1)

Galison thus sets the tone for the entire volume, which is then echoed by a number of contributors, including Nancy Cartwright and her collaborators. This is a tendency to attribute, in my view, an exaggerated influence to political activity in the sphere of scientific knowledge. For example, Galison claims that unity was raised to a scientific ideal in the German speaking countries in the mid nineteenth century.

For it was there, amidst the protracted political struggle for German unification, that scientific unity was raised to a scientific-philosophical ideal (Galison 1996, p. 3)

Meanwhile, Cat et al. (1996) devote an entire chapter to analyzing the work of Otto Neurath, one of the founders of the Unity of Science program, and claim that his apparent support for unity is to be explained by political motivations concerning the times and circles which Neurath moved in. In addition Cat et al. (1997) have produced an entire book which attempts to make much the same case in greater detail.

Surely such concern for political motivations for scientific and philosó-

phical ideals represents a rather narrow conception of what motivates scientific and other attempts to gain knowledge about the world. One dimension which seems to be completely absent from the Galison and Stump volume is the possibility that science might also be motivated by spiritual, religious and other such cosmological or philosophical aspirations, in the widest sense of the word. I suggest that a desire to understand nature in a unified way did not have to wait for a particular set of political conditions to prevail in Germany, or anywhere for that matter, but that it has existed since time immemorial in mystical, spiritual and religious world-views which themselves regard the natural world as a unified whole.

Without wishing to elaborate too much on this theme one might mention the work of Wilber who has analyzed the writings of the founders of twentieth century physics. Wilber concludes that the likes of Einstein, Schrödinger, Heisenberg, Bohr etc. all adopted what he terms an essentially mystical attitude towards their scientific research but he rejects the facile connections between mysticism and physics which were much discussed in numerous books and articles in the 1970s and 1980s (Capra 1974, 1976; Zukav 1979).

Where Galison does venture to consider specific scientific issues to support the claim for disunity we discover a number of rather dubious arguments. We are informed of the recent plea for autonomy from the "guiding principles of particle physics" made by the solid state physics community. Given that these pleas came in the midst of protracted discussions over the funding of the proposed Super Colliding Super Collider project, as Galison acknowledges, this is probably one case in which political factors may have contributed to the public pronouncements of a scientific community which rightly regards itself as being underfunded. Galison goes on to say,

More recent twentieth century physics has sought unity, in a great number of ways, from Einstein's embedding of electromagnetism in a general relativistic space-time, to John Wheeler's minority bid to reduce all of physics to geometry, the unified gauge theories of the 1970s, or the string theories of the 1980s and 1990s (Galison 1996, p. 6).

He then almost immediately adds,

What these various pleas for unity had in common was a hope that an international scientific worldview could curb the divisive racial and nationalistic worldview against which the Unity of Science saw itself in mortal combat (Galison 1996, p. 6)

It would indeed be very interesting to solicit reactions to this view from John Wheeler or a field theorist active in recent times. I cannot help doubting that they would concur with Galison's analysis. In addition Galison says,

In the sciences biology departments splitting into organismic and microbiological, (Galison 1996, p. 6)

as though the reader is supposed to conclude that this shows the sciences

to be fundamentally disunified rather than the more plausible interpretation of inevitable and periodic realignments in areas of research and the formation of new scientific sub-disciplines.

Ian Hacking is another philosopher who has been associated with the disunity of science thesis. This comes about mainly from his championing the cause of philosophy of experimentation and his urging, as does Galison, that experiments appear to take on a life of their own with respect to theories in science. But it should also be noted that Hacking has taken a far more circumspect approach to disunity. Rather than taking sides over this question he often appears to be more concerned with laying out the varieties of claims concerning unity or disunity (Hacking 1996). He suggests that when scientists talk of unity they frequently mean harmony between different parts of science or different phenomena and not singleness. For example, he cites Faraday as wanting to discover harmony between the properties of light and magnetism, something which he indeed succeeded in doing.

Hacking correctly points out the rift which exists between the way in which scientists and philosophers view the unity of science. Philosophers in the Anglo-American tradition have analyzed unity by means of language and logic and have been inclined to lean towards disunity, if formal reduction, or what Hacking terms global reduction of the sciences has not been forthcoming. As he cogently points out,

Contrary to what is commonly made out, global reductionism is not of great interest in scientific work – it is something that philosophers read into science (Hacking 1996, p. 50).

and also,

The philosophers who want to unify seem not just to be playing in another ballpark [from scientists] or even another league: they are playing a different game (Hacking 1996, p. 60).

