REDUCTION, EMERGENCE AND PHYSICALISM

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1 INTRODUCTION

There are two main reasons why the subject matter of physics might be thought ontologically prior to that of chemistry. The first is mereological: properties of wholes depend in some way on the properties of their parts. If physics studies the parts of the kinds of things that chemistry studies, the priority claim follows. And this makes physics basic to the explanatory aims of chemistry itself, for chemistry, so the argument goes, is explanatorily analytical: to explain what things do, it looks to their parts. The second line of thought is that the science of physics is unique in that it aims at full coverage. Physical laws cover *everything*, but the laws of other sciences, including chemistry, are of restricted scope: their truth does not require their full generality. Since physical laws cover everything, including chemical systems and their parts, if possession of a chemical property confers genuine causal powers, this must be in *virtue of* some relationship that that chemical property bears to some property that falls under a physical law. Both these considerations are empirical, and are also supported historically by the close interaction between the two disciplines that began in the nineteenth century, when physical methods of investigation like spectroscopy began to be accepted in chemistry. The relationship was cemented by the appearance of accurate physical models of atoms early in the twentieth century. Before that, it was an open question whether the chemists' atoms would turn out to be the same as the physicists' atoms (see [Knight, 1995, Chapter 12]). But can these considerations be turned into arguments that chemistry is reducible to physics? Clearly the *discipline* of chemistry is distinct and autonomous from the point of view of its practice and history [Bunge, 1985; Nye, 1993, Chapter 2], but what of its entities, theories and laws?

The classical models of intertheoretic reduction are now widely rejected by philosophers, but in Section 2 I will consider how well they fit the relationship between physics and chemistry, if only because they are so well understood. The central point is that the failure of the explanatory relationship between physical and chemical theories to fit some model of intertheoretic reduction does not settle the question of whether chemistry is reducible 'in principle.' There are many

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reasons why intertheoretic reductions can fail that are independent of 'in principle' reducibility, including mathematical intractability, complexity and conceptual mismatch between different sciences. Faced with a failed intertheoretic reduction, temperamental reductionists will blame these other factors (for further discussion of this point, see [Hendry, 2010]). That is why, from Section 3 onwards, I concentrate on the ontological issues, which promise a more direct approach to the question of reducibility in principle.

2 CHEMISTRY AND CLASSICAL REDUCTION

Reduction, in Ernest Nagel's classic description, is 'the explanation of a theory or a set of experimental laws established in one area of inquiry, by a theory usually though not invariably formulated for some other domain' [Nagel, 1979, 338]. Nagel distinguishes two kinds of intertheoretic reduction. (i) In a 'homogeneous' reduction, the descriptive terms of the reduced theory appear also in the reducing theory, as in the joint subsumption of Kepler's and Galileo's laws by Newtonian mechanics. (ii) Where the reduced science makes use of a distinct set of descriptive terms, a reduction is 'heterogeneous': Nagel cites 'temperature' in the relationship between thermodynamics and statistical mechanics. In this second kind of case, the connection between the vocabularies of the two theories must be forged by means of 'bridge laws', widely assumed (though not by Nagel) to be biconditionals relating predicates of the two theories. Nagel allowed that the bridge laws may either be: (i) analytical (i.e. true in virtue of the established meanings of the theoretical predicates); (ii) conventional (i.e. established by fiat); or (iii) physical hypotheses [1979, 354]. Different kinds of bridge law would presumably yield reductions of different kinds and degrees of scientific and philosophical interest and importance. In the reduction of thermodynamics to statistical mechanics, it would be too easy, and of dubious explanatory value, merely to *redefine* 'temperature' as 'mean molecular kinetic energy.' 'Temperature' already means something in thermodynamics, so the effect of redefinition would be ambiguity: occurrences of the word 'temperature' in thermodynamics and statistical mechanics would differ in meaning, and it would be a mistake to equate the numerical values associated with them. A physical hypothesis would still be required to relate thermodynamical and mechanical temperature, though not one that could be tested directly [Nagel, 1979, 358-9]. Connectability through bridge laws, then, is one necessary condition on intertheoretic reduction. The second condition, reflecting the broadly explanatory nature of reduction, is that the laws of the reduced science are derivable from those of the reducing science.

A more explicitly mereological account of reduction is offered by Paul Oppenheim and Hilary Putnam [Oppenheim and Putnam, 1958], who argue that the explanation of the properties of complex systems in terms of the properties of and relations between their parts (microreduction) is a characteristic and fruitful scientific project. Microreduction is mereological because theory T_1 microreduces a theory T_2 when the phenomena explained by T_2 are explained by T_1, and T_1

describes the parts of the objects described by T_2. On the assumption that the microreductive explanation takes the form of a deduction, microreduction will be a kind of Nagel-reduction. Oppenheim and Putnam do not explicitly identify explanation with deduction, but the identification is suggested by their assumption that reduction is a transitive relation: explanation is not obviously transitive, unless analysed in terms of some transitive relation like deducibility.

Three features of these classical accounts of reduction are worth emphasising. Firstly, intertheoretic reduction is a kind of subsumption, in which a more generally applicable theory replaces one of more restricted application. Secondly, intertheoretic relationships may show how to correct the laws of the reduced theory, as when the atomic theory showed how to correct the ideal gas laws to reflect the molecular structure of gases, via the van der Waals equation of state. Thus the laws of the reduced theory may be recovered only approximately. Thirdly, because reduction is an intertheoretic relation, the reduction of one discipline (or 'domain') by another is a scientific achievement secured at some specific time, when theories with the requisite explanatory resources become available.

