Chapter 14
The Prospects for Fusion Emergence

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14.1 Introduction

In a number of articles, Humphreys (1996, 1997a,b, 2008) has offered an account of emergence which aims to provide the grounds for an ontology of the special sciences. Humphreys' account (called *fusion emergence*) presents a series of challenges to at least three widely accepted assumptions about ontology: (i) that the right way to represent the relation between lower-level and higher-level properties is supervenience, (ii) that our world's ontology is wholly compositional, and (iii) that the physical domain is causally closed.[1]

Humphreys has argued not only that fusion emergence can be consistently described (1997b), but also that our own world exhibits cases of this kind of emergence (2008). According to Humphreys, covalent bonding is a "core example of fusion emergence" (2008, p. 7). The purpose of this paper is to raise some concerns about Humphreys' account in general and about his core example of fusion emergence in particular. It will be suggested that the extent to which covalent bonding undermines the second assumption mentioned above has been overstated.

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[1] (i) Has been discussed extensively by Kim and Lewis, (ii) by Lewis, (iii) by Papineau.

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14.2   Humphreys' Fusion Emergence

Humphreys' account of emergence was motivated by the desire to avoid the exclusion argument or a generalized version thereof, whose conclusion is that higher-level emergent properties are excluded from affecting lower-level properties, since all the causal work is done by the latter (see Kim 1992, 1999, 2006). The exclusion argument has unwelcome consequences for the ontology of the special sciences. If one thinks of the special science properties (e.g., chemical or biological) as occupying higher levels than do physical properties, then the exclusion argument entails that no event involving a special science property could ever causally influence a physical event. The idea of special science causation is thus threatened. Also, the exclusion argument challenges the idea that special science properties deserve a place in our ontology: if special science properties are causally idle, what is the point of having them in our ontology? The exclusion argument has unwelcome consequences for physics, too. If one thinks of physics itself as stratified (e.g., with high energy physics, solid state physics and thermodynamics occupying different strata), the exclusion argument entails that only the most basic physical properties can be causally efficacious, and – as a result – all other causal claims within contemporary physics are false.

While the exclusion argument denies that the higher-level properties that special sciences are concerned with are capable of downward causation, emergence seems to require it explicitly. It has been argued that the only way to cause an emergent property to be instantiated is by causing its emergence base property to be instantiated (Kim, 1992, p. 136). This is known as the downward causation argument, and it shares with the exclusion argument the assumption that the right way to represent the relation between lower-level and higher-level properties is supervenience.

In his work, Paul Humphreys challenges both the exclusion argument and the downward causation argument by explicitly denying their common assumption, namely that supervenience is the right way to represent the relation between lower-level and higher-level properties (1997a). He also argues that thinking of higher-level emergent properties in terms of supervenience is mistaken. Instead, he links the possibility of emergence with the existence of a *fusion operation* that operates on i-level properties and outputs $i + 1$-level properties, which have novel causal powers.[2]

The process of fusion is formally represented as follows. Let $P_m^i(x_r^i)t_1$ represent an i-level entity, x_r, instantiating an i-level property, P_m, at time t_1. $P_n^i(x_s^i)t_1$ will denote another i-level entity, x_s, instantiating another i-level property, P_n, at time t_1.

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[2]For the sake of brevity, sometimes I will use "property" instead of "property instance". It should be noted however that for Humphreys the arguments of the fusion operation are property instances.

Humphreys introduces the *fusion operation* symbolized by [. ∗ .], which takes as arguments the two property instances $P_m^i(x_r^i)t_1$ and $P_n^i(x_s^i)t_1$ and fuses them: $[P_m^i(x_r^i)t_1 * P_n^i(x_s^i)t_1]$. The fusion operation is a i-level operation, i.e., an operation of the same level as its arguments. The result of the fusion operation is the fused property $[P_m^i * P_n^i][(x_r^i)+(x_s^i)](t_2)$ at the $i+1$-level, which can also be written as $[P_l^{i+1}][x_l^{i+1}](t_2)$. The fused property is a unified whole in the sense that its causal effects cannot be represented in terms of the separate causal effects of the original property instances. Also, within the fused property instance $[P_m^i(x_r^i)t_1 * P_n^i(x_s^i)t_1]$, the original property instances $P_m^i(x_r^i)t_1$ and $P_n^i(x_s^i)t_1$ no longer exist as separate entities and they do not have all of their i-level causal powers available for use at the $i+1$-level (Humphreys, 1997b, p. 10).