What Hacking might have added is that if there is any glaring disunity anywhere then it is to be found in the different way in which scientists and philosophers regard the special sciences. Before ending this section on disunity I should stress that I have highlighted the more startling aspects of the thesis and I fully accept that I have probably not done justice to many of the subtle arguments concerning the, mostly philosophical, benefits of adopting such a view.⁹

ANOTHER APPROACH

Of course there are other possible responses to the realization that the special sciences cannot be reduced to physics. For example, Kincaid offers one such alternative in a study on molecular biology (Kincaid 1990). On one hand he maintains that molecular biology cannot be reduced to chemistry, citing the recent work of Blobel, Dobberstein and others. The

latter researchers have proposed the signal hypothesis whereby a protein knows where to go in a cell in the course of DNA transcription to form polypeptides.

Reporting on these studies Kincaid concludes that reduction fails in the following three senses.

1. The predicate signal sequence has multiple realizations in biochemical terms given that at least 200 different amino acid sequences have been found to act as signals in this way.
2. The problem of context-sensitivity manifests itself since particular sequences may or may not serve as signals depending on the cellular context in question.
3. The very concept of a signal sequence is defined in terms of its biological function, thus raising the problem of presupposing higher level explanations in the putative reductive account.

And yet in spite of this seemingly overwhelming evidence for the breakdown of reduction, Kincaid is perfectly happy to claim that molecular biology nonetheless provides an excellent example of . . . non-reductive unity (p. 589).

As he concludes,

Thus while molecular biology does not support the reducibility of biology to chemistry, it certainly argues for their unity. Molecular biology leaves biological explanations their role, yet combines them in a systematic fashion with those of biochemistry. As such, molecular biology presents a paradigm of non-reductive unity in the sciences. (Kincaid p. 591)

As I will claim in the following section, the relationship between chemistry and physics, or more precisely quantum mechanics, could be construed as another example of such non-reductive unity. Quantum mechanics fails to strictly reduce chemistry in various senses and yet provides a unified approach to the calculation of atomic and molecular properties and an excellent tool for rationalizing an increasing part of chemistry. For example, the Schrödinger equation for any chemical system can be solved approximately and this may be taken to be the unification afforded by quantum mechanics. But we are unable to obtain exact solutions in many-electron systems and this represents the failure of strict reductionism. Nevertheless, I prefer to avoid following Kincaid too closely and shall be arguing that the relationship between chemistry and quantum mechanics is one of autonomy of chemistry. This position can be situated in the middle ground between complete unity as advocated by Kincaid and disunity of the sciences as envisaged by Dupré and others.

CHEMICAL EDUCATION

I come now to the relationship of these philosophical discussions to the question of science education and in particular the question of teaching chemistry. To put the question starkly, how is it that if chemistry has

not been reduced to quantum mechanics, nevertheless many chemistry textbooks begin with a thorough treatment of quantum mechanics, atomic structure, electronic configurations and the like? Are chemical educators merely oblivious of the work of philosophers who generally maintain that reduction is no longer tenable? Is it because the reduction of chemistry is one case in which one can ignore the pronouncement of philosophers, perhaps because chemistry lies so close to physics? Or is it perhaps due to some as yet unarticulated justification which implies that chemical educators know what is best for teaching chemistry regardless of these philosophical debates?

Of course although I have been taking it for granted in the present article that all hope of reduction has collapsed, this conclusion is only prevalent in philosophy of science. Scientists themselves continue to regard reductionism as a very fruitful path to gaining knowledge. If reduction of chemistry is considered from a naturalistic viewpoint as I have advocated previously, the question as to whether or not chemistry has been reduced to quantum mechanics depends on the present state of computational quantum chemistry and in particular *ab initio* calculations of chemical properties. In this sense, one might want to concede that chemistry has been approximately reduced to quantum mechanics, although even the notion of approximate reduction is problematical (Scerri 1994, 1998). But since this reduction is not sufficiently clear-cut one response has been to claim that chemical educators are wrong to base the presentation of chemistry so closely on quantum mechanics. Indeed I have urged this response myself in the past (Scerri 1991), but in the present article I wish to revise my view in an important way.