Nagel, Oppenheim and Putnam saw the explanatory application of physical laws to chemistry as the paradigm example of reduction, and it is still cited as such. So how accurately does classical reductionism portray the undoubted explanatory success of physical theory within chemistry? Two main examples are cited in the literature: (i) the relationship between thermodynamics and statistical mechanics; and (ii) the explanation of chemical valence and bonding in terms of quantum mechanics. The former reduction is widely presumed to be unproblematic because of the identification of temperature with mean molecular kinetic energy, but Needham [2009] points out that temperature can be identified with mean energy only in a molecular population at equilibrium (one displaying the Boltzmann distribution), but the Boltzmann distribution depends on temperature, so any reduction of temperature will be circular (for a survey of the issues see [van Brakel, 2000, Chapter 5].

What of the second reduction? The emergence of quantum mechanics in 1925 and 1926 encouraged many physicists and chemists to hope for a deductive mechanical theory of atoms and molecules. In a passage that is often quoted, Dirac remarked, only a few years after the birth of quantum mechanics:

> The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. [Dirac, 1929, 714]

Quantum mechanics describes the motions of subatomic particles like electrons and nuclei in terms of wavefunctions and the Hamiltonians that govern them, much as Newton's physics describes the trajectories of mechanical systems like the planets, and the forces that govern them. In a deductive chemistry, physicists and chemists would apply quantum mechanics to atoms and molecules just as Newton and his scientific heirs applied Newtonian mechanics to the solar system, explaining the motions of the planets. Applied to the motions of electrons within atoms and molecules, quantum mechanics would provide a physical understanding of their inner workings, and of their interactions with other atoms and molecules. From this account would flow an explanation of the structure and bonding of molecules, and the properties of chemical substances.

The recipe for the required application is easy to describe, but complex to execute. One must first enumerate the constituent particles (electrons and nuclei) of the atom or molecule, their charges and masses, and any incident forces on the system. This determines a Hamiltonian for the molecule — a second-order differential operator representing its energy. Textbooks of quantum chemistry typically consider only Hamiltonians representing purely Coulombic interactions between particles. This means that a certain amount of idealisation has already occurred: other interactions and relativistic effects are ignored, and if incident forces are left out, the resultant Hamiltonian will describe only an isolated molecule, of which there are none in the real world. However, these factors can be shown to make little difference in most chemically interesting situations, and can be re-introduced if more accurate calculations are required. The Hamiltonian generates a Schrödinger equation, a second-order differential equation whose solutions — the eigenfunctions of the full atomic or molecular Hamiltonian — describe the states of the atom or molecule.

In physics, it is often easier to write down an equation for a complex system than it is to solve it. Newtonians struggled for years with the equations describing the orbit of the moon in the gravitational fields due to the Earth and the Sun [North, 1994, Chapters 13-14]. As a *sine qua non* for the acceptance of quantum mechanics, the Schrödinger equation for the hydrogen atom was written down and solved exactly in the early years of the theory's development, allowing direct calculation of its atomic spectrum. Physically, though, the hydrogen atom, like other one-electron systems (for instance He^+ and Li^{2+}), is a special case, because it involves no interactions between electrons. This makes it a special case mathematically, too. As Dirac pointed out, the exact application of quantum mechanics to more complex atoms and molecules 'leads to equations much too complicated to be soluble.' In these cases, further idealisations and approximations become necessary. These include simplifying the interactions between the subsystems of a composite system: Hartree-Fock self-consistent field methods (for atomic calculations) ignore electronic correlations as a starting point, then factor back in electrostatic interactions and electron exchange. In molecular calculations, nuclear and electronic motions are separated via the adiabatic approximation, the Born-Oppenheimer approximation then setting nuclei instantaneously at rest, so that electrons move in the resultant nuclear potential. Structural features of the molecule are then explained by calculating the effect of changes in nuclear configuration on electronic energy: for instance, the equilibrium structure for the molecule will correspond to a minimum in the molecule's potential energy surface. How is the electronic problem solved? One obvious approach is to construct molecular wavefunctions from atomic wavefunctions, although how exactly to do this has been a matter of contention in the history of quantum chemistry, between the valence-bond and molecular-orbital approaches. The molecule's *chemical* behaviour, that is, how it interacts with other molecules, can be investigated by determining the occupancy of its molecular orbitals, molecular geometry, charge distribution, and so on. Another approach, common in molecular spectroscopy, is the direct quantisation of the motion of subsystems of the molecule (Hückel models of π-bonding provide another example: see [Needham, 1999]). The molecular structure is again assumed, and quantum-mechanical models are applied to its rotations, and to the vibrations of its bonds.

Does the computational complexity of quantum chemistry raise any special problems for the reduction of chemistry to physics? The use of these approximate models in the explanation and prediction of chemical behaviour clearly does raise a number of issues in the epistemology of idealisation and approximation (see [Hendry, 1998b]). The model Hamiltonians differ from the intractable 'exact' Hamiltonians in that they neglect electronic interactions, and hold nuclei fixed, but electrons do interact and nuclei do move. Reductionists will respond that approximation and idealisation are ever-present features of physics: think of frictionless planes in mechanics, or ideal gases. But caution is required if some serious mistakes are to be avoided:

(i) If a model is not to be a mere *ad hoc* device, its guiding assumptions should be justified either by fundamental theory or collateral information about the system to which it is applied.

(ii) Conclusions derived from the model should be assumed to hold true only for systems in which the guiding assumptions hold.

(iii) Where the guiding assumptions are calibrated by collateral information, the model should not itself be thought to explain that information.

(iv) Approximations are often justified by appeal to limit theorems, according to which a dynamical variable in the model (like energy) approaches the value it would take in an exact treatment as the idealisations are relaxed. In this case, it should not be assumed without argument that other quantities also approach their exact values smoothly.