Humphreys argues that this particularity of fusion emergence is what enables this brand of emergentism to avoid the threats of the exclusion and downward causation arguments. At the time when the fused property instance $[P_m^i(x_r^i)t_1 * P_n^i(x_s^i)t_1]$ comes into existence, the original property instances $P_m^i(x_r^i)t_1$ and $P_n^i(x_s^i)t_1$ go out of existence. Therefore, it is a fortiori the case that they cannot compete as causes with the emergent property instance. On Humphreys account, emergents don't coexist with their bases, and this feature prevents the exclusion argument to get off the ground.

Humphreys' fusion emergence also deals with the downward causation argument. This argument is also committed to the idea that emergent properties supervene on lower-level properties. The argument assumes that the *only* way to bring about an emergent property instance at time *t* is by bringing about its subvenience base at time *t*. But if fusion emergents are not synchronous with their bases, this assumption is unwarranted. There is no reason to suppose that an $i + 1$-level property instance could not *directly* produce another $i + 1$-level property instance e.g., by directly transforming into it or by transforming another, already existing, $i + 1$-level property instance – in both cases, other property instances may contribute (1997b, p. 13; 2008, p. 8).

By avoiding the threats to the ontology of the special sciences posed by the exclusion and downward causation arguments, Humphreys' emergentist account attempts to rescue the autonomy of the special sciences and to depict an ontologically antireductionist image of the world in which the subject matters of the various special sciences correspond to irreducible ontological strata.[3] For Humphreys, there is a hierarchy of levels of properties $L_0, L_1, \ldots L_n \ldots$ of which at least one distinct level is associated with the subject matter of each special science, and L_j cannot be reduced to L_i for any $i < j$ (Humphreys, 1997a, p. 5).

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[3]Humphreys admits however that the boundary between the physical level and other levels is not sharp (Humphreys, 1997a, p. S345).

14.3   Previous Criticisms of Fusion Emergence

Humphreys remarks that philosophers have long thought of the ontology of the special sciences in terms of supervenience. On this view, the higher-level properties are "composed of" or "supervenient upon" lower-level properties.[4] But Humphreys finds supervenience unsatisfactory. He complains that supervenience does not provide any understanding of ontological relationships holding between levels.[5] If these levels are emergent, they contain emergent properties. According to Humphreys, an important characteristic of emergent properties is that they result from the interaction between their constituents.[6] However, the level of detail that emergent properties demand makes the use of supervenience relations seem simplistic. This is one of the reasons why Humphreys argues that emergence should not be understood in terms of supervenience. Add to this the threats posed by the exclusion and downward causation arguments, and supervenience seems completely inappropriate for providing the grounds for an ontology of the special sciences.

As mentioned in the previous section, on Humphreys' account, emergents are not co-instantiated with their bases. Wong (2006) has called this the *basal loss* feature of fusion emergentism, and he has claimed that it is both problematic and unmotivated (2006, p. 346). According to Wong, the dissapearance of the lower-level properties of an entity is problematic for two reasons. First, because it threatenes the structural properties crucial to the proper functioning of that entity. The basal properties that fuse to become emergents may also constitute nonemergent, structural properties which may be indispensable to the proper functioning of the system. However, if basal properties are destroyed by the fusion process, then so would the structural properties. Second, the dissapearance of the lower-level properties generates what Wong calls "the correlation problem". It is empirically established that many special science properties have lower-level correlates with which they are copresent (e.g., mental properties are synchronously correlated with neurophysiological properties). However, if we are to treat the special science properties as fusion emergents, then we deny the copresence of their lower-level correlates, which Wong sees as empirically implausible.