The view which I will be advocating here is that chemical educators should continue to use concepts like orbitals and configurations but only while recognizing and emphasizing that these concepts are not directly connected with orbitals as understood in modern quantum mechanics, but are in fact a relic of the view of orbits in the so-called old quantum theory. One might even consider calling them 'chemists orbitals'. After describing this case in chemical education in more detail I will conclude by trying to see what methodological lessons, if any, can be gained from this case about the more general philosophical debate which I briefly mentioned above. My overall message will be to argue for an autonomy of the sciences which I regard to be a far less radical position than the claim of disunity. The autonomy which I espouse consists more specifically of the view of autonomous though related levels of reality. The relationship between the sciences or sub-disciplines in question can be spelled out as a causal though discontinuous link between the use of terms in one field and those in another, by examining the historical development of these terms. I should add that I do not wish to claim any originality for the notion of autonomous but related levels and would point the reader to the work of Campbell and Wimsatt, among others (Campbell 1974; Wimsatt 1976).

ORBITALS AND CONFIGURATIONS IN CHEMICAL EDUCATION

The following quotations are taken from a chemistry textbook and a journal article respectively. They show the overwhelming ubiquity of 'orbital talk' in contemporary chemistry and the apparent disregard for the ontological redundancy of orbitals which as I shall argue is dictated by quantum mechanics.

Continuing on from mercury, which follows gold, we come via the noble gases radon and the radioelements Fr and Ra to actinium, with the outer configuration $7s^26d$. Here we might expect, by analogy to what happened at lanthanum, that in the following elements electrons would enter the 5f orbitals, producing a lanthanide like series of fifteen elements. What actually occurs is, unfortunately, not so simple. Although immediately following lanthanum the 4f orbitals become decisively more favorable than the 5d orbitals for the electrons entering in the succeeding elements, there is apparently no great difference between 5f and 6d orbitals until later. Thus for the elements immediately following Ac, and their ions, there may be electrons in the 5f and 6d orbitals or both. (Cotton and Wilkinson 1986, pp. 626–627).

The main difference between the elements of the 4th and 5th periods and those of the 6th period is due to the fourteen 4f electrons filled in between filling of the $6s^2$ and 5d electrons. The filling of the 4f shell shields the less penetrating 5d orbitals more effectively than the 6s orbitals, because the d electrons are more effectively kept away from the inner parts of the atom by the centripetal force $1(1 + 1)/r^2$, so that the stability of the $d^m s^2$ configuration is increased in the 6th period (except for Pt and Au). This effect will be even greater for the 6d elements, because the 7s electrons should drop relatively deeply into the atom and thus feel the very strong potential near the nucleus, whereas the 6d electrons are expected to be shielded more strongly by the 5f electrons. (Fricke and McMinn 1976)

A few years ago a controversy erupted in a chemical education journal, following the publication of an article by Ogilvie in which he claimed in his subtitle that "there are no such things as orbitals" (Ogilvie 1990). This article was, in part, an attack on the views of Linus Pauling which Ogilvie claimed were continuing to cause problems in the manner in which chemistry is taught. The article provoked a number of responses including one from Pauling himself in which he unrelentingly defended his original views (Pauling 1992; Scerri 1992; Scott 1992).

Without wishing to re-open this debate I would like to raise a couple of issues arising from it in passing on to the main theme of the present article. Ogilvie's main claim for the non-existence of orbitals appears to hinge on the fact that there are several formulations of quantum mechanics including, at the most elementary level, Heisenberg's matrix mechanics and Schrödinger's wave mechanics. Ogilvie maintains that orbitals cannot be regarded as being fundamental since they only emerge from one of these formulations, namely Schrödinger's wave mechanics. However, throughout his long and detailed article he fails to cite the one important criterion which renders the existence of orbitals redundant even within the Schrödinger formulation. Since this feature will be discussed in some detail in a subsequent section of this article I will not elaborate at this point except by saying that it occurs because the assignment of quantum

numbers is strictly invalid in many-electron atoms. Instead of concentrating on the startling announcement in his subtitle, "There are no such things as orbitals", Ogilvie proceeds to argue for the lack of experimental evidence for the real existence of hybrid orbitals in molecules such as methane.

Pauling's response in a later issue of the same journal consists mainly of an *ad hominem* assault in which he accuses Ogilvie of failing to understand quantum mechanics. One rather interesting remark made by Pauling in response to Ogilvie's claim that orbitals do not exist is the following,

The subheading of the Ogilvie paper "There Are No Such Things As Orbitals!" contains a misconception of the meaning of the word "thing". One of the dictionary definitions of "Anything that is or may become an object of thought"; in other words, a thing need not be tangible, but it could be represented by a symbol . . . Quantum mechanical expressions for orbitals, such as those that Mulliken and I and scores of other theoretical physicists have formulated, are clearly objects of thought, and hence are things (Pauling 1992, p. 520).