Let us begin with the quantum-mechanical understanding of the electronic structure of atoms in terms of one-electron orbitals: the 'orbital model.' Eric Scerri [1991] argues that although the orbital model is fruitful, its success should not be misinterpreted. Firstly, the assignment of electrons in multi-electron atoms to one-electron states is at best an approximation, a hangover from the interpretation of atomic spectra within the old quantum theory prior to the emergence of quantum mechanics proper in 1925. Secondly, the determination of the electronic structure of individual atoms is not a principled affair, but is tailored to accommodate empirical information from spectroscopy: the problem is not now the quantum-mechanical understanding of the shells themselves, but the order in which they are filled [Scerri, 1998a]. Thirdly, the correlation of electronic structure with chemical properties is far from perfect [Scerri, 1997]. Chemical behaviour ought, he argues, to be determined by outer-shell electron configuration. But vanadium, tantalum and niobium are grouped together in the periodic table due to their chemical similarities even though niobium has a different outer–shell configuration. Overall, the physical structure and chemical behaviour of atoms cannot be said to have been explained within a principled application of quantum mechanics (see point 3, above). Scerri [1994; 1998b] further worries whether the accuracy of complex computations in quantum chemistry masks their *ad hoc* character. The problem is that approximate calculations model atomic and molecular wavefunctions using bases of (typically Gaussian) functions. The fuller the basis, the more assured one can be in advance that theoretical and empirical energies will match, regardless of how good the approximation is from the point of view of exact quantum mechanics. If a good match is achieved, is this a success for theory, or an artefact of the approximate method?

However, Paul Needham [1999], argues that Scerri requires too much of reductive explanation. Firstly, although Nagel's model of reduction requires a deduction of the reduced theory from the reducing theory, this was always something of an idealisation. Philosophers of explanation like Hempel and Duhem allowed that looser approximate derivations can still be explanatory. Smith (1992) and Field (1992) also point out that the messy and approximate intertheoretic relationships that characterise real science should not be taken too quickly as a refutation of reductionism. Furthermore, genuine justification for the assumptions grounding a model may come from empirical information about the system to be described: there is nothing wrong with semi-empirical models *per se* (a point that is often made by Nancy Cartwright, see for instance her [1983]). This acknowledgement limits the inference to reductionism, however, if the third 'serious mistake' on our list is to be avoided. (See [Scerri, 1999] for a reply to Needham.)

Chemical physicist R.G. Woolley [1978; 1985; 1998] focuses on the Born–Oppenheimer approximation, although 'approximation' is, he argues, a misnomer. An 'exact' quantum mechanical treatment of a molecule fails to distinguish between isomers, which are distinct molecules which contain the same numbers of electrons and nuclei. Thus, for instance, cubane, cyclooctatraene and vinylbenzene are chemically very different molecules which share an 'exact' molecular Hamiltonian, each having eight carbon nuclei, eight protons and 56 electrons. The problem is that the mathematical form of the 'exact' Schrödinger equation is determined only by the nuclei and electrons present in a molecule. It may be that the different molecular species correspond to different sets of eigenfunctions of the molecular Hamiltonian, but this is not a possibility that has been articulated in detail.

A further problem concerns the symmetry of Hamiltonians for isolated molecules, which exhibit nuclear permutation and rotational symmetries, although Born-Oppenheimer structures — and real molecules — do not (see [Woolley, 1976, 34; Hendry, 1998b] for discussion). The lower symmetries of real molecules are explanatorily relevant, so if, as Woolley argues, structure needs to be put in 'by hand' we face 'serious mistake' number 3 again. The problem is not that there are no explanations of empirically-determined molecular shapes, or even that the explanations are *ad hoc*, or of poor quality. Rather it is that the explanation assumes determinate nuclear positions. Hence it would be quite wrong to conclude that 'exact' Schrödinger equations fail to appear in chemical explanations merely because of their mathematical intractability, or that 'in principle' exact quantum mechanics would do the job. According to Woolley, only the Born-Oppenheimer structures are explanatorily adequate.

So quantum chemistry does not seem to offer explanations that look like classical intertheoretic reductions. It is not just that the calculations are too complex: Woolley's arguments suggest that they cannot succeed. But clearly, physics has done some explanatory work in chemistry. Is this not evidence for ontological dependence?

3 CHEMISTRY IN A PHYSICAL WORLD

Chemistry deals with substances, with chemical microspecies like molecules, and also with their physical bases. There would then seem to be two layers to the question of reduction in chemistry [Hendry and Needham, 2007]. One, in a sense, is internal to chemistry: are chemical substances nothing but their constituent microspecies? The second concerns the relationship between molecular structure and physics: are molecules just quantum-mechanical systems of charged particles? I will address the first question only to note that microstructuralism about chemical substances does not commit one to reductionism about the first. Even if substances are just types of collections of molecular species, the properties of such collections may be emergent. The second reduction issue merits a longer discussion because of the symmetry problem about molecular structure.