Wong considers the basal loss feature of fusion emergentism as unmotivated for the reason that on Humphreys' account, basal and emergent properties don't have causal profiles that overlap significantly and thus cannot compete as overdeterminers of their effects. According to Wong, emergents supplement the underlying dynamics rather than merely overdetermine physical effects (2006, p. 361).

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[4]The notion of supervenience that Humphreys uses is Kim's strong supervenience: "A family of properties M strongly supervenes on a family N of properties iff, necessarily, for each x and each property F in M, if F(x) then there is a property G in N such that G(x) and necessarily if any y has G it has F" (Kim, 1993, p. 65).

[5]This worry is in fact shared with Kim.

[6]Humphreys sees this interaction as nomologically necessary for the existence of emergent properties (1997a, p. S342)

In his response to Wong's criticisms, Humphreys (2008) argues that most systems possess multiple properties, some of which are essential to carrying out the system's function, whereas others are not. In general, the fusion process will affect only the latter. If a system's state is given by <P,Q,R,...Z> (x), the fusion between P(x) and Q(x), will leave R...Z unchanged and able to sustain the proper functioning of the system. Also, given that most properties are quantitative, part of P and part of Q will fuse, leaving the remainder to maintain the state. Wong's challenge to Humphreys is to show that this is will *always* be the case (Wong, 2006, p. 357). However, Wong's demand is unreasonable. If Humphreys can show that at least some of the special science properties are examples of fusion emergence, then this is enough to challenge the three assumptions mentioned at the beginning of the paper. But are Humphreys' examples able to do this? Before addressing this question, a couple of quick general points about Humphreys' account of emergence are in order.

14.4 The Division of Labor Between Properties and the Notion of a Physical Operation

Although Humphreys does not say it, his distinction between properties which are able to undergo fusion and those which are essential in the functioning of the system does in fact rely on two other dichotomies: first, between properties that are able to undergo fusion (PAUF) and properties that are not (PNAUF); and second, between properties which are essential in the functioning of the system (PEFS) and those that are not (PNEFS). Thus, Humphreys' distinction results from crossing two criteria: first, whether the properties are able to undergo fusion; second, whether the properties are essential in the functioning of the system. Humphreys assumes that the application of these two criteria delivers co-extensive subsets of properties, so that the properties which are able to undergo fusion will also be the ones that are not essential in the functioning of the system. Humphreys can, of course, maintain his distinction between properties without threatening the coherency of his account. That is, he can maintain that in any given entity there will be a "division of labor" between properties: some will undergo fusion, while others will preserve the functioning of the system. In this case, the properties to which the emergent character of an entity is due will not also be structural properties with a role in the in the functioning of that entity. Conversely, the structural properties that are crucial to the proper functioning of an entity won't participate in the fusion processes that that entity may undergo. However, these two last claims are far from trivial. Unless we have an independent justification of why the two dichotomies overlap, one may worry that Humphreys' division of labor between properties constitutes an ad hoc response to the problem of basal loss (Fig. 14.1).

The other point has to do with the nature of the fusion operation. On Humphreys' account, the fusion operation is not necessarily causal. However, fusion is supposed

Fig. 14.1 The dichotomy
between the properties that
are able to undergo fusion
(PAUF) and those that are not
(PNAUF) overlaps with the
dichotomy between the
properties that are not
essential in the functioning of
the system (PNEFS) and
those that are (PEFS)
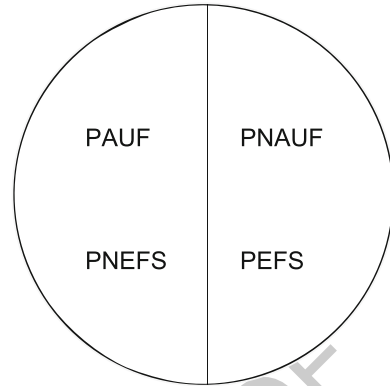
to operate on real properties in the world, not on their representations. Humphreys
claims that the fusion operation is "a real physical operation" as opposed to a merely
logical one like conjunction or disjunction (1997b, p. 10).