One does not need to be a philosopher to appreciate the folly of Pauling's remark. Surely the mere fact that unicorns and fairies, for the sake of argument, might be objects of thought does not imply that they exist in the real world. One wonders whether Pauling would have accepted a subheading which had simply stated "Orbitals do not exist" which would have avoided the use of the word "thing" and would still have conveyed Ogilvie's intention.

Although this particular controversy was terminated by editorial fiat, the question of how to teach chemistry and in particular whether to put quantum mechanics, before the chemical facts, continues to be a source of discussion in chemical education circles (Basolo and Parry 1980; Bent 1984, 1987; Gallup 1988; Gillespie et al. 1996; Hudson 1980; Pilar 1981; Sanderson 1986; Schaffrath 1983; Zuckerman 1986). In previous articles I sought to remind chemical educators that the orbital concept which is so prevalent in chemistry is not underwritten by theoretical physics, and in particular quantum mechanics, from which the concept is commonly supposed to emerge. I implied that chemical educators were mistaken in emphasizing atomic structure and quantum mechanics thus putting physics before chemistry, since the orbital concept which chemists concentrate their attention upon, does not in fact 'exist' (Scerri 1991).

I was emphasizing, as some philosophers of science might, that the term orbital does not refer according to quantum mechanics. That is to say, according to quantum mechanics à la Schrödinger and Heisenberg, orbitals should not be regarded realistically although in the old quantum theory, orbits, as they were then termed, could be so interpreted. I therefore urged a partial return to teaching chemistry according to qualitative concepts rather than falling prey to the seductive influence of quantum mechanics and atomic structure. Recently I have come to a new view of these matters, which I now turn to.

First of all, it would appear that the use of orbitals and configurations

in chemistry has continued to increase and the chances for a return to the nostalgic days of chemistry based upon 'smells, bangs and colors' appear increasingly dimmer. However, there is a deeper philosophical reason why one should stay loyal to orbitals in chemistry education while at the same time not committing any errors from the point of view of quantum mechanics. I believe that in pronouncing on the situation from the perspective of theoretical physics I was myself falling prey to the ever lingering reductionist view which considers that physics rules all of science, or what has sometimes been termed 'physics imperialism'. A more enlightened way to regard such questions would be to bite the bullet and assert that physics imperialism is at fault and that the special sciences are, as I suggested above, autonomous and thus not entirely dependent upon the latest pronouncements from theoretical physics.

To return to the question of chemical education and how one should present chemistry, what I now wish to urge is that given the generally accepted failure of reduction of the sciences, we should embrace this state of affairs and incorporate this knowledge into the way in which we teach subjects like chemistry. My suggestion is that the downfall of the notion that all the sciences reduce to physics leads to a form of liberation in that one may continue to use concepts like orbitals in chemistry, despite the strictures from quantum mechanics that orbitals do not truly exist.

However, one important change must be made in the presentation of the subject and that is that we must cease to pretend that the chemists orbitals are the same as those of the theoretical physicist. In other words we should continue to use the highly productive paradigm of orbitals and configurations but only while claiming it as a distinctly chemical paradigm, not one which is strictly compatible with quantum mechanics. Only by upholding such an independence from the quantum mechanician's orbitals can the chemist attribute any reality to what I have dubbed as chemical orbitals with, as it were, a clear conscience.

The link between physicists and these chemist's orbitals is a causal but discontinuous connection which may be discerned by considering the historical development of the concept of an orbit and later an orbital. My claim is that what chemists refer to as an atomic orbital began as the theoretical term, orbit, which was considered to refer in theoretical physics between approximately the years 1900 and 1925. Following the invention of quantum mechanics, physicists realized that orbits do not refer to real entities in the world and the advent of a probabilistic interpretation of electron motion led to the adoption of the new term orbital. It would appear that while chemists have adopted the probabilistic notion of electronic motion in the form of the orbital they retain the ontological appeal of the older term orbit as an entity which refers. It is necessary to briefly recap on the historical changes which the concepts of orbit, orbital and electronic configuration underwent in order to appreciate the situation in question here. These changes are interconnected with the historical development of the periodic system as will be outlined below.

HISTORICAL DEVELOPMENT OF ORBITALS AND CONFIGURATIONS

For the benefit of readers who may not be well versed in chemistry it should be explained at the outset that in arriving at the electronic configurations of an atom a procedure is used in which electrons are assigned to particular orbitals. This way of obtaining the electronic configuration of any atom is called the aufbau procedure and was introduced by Niels Bohr. The concept of electronic configuration is thus inextricably linked to that of orbits and orbitals. I now proceed to give a historical overview of the development of electronic configurations.