Quantum chemistry is the interdisciplinary field that uses quantum mechanics to explain the structure and bonding of atoms and molecules. For any isolated atom or molecule, its non-relativistic Schrödinger equation is determined by enumerating the electrons and nuclei in the system, and the forces by which they interact. Of the four fundamental physical forces, three (gravitational, weak and strong nuclear) can be neglected in calculating the quantum-mechanical states governing molecular structure. As we saw in Section 2, classical intertheoretic reduction would require the derivation of the properties of atoms and molecules from their Schrödinger equations. There is an exact analytical solution to the non-relativistic Schrödinger equation for the hydrogen atom and other one-electron systems, but these cases are special owing to their simplicity and symmetry properties. Caution is required in drawing any consequences for how quantum mechanics applies to chemical systems more generally. The Schrödinger equation for the next simplest atom, helium, cannot be solved analytically, and to solve Schrödinger equations for more complex atoms, or for any molecule, quantum chemists apply a battery of approximate methods and models which have become very accurate with the development of powerful digital computing. Whether they address the electronic structure of atoms or the structure and bonding of molecules, many explanatory models are calibrated by an array of theoretical assumptions drawn from chemistry itself. In short, quantum chemistry does not meet the strict demands of classical intertheoretic reduction, because its explanatory models bear only a loose relationship to exact atomic and molecular Schrödinger equations (see for instance [Bogaard, 1978; Hofmann, 1990; van Brakel, 2000, Chapter 5; Scerri, 2007, Chapters 8 and 9; Hendry, 2011, Chapter 7]). In the case of atomic calculations, quantum-mechanical calculations assign electrons to one-electron orbitals that, to a first approximation, ignore interactions between electrons. Scerri [2007, Chapters 8 and 9] argues that although the orbitals are artefacts of an approximation scheme, they seem to play an important role in explaining the structure of atomic electron shells, and the order in which they are filled is determined by chemical information rather than fundamental theory. In the case of molecular calculations, the nuclei are constrained within empirically calibrated semi-classical structures, with the electrons moving in the resultant field [Hendry, 2011]. Only the electrons are assumed to move quantum-mechanically, and the molecular structure is imposed rather than explained.

Reductionists can make two responses here. The first is that the models are just *ad hoc*, but since these models provide much of the evidence for the explanatory importance of quantum mechanics in chemistry, this response would seem to undermine the motivation for reductionism. The second response is that inexact models are common in computationally complex parts of physics, and do not signal any deep explanatory failure. There is something in this response, but it requires that the atomic and molecular models that are used in explanations are justifiable as approximations to solutions of exact Schrödinger equations, and stand in for them in explanations of molecular properties (hence call this the 'proxy defence' of inexact models). This is a more stringent condition than it may sound, requiring that the inexact models attribute no explanatorily relevant features to atoms or molecules that cannot be justified in the exact treatments. The Born-Oppenheimer or 'clamped nucleus' approximation seems to offer just such a justification for the assumption of semi-classical molecular structures because the masses of atomic nuclei are thousands of times greater than those of electrons, and so move much more slowly. Fixing the positions of the nuclei makes little difference to the calculated energy, so in calculating the electronic motions the nuclei may be considered to be approximately at rest. But if Woolley's symmetry argument is one of mathematical principle, the problem is not that the calculations are difficult to execute. The question is whether there are any determinate molecular structures in quantum mechanics.

But the reduction issue does not begin and end with relationships between theories. Robin Le Poidevin [2005] distinguishes intertheoretic (or as he calls it, 'epistemological') reduction from ontological reducibility, arguing rightly that the unfeasibility of intertheoretic reduction does not settle the issue of ontological reducibility. He attempts to identify just what could count as an argument for ontological reducibility of the chemical to the physical: chemical properties, he argues, are more than merely correlated with microphysical properties, they are exhausted by them. All *possible* instances of chemical properties are constituted by combinations of discretely varying physical properties. It is just not possible that there is an element between (say) helium and lithium. There are two lines of objection to an argument of the kind Le Poidevin envisages (see [Hendry and Needham, 2007]). Firstly it applies only to properties that vary discretely, like the elements. The elements do not exhaust the whole of chemistry, however, because as we have seen, isomers are distinct substances that are identical in respect of their elemental composition, yet differ in respect of their molecular structures. Furthermore molecular structure is defined in terms of continuously varying quantities like bond lengths and bond angles. Secondly, it is not clear just why the exhaustion of chemical properties by combinations of physical properties would establish the ontological reducibility of the chemical. Here's why not. In recent philosophy of mind, ontological reducibility has been understood in terms of causal powers: A is ontologically reducible to B just in case the causal powers conferred by possession of A-properties are exhausted by those conferred by possession of B-properties (see [Kim, 1998, Chapter 4]). On this formulation neither Le Poidevin's combinatorial determination nor microstructuralist supervenience is sufficient for ontological reduction, for the A-properties may confer 'additional' causal powers. If, for each cluster of B-properties corresponding to an A-property there is a *sui generis* law of nature conferring distinct causal powers that are not conferred by more fundamental laws governing the B-properties, then the A-properties are irreducible to the B-properties in a robustly ontological sense.

Is this more than a mere logical possibility? The symmetry problem discussed earlier would seem to indicate that it is. For over a century, chemical explanations of the causal powers of molecules, and of the substances they compose, have appealed to molecular structures attributed on the basis of chemical and physical evidence. Yet the existence of such structures does not seem to have an explanation in exact quantum mechanics. To be an ontological reductionist is to think that molecular structures are determined by more fundamental laws, and that the required explanation must in some sense exist, even if it is unfinished business for physics. The emergentist interpretation of the situation is that for each molecular structure there is a *sui generis* law of nature that can be expressed in the language of quantum mechanics, but is an instance of no deeper physical law. So it seems that the issue of ontological reduction is settled neither by the existence nor the non-existence of quantum-mechanical explanations of molecular structure and bonding. Both reductionism and emergence are compatible with there being such explanations, differing over their structure, and the degree to which the laws that appear in them are unified. To address the issue of the ontological reduction of chemistry is to assess the relative plausibility of these two interpretations (see [McLaughlin, 1992; Hendry, 2010; 2011, Chapters 9 and 10] for differing views).

4 PHYSICALISM

Given the consensus that *classical* reductionism is utopian, attention understandably turns to the question of whether the dependence of the chemical on the physical is of some looser kind, as might for instance be elucidated by the relation of supervenience. Within contemporary philosophy of mind there is an emerging consensus that the central question of physicalism is whether — and in what sense — the physical is causally closed, an issue that goes back to Descartes.