At this point, one may pause and ask what a *physical* operation is. We know
what a *logical* operation like conjunction or disjunction is because there are
logical/mathematical theories in which such operations are defined (e.g., sentential
logic, predicate logic, Boolean logic, etc.). In the absence of these theories, our
understanding of the logical operations will be greatly impoverished. What is the
corresponding theory for the fusion operation? Humphreys claims that fusion is a
physical operation. However, what it means for something to be a physical operation
is not entirely clear. For example, in physics textbooks one does not find such an
operation being defined. Humphreys may be taken as being uncommitted to the
exact nature of the fusion operation pending futher empirical work (Wong, 2006,
p. 352). It may turn out that fusion is implemented by single physical process
(already discovered or yet to be discovered), or by a host of physical processes.
In any case, an understanding of fusion as a physical operation depends on how
well one understands its physical implementation. In order to achieve this, one
needs to engage with empirical issues. It is to these empirical issues that I will now
turn.

14.5 Humphreys' Examples

Whether the theory of fusion emergence can be coherently formulated is one
thing; whether it applies to anything in the world is quite another. The former is a
theoretical aspect that can be addressed largely on a priori grounds, while the latter
is a an empirical issue. To argue that fusion emergence is not a metaphysician's
fiction but a real phenomenon, one needs more than appeals to imagined scenarios;
one needs concrete examples taken from the sciences. Humphreys presents such

examples. According to Humphreys, "the clearest cases of fusion emergence is the entangled states of quantum systems" (2008, p. 4).[7]

According to Humphreys, the existence of such cases of emergence entails that our world's ontology is not wholly compositional. By a compositional ontology Humphreys means an ontology in which "all non-fundamental entities are aggregated or structured collections of other entities that can be generated by the use of explicitly stated rules of combination, where the constituent entities retain their identities within the structure" (2008, p. 2).

Humphreys thinks that the entangled state of a composite quantum system does not conform to the requirements of a compositional ontology because it is non-separable – the state of the system cannot be written as a tensor product of the states of its parts. Although there may be worries that a theory whose physical interpretation is still heavily debated might not be our best guide to ontology, let's grant that the entangled state in quantum mechanics is a *bona fide* example of fusion emergence. The question then becomes whether there are other examples of fusion emergence in our world, preferably in the special sciences.[8] Humphreys' answer is affirmative. The example of fusion emergence that is discussed in most detail by Humphreys is that of the covalent chemical bond. As mentioned, according to Humphreys, covalent bonding is a "core example of fusion emergence"(2008, p. 7).

Why does Humphreys think that the covalent bond exemplifies fusion? Humphreys notes that a covalent bond occurs when a pair of electrons is shared by two atoms; he also notes that the electron density of the electrons which participate in the covalent bond is distributed over the entire molecule rather than the individual atoms. Humphreys also claims that while some properties remain unchanged after the fusion (e.g., the charge and mass of the nucleons, the total charge of the molecule), others are affected by it; for example, there is a slight lowering of the energy of the combined molecular arrangement compared to the energies of the atoms before fusion. According to Humphreys, this energy that emerges upon fusion is responsible for the characteristic properties of the molecule.

Humphreys contrasts the covalent bond with the ionic bond. He suggests that ionic compounds are the result of electrostatic forces between positively and negatively charged ions and can be understood within the framework of a compositional ontology. On the other hand, molecules (resulting from covalent bonding) exemplify fusion and therefore are non-compositional in the sense explicated above. Humphreys does not elaborate much on why ionic bonding is compositional and covalent bonding isn't. He only claims that there is a contrast between the two types

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[7]Humphreys' suggestion that the entangled state is an example of fusion emergence has been developed in more detail by Kronz and Tiehen (2002), who also discussed its ramifications and limitations.

[8]The exclusion argument to which fusion emergentism is an objection threatens the special sciences to a greater extent than physics.

of bonding and that the fact that "the molecule is not simply a spatial arrangement of the two atoms (...) is one of the things that distinguishes fusion from composition." (2008, p. 7).

14.6 Questioning the Ionic-Covalent Dichotomy

Insofar as Humphreys takes the two types of bonding as having different ontological requirements (and thus supporting incompatible ontologies), he is committed to a contrast between them that is not simply a matter of degree. However, the sharp contrast between ionic and covalent bonding that Humphreys' example assumes does not receive as much support from physical chemistry as one may think.