The discovery of the electron shortly before the turn of the century saw a shift towards attempts to understand the periodic system in terms of microscopic properties, namely the electronic configurations of the atoms of the elements. Within four years of J. J. Thomson's discovering the electron in 1897, the Frenchman, Jean Perrin, had postulated a planetary model of the atom in which a central positive charge, or sun, was surrounded by a number of electrons or negative planets. This may be regarded as the first model of the atom having orbiting electrons. A similar planetary model, more specifically called a Saturnian model, was suggested by Nagaoka in Japan. In this case the electrons were thought of as moving in rings around the nucleus just as the Saturnian rings circulate around the planet Saturn. In the same year, 1904, J. J. Thomson introduced his 'plumb pudding' model of the atom (Thomson 1904).

Already in 1897 when he had announced the discovery of the electron, Thomson had postulated that this particle might provide the key to explaining chemical periodicity. Soon thereafter, he made the first detailed attempt to explain periodicity, and produced a set of electronic configurations of atoms, the earliest precursor of today's electronic configurations. The electrons in Thomson's model were thought of as being imbedded in the positive charge, the 'pudding', while also circulating in concentric rings. Another essential idea which Thomson introduced in the same paper was that atoms of successive elements differ by the addition of a single electron.

Thomson calculated the number of electrons needed in each ring from considerations on mechanical stability and connected this feature with periodicity in electronic configurations. His configurations involved variations in inner rings and are not of great interest particularly as they did not correlate in any simple way with the valences of the chemical atoms. Thomson's model was soon discarded by Ernest Rutherford whose experiments with the scattering of alpha rays led him to postulate a return to a solar system model of the atom. Rutherford did not however venture to attack the problem of chemical periodicity and made no attempt to assign electronic configurations as Thomson had.

As all students of chemistry know, in 1913 Niels Bohr solved the problem of the mechanical instability of Rutherford's model by postulating the quantization of the angular momentum of electron in the hydrogen atom.

As historians Heilbron and Kuhn have argued, Bohr's initial motivation for his famous trilogy article, in which he announced his quantum theory of the atom, was a desire to explain chemical periodicity (Heilbron and Kuhn 1969). In the course of this article Bohr returned to Thomson's search for electronic configurations as an explanation for the form of the periodic table. Even with his first attempt he obtained a set of configurations which were well correlated with the valences of the atoms. Essentially, the valency of each element was found to coincide with the number of outer-shell electrons in Bohr's atomic configurations.¹⁰

The chemical similarities shown by the elements in the same group of the periodic table could now be explained as resulting from sharing the same number of outer-shell electrons, a view that remains at the heart of modern chemistry. The view which arose from Bohr's work is that the configurations of atoms can be built-up systematically using the 'aufbau principle' in which nuclear charge increases by one unit and an additional electron is added to the atom of the previous element in the periodic table, while not altering any of the 'locations' of the electrons which are already present.

Over the next few years, further small improvements were made to the tables of electronic configurations by Langmuir, Bury and others. Bohr returned to the question of chemical periodicity in 1923 and gave an account based on two quantum numbers, making use of Sommerfeld's newly discovered azimuthal quantum number for each of the electrons. This new scheme extended Bohr's previous theory of periodicity, which had used just one quantum number, and thus revealed greater detail in the electronic arrangements. For example, the configuration of the atom of sulfur now emerged as 2, 4, 4, 6 thus maintaining a valency of six in accordance with the chemical facts about this element. However, sulfur can also show valences of 2 or 4 depending on which compound is considered. Such anomalies contributed to the next development, which was the introduction of a third quantum number in attempts to understand periodicity.

In 1924, Stoner produced tables of electronic configurations based on the inner quantum number, also introduced by Sommerfeld, in addition to the two quantum numbers which Bohr had used. The configuration of sulfur became 2, 2, 2, 4, 2, 2, 2 where the last three numbers represent the outer-most electrons. The observed valences of two, four or six shown by the element could therefore be easily accommodated for by this new version, depending on how many of the outermost electrons are regarded as entering into chemical combination (Stoner 1924).