Physicalism is the ontological position according to which the physical facts determine all the facts. Physicalists are therefore committed to one of two positions with respect to chemistry: either chemical facts are determined by physical facts, or there *are* no chemical facts, strictly speaking. The second kind of position, involving an instrumentalist stance towards chemical laws and entities, is implied by at least one anti-reductionist commentator on chemistry [Primas, 1983], while analogous positions have been taken with respect to biology [Rosenberg, 1994]. It is the purpose of this chapter to explore the content and standing of the first kind of position, however: to do that requires some account of what it is for one set of facts to determine another (and conversely, for one set of facts to *depend* on another), and also some account of what it is for a set of facts to count as 'physical.'

An initial, and well known attempt to explain how the facts, entities or laws associated with one domain could determine those of another proceeded in terms of *reducibility.* To borrow a formulation from Field [1992, 272-3], the classical reducibility of chemistry to physics would require that for every true sentence in the language of chemistry there would be a physical transcription: a sentence in the language of physics that (as Field puts it) "expresses the same facts" [1992, 272]. A second (and arguably subordinate) requirement concerns explanation: that every good chemical explanation could be recast as a physical explanation, although the physical explanations may well be less illuminating than their higher-level counterparts. So the reductionist picture required chemical and physical laws to be bound together by *bridge laws* from which, together with a precise physical description[1] of the physical entities, the chemical laws (or approximations to them) could be deduced. The difficulties associated with the reductionist picture are well known, and centre on the bridge laws. Even if everything is, at bottom, physical, higher-level properties might admit of multiple physical realisations that would make the disjunctive lists of properties on the physical side of bridge laws open-ended. Furthermore the length and complexity of those disjunctive lists might debar them from counting as genuine physical properties, and hence appearing in genuine physical explanations, all of which presents reductionism with a major difficulty in meeting its explanatory commitment.

Clearly an argument for physicalism should not require that a classical reduction be displayed for *every* chemical law. Hence Field [1992] and Smith [1992], by

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[1] 'Physical description' is here used in the broad sense, encompassing the physical laws that are taken to govern the target systems.

way of refining and defending reductionism, have presented plausible relaxations of the physical transcription requirement, and along with it, a response to the explanatory problem. Field and Smith require only what Field calls 'sketches' [1992, 274] and Smith calls 'quasi-reductions' [1992, 29-30]. Sketchy, approximate quasi-reductions fall short of offering the tight bridge laws that would allow replacement of the dependent ontology within science (in this case, that of chemistry): the dependent ontology might remain indispensable in explaining higher-level regularities. But the reductionist dependence claim surely would require successful reductions (or quasi-reductions) of at least a representative sample of dependent systems, plus reasons for thinking that this good fortune will continue, with further reductions and quasi-reductions forthcoming.

According to classical reductionism, the dependence of chemical facts on physical facts would be reflected in tight *logical* relationships between chemical and physical theories. Given that physicalism is driven by an ontological intuition, it would make sense, if the reductionist picture is rejected, for the physicalist to detach the logical and ontological claims. At the heart of *non-reductive* physicalism would be a relation that could hold between the entities, properties, events or processes associated with two sciences that would capture the idea that one science's facts determine the other's, without making too many hostages to fortune as to logical relationships between the *theories* that describe those entities, properties, events or processes. One move is to require only token identity of higher-level with lower-level entities or events, leaving type-identity open (another is to relativise the type-identities to particular higher-level species, but that is a form of reductionism). Another alternative is, of course, supervenience, which allows for the distinctness of the higher-level entities, properties, events or processes, but attempts to capture the sense in which they are nevertheless dependent on lower-level entities, properties, events or processes.

However, supervenience is a family of relations, and an extended family at that. Supervenience is usually characterised as a relation between groups of properties (see [Kim, 1984]). Roughly, a group of properties, A (the supervenient group), supervenes on another, B (the subvenient, or base group) when there cannot be variation in respect of A without variation in respect of B. Supervenience does seem to be a plausible determination relation in that it shows how the A-properties are fixed along with the B-properties. Not only that: coupled with a claim about the causal completeness of the physical and a denial of causal overdetermination, we could add that causal (and possibly explanatory) claims associated with the 'higher level' science in which the supervenient properties are discussed fail to be autonomous. Causal powers conferred by the possession of supervenient properties are really conferred 'in virtue of' the subvenient properties, since we can always look to the lower-level change as the real cause of any effects apparently brought about by changes among the supervenient properties. Hence supervenience offers something parallel to the explanatory commitment in reductionism: although we may not have physical explanations of higher-level regularities, we do have an assurance that the causal processes that constitute the basis of higher level explanations are, in fact, physical processes.

However, the situation is a bit more complicated: for A to supervene on B requires some modal force to the covariation of A and B (hence 'cannot' rather than 'does not'),[2] and how closely the A-properties are determined by the B-properties depends famously on the strength of the modal force. Weak supervenience requires that B-identical systems within the same possible world must be A-identical, but allows A-discernibility between B-indiscernibles in different possible worlds. Strong supervenience requires in addition that B-indiscernibility entail A-indiscernibility *across* different worlds. If we think of supervenience as a consistency requirement on the attribution of supervenient properties given the fixation of the base properties, weak supervenience requires consistency only within possible worlds, strong supervenience requires consistency also between them. There are, of course, significant differences between physicalist claims formulated in terms of the various kinds of determination. It is sometimes held that too much variation is allowed among weakly supervenient properties for it to be said that they are determined by the assignment of subvenient properties. However, there are contexts in which weak supervenience is a very plausible way of capturing determination. On a projective or response-dependent account of the supervenient properties (think for example of evaluative properties supervening on descriptive ones), there might well be differences among supervenient-property attributions between counterpart-communities of supervenient-property attributers in different possible worlds. On the other hand, strong supervenience has sometimes been argued to require such *close* determination of supervenient by subvenient properties that it threatens to collapse the new, supposedly non-reductive physicalism into reductionism after all, although the seriousness of that threat depends on the extent to which one thinks that properties are closed under logical operations (see [Kim, 1984]). One further objection to the kind of physicalism that is limited to a strong supervenience claim is that, to accompany correlations among higher-level properties, it posits correlations among base properties. Such correlations are unexplained except by the reductionist (see [Field, 1992; Papineau, 1992; Smith, 1992; Kim, 1997]). Hence in a world where strong supervenience holds, epistemic values will force us to seek reductions, to the extent that explanation is a telling epistemic requirement.