Ionic and covalent bonding are viewed as two extreme models of the chemical bond (Atkins and Jones, 2002, p. 92). With the exception of the bonds of homonuclear diatomic molecules, all chemical bonds lie somewhere between purely ionic and purely covalent. If the electronegativity difference $\Delta\chi$ increases, so does the ionic character of the bond.[9] Generally, if $\Delta\chi > 1.6$, the bond is considered ionic. If $\Delta\chi < 0.5$, the bond is considered covalent non-polar. And if $\Delta\chi$ is between 0.5 and 1.6, the bond is considered covalent polar. However, there is no principled way to choose these values and they may vary slightly from one chemistry textbook to another. There is no sharp distinction between an ionic and a polar covalent bond; rather, the difference between them is a matter of degree. If the difference between the two types of bonding is only gradual, then how can they be accomodated within different ontological frameworks? Where should the boundary between compositional and non-compositional be placed?

One may argue that as long as there exist clear cases of covalent and ionic bonding, this should be enough to justify the requirement of different ontological frameworks. However, while pure covalent bonding exists (between the atoms of homonuclear diatomic molecules such as Cl_2, H_2, O_2), pure ionic bonding cannot exist, since it would require that the electronegativity difference $\Delta\chi$ between the atoms be infinite or at least exceedingly large (Carter, 1979, p. 124). Therefore, all bonds have some covalent character. Does non-compositionality characterize only those pure cases of covalent bonding, or should all types of bonding be accountable within a single (non-compositional) ontology? If neither, how should the discrete border between two distinct ontological frameworks be superimposed onto the covalent-ionic continuum? These questions are not in themselves sufficient to show that Humphreys' account fails, but they are certainly indicative of a lack of harmony

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[9]On the Pauling scale, the difference in electronegativity between atoms A and B is a dimensionless quantity: $\chi_A - \chi_B = (eV)^{-1/2}\sqrt{E_d(AB) - [E_d(AA) + E_d(BB)]/2}$, where $E_d(XY)$ represents the dissociation energy between atoms X and Y in electronvolts. Pauling defined the amount of ionic character of a chemical bond as $1 - e^{-1/4(\chi_A - \chi_B)}$ (Pauling, 1960, p. 98).

between the sharp character of the boundary between a compositional and a non-compositional ontology and the non-sharp character of the boundary between ionic and covalent bonding.

There is another problem with viewing chemical compounds through the ionic-covalent dichotomy. These two types of chemical bonding are models, i.e., they are idealizations which have their virtues but distort reality in some respect. For example, they represent the pair of electrons participating in a covalent bond as being shared by just one pair of atoms, even when the molecule is polyatomic. Chemical bonds between atoms can be described more accurately using the concept of resonance. Resonance refers to the representation of the electronic structure of a molecular entity in terms of distinct contributing structures (also called resonance structures). Electrons involved in resonance structures are said to be delocalized: for example, in the case of a polyatomic molecule the sharing of an electron pair is distributed over several pairs of atoms and cannot be identified with just one pair of atoms. A resonance hybrid is a blend of the contributing structures.

All compounds, regardless of whether they are considered ionic or covalent, can be viewed as resonance hybrids of purely covalent and purely ionic *resonance structures*. For example, the structure of a homonuclear diatomic molecule, in which two atoms of the same element are covalently bonded to each other, can be described as a resonance hybrid of two ionic structures (Atkins and Jones, 2002, p. 93).

$$A{-}A \longleftrightarrow A^{\delta-}A^{\delta+} \longleftrightarrow A^{\delta+}A^{\delta-}$$

In the case of homonuclear diatomic molecules, the ionic structures make only a small contribution to the resonance hybrid. Also, the two ionic structures have the same energy and make equal contributions to the hybrid, so the average charge on each atom is zero. In a heteronuclear molecule, the resonance hybrid has unequal contributions from the two ionic structures – the structure with the negative charge on the atom that has a greater electron affinity will make a bigger contribution to the resonance hybrid.