However, one rather important problem remained regarding periodicity, that of the so-called closing of the electron-shells. The question was to try to understand the series of whole numbers starting with 2, 8, 18 and 32 which characterizes the total number of electrons which can be accommodated by successive electron shells around the nucleus of the atom. The solution was provided by Wolfgang Pauli who postulated yet

a fourth quantum number, which eventually became associated with electron spin.¹¹ Pauli further stipulated that no two electrons could share the same set of four quantum numbers. If two electrons had exactly the same three quantum numbers, they would differ in the fourth, one adopting a value of $+1/2$ units of angular momentum and the other one $-1/2$. The manner in which the problem was solved may be seen by reference to the table below,

TABLE I
Assignment of quantum numbers based on Pauli's scheme.

n	l	m _l	m _s	Number of electrons
1	0	0	+1/2	2
			-1/2	
2	0	0	+1/2	2
			-1/2	
2	1	-1	+1/2	2
			-1/2	
2	1	0	+1/2	2
			-1/2	
2	1	1	+1/2	2
			-1/2	
3	0	0	+1/2	2
			-1/2	

When the first quantum number or n takes the value of one, the second quantum number can only be zero, and likewise the third quantum number. According to Pauli's principle it is forbidden for more than one electron with the same value of n to have the same values for the remaining three quantum numbers. This gives a prediction, for the first shell, of a maximum of two electrons, which share the first three quantum numbers but differ in their value of the fourth quantum number which may adopt either of two possible values. For the $n = 2$ shell the situation is more complicated, since there are two possible values for the second quantum number, namely one and zero as shown in Table I. As noted above, when the second quantum number is zero, the third quantum number also adopts a zero value, and since the fourth quantum number can adopt two possible values, two electrons are accounted for. When the second quantum number in the second shell takes a value of one, the third quantum number may take on three possible values of -1 , 0 and $+1$ each of which can show two values for the fourth quantum number to account for a further six electrons. Considering the second shell as a whole, a total of eight electrons is therefore predicted, in accordance with the experimental evidence. Similar considerations for the third and fourth shells predict 18 and 32 electrons respectively, once again in accordance with the arrangement of the elements in the modern periodic table.

The closing of the various shells was thus seen to be a consequence of

Pauli's exclusion principle which prohibits any two electrons from having the same four quantum numbers, and the assumption that the fourth number itself can only adopt two possible values, while all the previous rules for assigning the values for the second and third quantum numbers for a given value of the first quantum number are retained.

Modifications to quantum theory were made by Heisenberg and Schrödinger in 1925 and 1926 to yield quantum mechanics in essentially the form used to this day. However, the impact of the new quantum mechanics on the periodic table has been rather minimal since the Schrödinger equation cannot be solved exactly except for the very first atom, hydrogen. This means that the electronic configurations of atoms, on which our modern understanding of the periodic table is based, cannot be strictly derived from first principles, although approximations used in quantum chemistry can account, after the facts, for all spectroscopically observed configurations (Scerri 1994c).

The apparent order imposed upon the periodic table by adopting a microscopic approach of using electronic configurations is far from perfect. Approximately twenty elements possess anomalous electronic configurations whereby they show unexpected arrangements of electrons in which they differ from other members in the same group of the periodic table.¹² For example, nickel, palladium and platinum occur in the same column of the periodic table and yet show different outer-shell configurations. There are also cases of atoms which do not adopt the configuration which might be expected on the basis of the ordering of energy of the various atomic orbitals in question. The element scandium represents such an example in that contrary to the account in most textbooks, calculations show that the 3d orbital has a lower energy than the 4s orbital and yet the order of filling orbitals requires the occupation of the 4s orbital before that of 3d. Such subtle effects are difficult to rationalize, even within a full blown quantum mechanical treatment (Melrose and Scerri 1996).

Furthermore, it is not possible to begin with quantum mechanics and to predict in a strictly deductive manner which electronic configuration is adopted by a particular atom. This is because existing calculations depend on assuming a particular basis set or set of orbitals, which are in turn obtained from spectroscopic observations. What can be done is to use quantum mechanical calculations to examine which of a number of alternative possible configurations might be the one with the lowest energy (Scerri 1994a). For example, in the case of scandium, three candidate configurations for the ground state are; $[\text{Ar}]4s^23d^1$, $[\text{Ar}]3d^3$ and $[\text{Ar}]4s^13d^2$. Calculations carried out through the Hartree-Fock method of approximation predict that the first of these configurations shows the lowest energy in accordance with experimental observations. Electronic configurations and the related orbital concept cannot therefore be strictly reduced to quantum mechanics for many-electron atoms.