So to the second dimension in the elucidation of physicalism: the boundary of the physical. In arguments concerning the dependence of the mental on the physical, a broad sense of 'physical' is typically at work: roughly, one according to which physical objects are those that are spatially located, and physical properties are those that can be borne only by physical objects. But this construal is obviously

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[2] Although supervenience now customarily involves a modal element, Quine formulated a 'nonreductive, nontranslational' physicalism that is recognisably a member of the supervenience clan despite (unsurprisingly) being non-modal: 'nothing happens in the world, not the flutter of an eyelid, not the flicker of a thought, without some redistribution of microphysical states' (Quine 1981, 98). Quine's thought is that physics alone is in the business of full coverage. For criticism of non-modal supervenience as a physicalist determination relation see [Field, 1992, 280-1].

far too broad for our present purposes, since it fails to exclude the chemical. If the physical includes the chemical in this way, then dependence claims of all kinds are established very easily, and are correspondingly uninformative. If, for instance, chemical properties are a subset of physical properties, then because supervenience is a reflexive relation among sets of properties (trivially, there cannot be change in respect of A without variation in respect of B when $A \subseteq B$), the chemical supervenes on the physical, but only because it supervenes on the chemical. This would be a terminological answer to the question of chemistry's dependence on physics because it would leave open what dependence relations hold between different subsets of 'physical' properties. A narrower, and therefore more informative, conception of the physical proceeds in terms of the *discipline* of physics. But this is not yet adequate, for physics itself studies a heterogeneous array of entities and processes. It is hard to see why theories constructed within such areas of physics as fluid dynamics and astrophysics should be thought more 'fundamental' than chemistry.[3] Nor do physicalists give much serious thought to which particular domains of phenomena have come to be studied in physics departments, rather than (say) departments of engineering or chemistry, or why historical accidents of this sort should give physics all the ontological authority. Rather, a well-motivated conception of the physical will presumably proceed in terms of the laws and categories associated with a few 'fundamental' — for which read, general or abstract — theories in physics, namely quantum mechanics and particle physics. This, to be fair, is how physicalists have tended to identify the physical: in a sense that allows it to contrast with the chemical, and be correspondingly informative (see for instance [Quine, 1981; Papineau, 1990; Field, 1992].

Thus we have physicalist positions of a variety of strengths, each of which seems to capture in its own way the one-sentence sketch of physicalism with which I began this section. Applied to the relation between chemistry and physics, they yield the following possibilities: that chemical facts are determined by (micro-)physical facts in the sense that the chemical entities, properties, events or processes to which they relate just *are*, or are reducible to, or supervene on, micro-physical entities, properties, events or processes. Having done all this work to review and distinguish the various kinds of physicalism, I propose to lump them all together again, at least for the purposes of appraising their support. For physicalists seem to agree that physicalism, properly so-called, involves a claim that has been called the *completeness* of physics: physics alone is self-contained; its explanations need make no appeal to the laws of other sciences, and its laws cover the entities, properties, events or processes that are studied by the special sciences. Hence all versions of physicalism, properly so-called, stand and fall together, along with that claim. This is not to say that they are all on a par: were the completeness of physics to be established, important work would have to be done in finding out, for

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[3] For discussion of these issues, see Crane and Mellor [1991 Sections 1 and 2]; Papineau [1990; 1991], and Crane [1991]. David Knight [1995, Chapters 5 and 12] charts the changing views of chemistry's place in the hierarchy of the sciences. The issue is further complicated by its entanglement with the identification of the dependence relation: see above.

each higher-level science, which version of physicalism best captures the detailed structure of relations between physical and higher-level properties. However, this is not a pressing task for those who think, as I do, that there is little reason to accept the completeness of physics.

5 THE COMPLETENESS OF PHYSICS

Why should every physicalist be committed to the completeness of physics? Perhaps physicalism of one sort or another can be argued for on independent grounds, with the completeness claim dropping out as a corollary. However, the completeness of physics typically appears as a lemma. In 1966, Lewis, arguing for (a restricted) type-identity of mental and physical, was explicit about his appeal to the completeness of physics, and the empirical nature of that claim:

> A confidence in the explanatory adequacy of physics is a vital part ... of any full-blooded materialism. It is the empirical foundation on which materialism builds its superstructure of ontological and cosmological doctrines. [Lewis, 1966, 105]

Papineau's argument that all facts (strongly) supervene on physical facts [1990; 1993; 1995] is similarly explicit in this commitment, as is Loewer [1995], Smith [1992], Smith and Jones [1986, 57-9]. Field [1992], Papineau [1992] and Smith [1992] begin their arguments for reductionist theses by criticising supervenience versions of physicalism on the grounds that supervenience fails to explain the physical correlations that underlie mental (or other) correlations. Supervenience physicalism and its basis in the completeness of physics is taken to be unproblematic, and the argument is about whether or not this is sufficient for reduction. On these arguments, (modern, reformed) reductionism too inherits the evidential route through the completeness of physics, although Field [1992, 283] also commits himself independently to the completeness claim. But how is the claim supported?