Indeed, strictly speaking, quantum mechanics in its most general form forbids any talk of electrons in orbitals and hence electronic configur-

ations. In technical terms this is because the operator representing the quantum number of any particular electron, for example, the angular momentum of an individual electron, fails to commute with the Hamiltonian of a many-electron atom. This means that the eigenfunctions corresponding to the angular momentum operator of single electrons are not strictly defined quantities. The assignment of individual quantum numbers to individual electrons become invalid as a result of this mathematical relationship. Since such labels can no longer be placed on individual electrons they must be regarded as indistinguishable. The Pauli Exclusion Principle remains valid, but must be re-expressed in such a way as to uphold the non-individuality of electrons and this is done by stating that the atomic wavefunction is anti-symmetric with respect to the interchange of any two electrons. The important point is not just that the new quantum mechanics forbids the visualization of atomic orbitals but that it also forbids us from even defining an orbital mathematically, through the assignment of individual quantum numbers to each electron, except in the case of the hydrogen atom. It is in this particular sense that quantum mechanics tells us that orbitals and configurations do not strictly exist, that is to say, they cease to refer to real entities in the natural world.

CONCLUSION

However, chemists, and incidentally many physicists, have felt no need to accept this refinement in the ontological status of orbitals and have continued to regard orbitals as referring terms. Chemists and applied physicists continue, to this day, to regard orbitals and configurations realistically, not because they are weak minded and enamored of pictures, as theoretical physicists often cynically imply, but because regarding orbitals realistically is appropriate to the practice of giving explanations and generally interpreting phenomena in chemistry and applied physics.

The mistake in chemical education has not been an excessive use of the orbital concept but rather the mistaken genuflection in front of the 'God of Quantum Mechanics'. This erroneous tendency has produced the illusion of falsely grounding the chemist's orbital in current quantum mechanics whereas the concept has in fact been inherited from the old quantum theory. Stated in slightly different terms, while the evolution of quantum mechanics has shown the orbital concept to be ontologically redundant, chemists¹³ have unwittingly retained it in its older form of the orbit which originated in Bohr's old quantum theory.

Herein I believe lies the autonomy, rather than the disunity, of chemistry from quantum mechanics. Whereas in one sense chemistry appears to lag behind theoretical physics, in another equally important sense chemistry has latched onto an extremely useful explanatory model. Chemists have rightly shown great reluctance to abandon the realistic interpretation of this model in spite of the theoretical pronouncements from physicists

who claim that the model does not correspond to anything in the real world. Chemists and chemical educators have thus instinctively resisted physics imperialism but at the same time have given the confusing impression that they wish to submit to it through their frequent appeal to quantum mechanics. I suggest that the gap between theoretical physics and chemistry in this example is quite appropriate due to the fact that chemists operate on an separate, though related, level which may require a less fundamental and hence usually an older version of any particular physical theory.

It is also important to draw a clear distinction between the use of orbitals and electronic configurations as an explanatory device in inorganic or organic chemistry from the way in which orbitals are interpreted in theoretical chemistry, or more specifically the branch known as computational quantum chemistry. In the latter field the practitioners, who are also sometimes referred to as chemical physicists, are under no illusions regarding the theoretical status of the orbital approximation. Highly sophisticated computational techniques have developed which involve the expansion of the wavefunction for any particular chemical system in question as a linear combination of terms involving atomic orbitals and taking the electronic configuration of atoms as a starting point. In this approach orbitals and configurations are most definitely not regarded realistically. These theoreticians know only too well that the central failing of the orbital approximation is the neglect of instantaneous, as opposed to time averaged, inter-electron repulsion. Indeed most of the computational effort is expended in trying to remedy the deficiencies of the orbital approximation which neglects the above mentioned phenomenon, also termed electron correlation. Needless to say, the distinction I have drawn in earlier sections of this article does not include work in this field at the borderland of chemistry and physics.¹⁴ I believe that researchers in computational quantum chemistry and closely allied fields would tend to regard the orbital approximation in a purely instrumental fashion, contrary to their colleagues in general and synthetic chemistry. I emphasize that it is the interpretation of orbitals and configurations by practicing inorganic and organic chemists which the bulk of the present article is concerned with and not with the mathematically more sophisticated use to which orbitals are put by quantum chemists. Not only is the question of the realistic as opposed to anti-realistic interpretation of the orbital concept contextual with regards to whether one considers chemistry or theoretical physics but even within chemistry it emerges that practitioners in different sub-fields generally adopt opposite interpretations. I suggest that this case study regarding the philosophical interpretation of orbitals in chemistry and physics should be considered in the wider debates which persist regarding the realistic versus anti-realistic interpretation of theoretical scientific terms.