Detailed arguments for the completeness of physics have been fairly thin on the ground, beyond claims that it is somehow built in to the methods of both physics and other sciences. I will examine those arguments in the next section. Papineau's exchange with Crane, however, is an exception (see [Papineau, 1990; 1991; Crane, 1991]), for Papineau offers what I will call a *contrastive* argument for the completeness of physics. The argument is 'of general significance' [Papineau, 1990, 66], in that it is intended to establish the supervenience on the physical of such diverse categories as 'the psychological, the biological, the meteorological, the chemical', although his examples concentrate on the psychological.[4] His argument is premised explicitly on the completeness of physics:

> all physical events are determined (or have their chances determined) entirely by prior physical events according to physical laws. [1990, 67]

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[4] This may seem like an irrelevant aside, but it is a pertinent point to which I will return shortly.

Papineau acknowledges one obvious objection to the completeness of physics [1990, 70], which arises from the pessimistically inductive thought that it is highly likely that there are kinds of event that current physics *doesn't* cover. Hence current physics is not complete. Given that one wouldn't want the provisional nature of physical knowledge to allow so easily for the independence of the mental, Papineau makes the completeness of physics *trivial* by identifying 'physics' with whatever body of scientific theory turns out to give a complete account of such *straightforwardly* physical events as stone-fallings.

Crane [1991] complains that Papineau's argument begs the question: if it supports a non-trivial physicalism (i.e. one that can reasonably exclude the mental from the physical), then it must appeal to just the sort of mereological supervenience intuitions that a non-physicalist will dispute. Otherwise it is only an *equivocation* between what he calls PHYSICS (the by-definition complete science) and *physics* (the discipline that is practiced in present-day physics laboratories) that allows us to claim that mental states are unlikely to be cited in explanations of physical events offered by PHYSICS. We don't know anything about what will turn out to be required by PHYSICS. But perhaps this is unfair to the kind of argument that Papineau is offering. As Papineau himself points out, the physicalism so defined is uninformative only if it turns out that (complete) PHYSICS must appeal to mental states. The intention is clearly that there is an *evidential* connection between (current) *physics* and (complete) PHYSICS, in the sense that what is appealed to in explanations offered by current physics gives us a guide, albeit a fallible one, to what kinds of states will be appealed to in explanations offered by (complete) PHYSICS:

> I take it that current physics is committed to developing a complete theory formulated in terms of the categories of energy, field and space-time structure. Now, it seems reasonably plausible to me that no such theory is possible, because of as yet unknown physical effects that cannot be accounted for in terms of these current categories, and that therefore a genuinely complete theory (PHYSICS) will need to appeal to further explanatory categories. What seems unlikely to me is that these further categories should include mental ones. [Papineau, 1991, 38]

Now some dependence claims are *transparently* generated, or at least supported by, reflection on the concepts whose use characterises the supervenient domain. Take, for example the view associated with G.E. Moore and R.M. Hare that evaluative properties supervene on natural properties: part of what makes this view plausible is that it would be *evaluatively* inconsistent to make differing evaluative judgements on two things that did not differ descriptively. Other supervenience claims do not so obviously turn on claims about the supervenient domain, but on further examination turn out to do so. To take a relevant example, functionalist approaches to the mental make plausible the supervenience of the mental on the physical, because functionalism has it that mental states are identified by their (physical) causes and effects [Lewis, 1966; Papineau, 1990; Loewer, 1995]. Hence a view of the supervenient domain (in this case the mental) motivates a view of its connection with its putative base domain. Mental states necessarily have physical causes and behavioural (i.e. physical) effects, which are then the subject of requests for physical explanation. The causal completeness of the physical and the implausibility of causal overdetermination are then raised to establish that if mental states are causally efficacious, they must be so in virtue their dependence on physical states of certain sorts, even if, as in the case of mental properties, multiple realisability means that characterisations of these physical states in physical terms might be very complicated.

Papineau's argument implicitly turns on intuitions about one supervenient domain — the mental — in another way, and in a way that means his argument cannot establish the physicalist claim with respect to the chemical. Let us accept for the sake of argument Papineau's (quite plausible) contention that reflection on the practice of present-day physics supports the view that mental categories will not be cited in the laws of a completed physics. Mental categories are rarely, of ever, cited in present-day physics,[5] and if final physics is anything like current physics — and we surely have no better model — then mental categories really are unlikely to appear in the laws of a completed physics. To establish the general claim that *all* facts — and not just mental facts — supervene on the physical, we need to know that categories appearing in theories of the biological, the meteorological and the chemical will *also* fail to appear in completed physics. What reasons have we been given for thinking that they won't appear? Papineau left them implicit, but whatever the science, the plausibility of the claim would presumably need to be established by inspection of current physics. Now one method is to think in a general way about how the relevant higher-level domain is marked off from the physical: biology, for instance, is the science of living things, and discourse in biology is characterised by functional concepts, concepts that (reflection quickly assures us) do not appear in the explanations offered by current physics. It is difficult to imagine how a similar argument would run in the case of (standard) chemical categories, most of which are hard to differentiate from physical categories in any principled way. So even supposing that versions of Papineau's contrastive completeness claim are true for some supervenient domains like the psychological and the biological, it is difficult to see how one could be made out in respect of chemical categories. So we are thrown back on physics itself — and more particularly its successes, methods and guiding assumptions — for support for the completeness claim.