It must also be said that arguments I have given for the autonomy of chemistry from quantum mechanics apply, though to a lesser degree, vis

a vis solid state physics. This and other applied branches of physics also show a degree of autonomy from quantum mechanics. The tendency to regard atomic orbitals realistically is also prevalent in these sub-disciplines, as are errors involving the indistinguishability of electrons. For example, it is not uncommon for textbooks and encyclopedias of physics to refer to 'free' or 'bound' electrons in discussing the topic of Fermi surfaces. This labeling of electrons, as free or bound, is contrary to the quantum mechanical stricture of electron indistinguishability.¹⁵ My claim is thus not so much that chemistry is autonomous from physics, as a whole, but rather that it autonomous from quantum mechanics.

As indicated in the introduction, the present study might also be of interest to those who have claimed that the sciences are disunified. I conclude that the relationship between the adjacent fields of chemistry, applied physics and quantum mechanics presents an argument for the autonomy of chemistry and applied physics and not their disunity or disconnection from quantum mechanics. Moreover, support for the autonomy of chemistry and applied physics which has been urged here can be rationally defended within the historical evolution of the orbital concept, as was argued above, and is by no means dependent upon sociological or other similar factors.

In some ways it might be thought that the current prevalence of the disunity of science thesis is a result of the work of Thomas Kuhn and his initial enthusiasm, at least, for the existence of distinct paradigms and the lack of unity even across theory changes. Even though I believe there to be an element of truth in this suggestion the debate appears to have moved on somewhat since Kuhn initiated such ideas. Indeed some of the proponents of the disunity thesis has seized upon is at a possible means of clarifying the present debate between realists and relativists (Stump 1996). Be that as it may, the possible means of healing of philosophical problems should not necessarily lead scientists, and especially science educators, to begin to regard the unity within modern science as being somehow under threat although they can gain great enrichment from being aware of the issues concerned in the disunity debate.

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NOTES

¹ The following references provide a survey of views in favor and against reduction of the special sciences in the philosophical literature. Darden and Maull 1977; Kemeny and

Oppenheim 1956; Nagel 1961; Kuhn 1962; Sklar 1967; Nickles 1975; Sarkar 1992; Schaffner 1967; Freidman 1980.

² Another response has been to invoke the notion of emergence of properties, a view which has been recently defended by Humphries among others but on which the present article will have very little to say (Humphreys 1996).

³ See for example Kim (1984). Some authors have even drawn on the relationship between chemistry and physics to illustrate their basic arguments about the supervenience relationship (Papineau 1993).

⁴ The role of smell in chemistry as an example of supervenience has previously been discussed in general terms by the author (Scerri and McIntyre 1997).

⁵ These authors include Dupré as well as Dennett, Garfinkel, Putnam and Wimsatt. See Kincaid (1990) for references to all of these except Dupré.

⁶ See Galison and Stump (1996), as well as Cartwright (1994) and Hacking (1983).

⁷ I learned this term in the course of a conversation with John Dupré. The 'godfather' from whom this disunity view originates is Patrick Suppes, a long-standing member of the Stanford philosophy department (Suppes 1978). Dupré, Galison, Cartwright and Hacking have all been associated with the Stanford department at some time. Coincidentally, Suppes is one of the few philosophers to stress the irreducibility of even quantum chemistry to quantum mechanics, which he does in his seminal 1978 article.

⁸ Rouse (1996)

⁹ See for example the articles by Stump and Rouse in the Galison and Stump volume (Galison and Stump 1996). In addition, Galison's earlier book argues persuasively against constructivist views in the context of experimentation (Galison 1987).

¹⁰ This was not altogether such a theoretical triumph since Bohr actually used the chemical valences to fix the configurations, although he gave the impression that they had been derived from the principles of the quantum theory of the atom (Scerri 1994)

¹¹ Pauli initially resisted the association of his fourth quantum number with the concept of mechanical spinning motion (Scerri 1995).

¹² The following elements show anomalous configurations; chromium, copper, niobium, molybdenum, ruthenium, rhodium, palladium, silver, lanthanum, platinum, gold, actinium, gadolinium, lutetium, thorium, palladium, uranium, neptunium, curium and lawrencium.

¹³ The same argument can be made throughout for the relationship between applied physics and theoretical quantum mechanics.

¹⁴ The people who work in computational quantum chemistry frequently show departmental affiliations to physics, chemical physics and even computation.

¹⁵ Such a version is given in the entry by Bohm and Tepley, entitled Fermi Surfaces in a well respected Encyclopedia of Physics (Bohm and Tepley 1974). Conversely the entry by H. G. Kuhn (no relation to Thomas Kuhn) under the title of Atomic Physics points out the limitations of the orbital approximation rather carefully.

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