There are two interlocking elements to the claim that physics is complete: (i) the *autonomy* and (ii) the *universality* of physics. A science is *autonomous* if its laws and explanations make no appeal to the laws or categories of other sciences. On the physicalist view, only microphysics is autonomous in this way, since only

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[5] The Copenhagen interpretation of quantum mechanics looks like an exception, but part of a claim like Papineau's may be the plausible bet that nothing like the Copenhagen interpretation of quantum mechanics will appear in a completed physics.

its laws are free of *ceteris paribus* conditions that must be expressed in the language of other sciences (that is, to the extent that *ceteris paribus* conditions can be expressed in any but the sketchiest terms). A science's laws are *universal* if they cover the behaviour of *every* real entity or process: note that the universality of physics need not beg the question of physicalism if 'coverage' is suitably understood to allow that a physical law may 'cover' (i.e. fix some truths about) an entity or process without determining *all* the truths about that entity or process. The universality claim for physics is made plausible by the ubiquity of microphysical entities: according to chemical theory itself, the parts of chemical entities are studied by physics (the same mereological intuitions work, *mutatis mutandis*, for the dependence of yet higher-level entities on chemical entities). The autonomy and universality claims work in partnership: the universality claim establishes that microphysical laws act everywhere (since everything has physical parts), while the autonomy claim establishes that microphysical laws *determine* the behaviour of whatever they cover, to the extent that that behaviour is determined by law, since there are no situations that must be covered by non-physical *ceteris paribus* conditions. Whatever physics' laws cover, they cover alone, and they cover everything.

What evidence is there for completeness, so understood? What physicalists have in mind, I take it, is straightforwardly scientific evidence of the kind that is considered by Nobel Prize Committees, and may subsequently appear in textbooks of physics and chemistry. The evidence, presumably, is of two sorts.[6] On the one hand are the well-known experiments which, according to physics textbooks, can be accounted for by only quantum mechanics, but not classical mechanics: take the behaviour of the Stern-Gerlach apparatus as a canonical example. On the other hand are the explanatory achievements of quantum mechanics within chemistry, starting with the opposing treatments of the hydrogen molecule due to Condon, and Heitler and London, and expanding outwards to provide all the well-known explanations of molecular structure and spectroscopic behaviour. Now the physicalist will concede that, for practical reasons, it might never be the case that there is a detailed quantum-mechanical treatment for every situation: the physicalist argument necessarily involves generalisation from a few cases. The physicalist and the non-physicalist will differ over whether this matters. Physicalists present their generalisation as an ordinary scientific inference, and view any resistance as unmotivated scepticism. Hence the onus appears to be on the non-physicalist to provide *specific* reasons to resist the generalisation.

Turning to the experimental evidence first, Cartwright [1999, Chapter 1] does indeed oppose the inference to the generality of quantum mechanics from its successful treatment of carefully controlled situations like (say) the Stern-Gerlach experiment, on the specific grounds that such situations *are* carefully controlled. Firstly, to perform the experiments that constitute the main evidence for fundamental physical theories like quantum mechanics requires a great deal of skill, involving detailed knowledge of the kinds of perturbation that can defeat the fleet-

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[6] This way of thinking about the evidence, and the following critical discussion are a developed version of arguments presented in Hendry 1998a.

ing effects that such experiments seek to display. Even if the physical states whose causal powers are displayed in these experiments persist in the wild, some assurance is required that in persisting, they make more than a negligible contribution to the systems of which they form part. No argument to that effect is forthcoming from physics, because theoretical descriptions of the wild behaviour are intractable even if they can be written down. Secondly, it is far from clear that quantum-mechanical accounts of the Stern-Gerlach experiment are autonomous, in the sense outlined earlier. Hasok Chang [1995] has argued that many experiments of central relevance to quantum mechanics are understood in terms of calculations that are grounded in classical electrodynamics and mechanics. Chang's examples include: the use of magnetic and electric deflection to measure the kinetic energy and momentum of microscopic particles, the charge-mass ratio for electrons (Thomson) and alpha particles (Rutherford); and also Millikan's study of the photoelectric effect and calculation of Planck's constant (see [Chang, 1995, 122-5]). On the face of it, the classical theories are incompatible with quantum mechanics, but the use of pre-quantum-mechanical theories might be sanctioned by the well-known convergences — Ehrenfest's theorem and Bohr's principle of correspondence — between quantum and classical predictions. But these convergences are limited, and in any case Chang [1995, 127] points out that *predictive* convergences mask *conceptual* inconsistencies: in deflection experiments, for instance, classical equations are used to deduce the *path* of a particle with a given energy, but under standard interpretations, quantum mechanics denies that microscopic entities *have* paths. Hence the universality of quantum mechanics is not, in practice, assumed in theoretical accounts of the very experiments that are adduced in its support. Surely an experiment supports a theory *as a universal theory* only if theoretical accounts of that experiment are understood in ways that are consistent with its universality. It is one thing to have a quantum-mechanical account of the spin states of a silver atom, quite another to have a quantum-mechanical account of the whole Stern-Gerlach apparatus: the universality of quantum mechanics demands the latter. Of course the physicalist will reply that classical physics is still physics. True, but classical physics certainly isn't microphysics. Part of the initial plausibility of the completeness of physics comes from what I called the ubiquity of physical entities. However, the price of the ubiquity argument is that it motivates only the universality of *microphysical* laws. The disunity of real physics is directly relevant to the completeness of microphysics.

The second kind of evidence concerned the explanatory applications of quantum mechanics to molecules. These explanations, I argue, fail to display the direction of explanation that physicalism requires. Remember Woolley's point that Born-Oppenheimer models assume but do not explain molecular structures. It is natural to read the attribution of such structures as the direct attribution of a state to the molecule as a whole, a state that is not further explained in terms of the more fundamental force laws governing pairwise interactions between the constituent electrons and nuclei. Given that this state constrains the quantised motions of the functional groups appearing in the spectroscopic explanation, the direction of explanation appears to be downwards — *from* the molecular structure *to* the motions of the parts — *contra* the intuitions about mereological determination that drive the physicalist argument.

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