The representation of chemical compounds in terms of resonance structures is more accurate than the ionic-covalent representation but it is strictly speaking incompatible with it. The resonance model challenges the view of chemical compounds as either ionic or covalent because resonance hybrids are a blend of resonance structures rather than the flickering of a compound between different structures, just as a mule is a blend of a horse and a donkey, not a creature that flickers between the two (Atkins and Jones, 2002, p. 80).

14.7 The Level-Relativeness of Fusion

According to Humphreys, the covalent bonding exemplifies a kind of ontological emergence which shows that the ontology of our world is not exclusively compositional. Why does Humphreys think that molecules cannot be understood in the

framework of a compositional ontology? Molecules consist of atoms, so at a first glance, the compositionality condition would seem to be satisfied. However, at a closer look, one realizes that molecules are not simply the result of the combination or spatial juxtaposition of atoms. A molecule is the *sharing* of electrons between two or more atoms. Because of this, Humphreys is justified in claiming that the molecule can be described as the *fusion* of two or more atoms, not as a combination or aggregation of atoms.

However, if one thinks of molecules not as collections of atoms but as collections of nuclei and electrons, what looks like fusion between two atoms can be described as composition of nuclei and electrons. The Aufbau principle consists in a number of explicitly stated rules that allow us to understand the atom (any atom) as a physical system that is built by successively adding electrons around the nucleus.

1. The principle of the minimum energy: the electrons occupy atomic orbitals in such a way that the total energy of the atom is a minimum; they fill orbitals starting at the lowest possible energy states before filling higher states.
2. The Pauli exclusion principle: every electron in an atom is described by its own distinct set of four quantum numbers, not shared with any other electron. This entails that a given orbital is to be occupied by no more than two electrons, case in which their spins, denoted by the m_s quantum number, are paired.
3. The Madelung rule: orbitals with a lower $n + l$ value are filled before those with higher $n + l$ values.
4. Hund's rule of maximum multiplicity: electron pairing will not take place in orbitals of the same sub-shell until orbitals are singly filled by electrons with parallel spin.

It should be recognized that the Madelung rule and Hund's rule of maximum multiplicity are not exceptionless. They are rules of thumb, but they are helpful. There must be some deeper reason of why these rules work (when they do), although deriving these rules from deeper physical principles has proven to be not an easy task. What these four rules show is that the atom is a complex physical system in which the nucleus and the electrons are subject to a number of physical constraints and interact with each other according to physical laws. It is these physical laws and constraints that are the more basic rules of composition in the multi-electron atom. The atom appears to be more than just a collection of individual particles because of the complexity of the interactions between these particles.

In contrast with the entangled state, which is non-decomposable into separate states of each of the two electrons and thus cannot be written as a tensor product of the states of the individual electrons, the wavefunction of a multi-electron atom can be thought of as resulting from the separate contributions of each electron wavefunctions, and it can be written as a product of individual atomic orbitals: $\psi(r_1, r_2, \ldots . r_n) = \phi_1(r_1)\phi_2(r_2)\ldots.\phi_n(r_n)$. This strategy of learning about the wavefunction of a multi-electron atom on the basis of the individual electrons

is known as the *orbital approximation* and is a remarkably useful tool in the attempts at solving the Schrödinger equation for atoms that have more than one electron. When applied to multi-electronic atoms, the (atomic) orbital approximation assumes that each electron behaves independently of the others, and thus the electronic Hamiltonian can be separated into as many components as there are electrons: $\hat{H}_e = \hat{H}_1 + \hat{H}_2 + \ldots + \hat{H}_n$.

The treatment of the multi-electron atom in physical chemistry is, I think, an illustration of compositionality. Admittedly, the orbital approximation is an approximation – the inter-electronic repulsion forces which are due to the Coulomb potential are deliberately ignored, to make the Schrödinger equation more tractable. However, the existence of such forces does not show that the atom cannot be understood compositionally; after all, the electron-electron repulsion itself obeys compositionality – the repulsive force depends on the charge and and distance between the individual electrons.

The presence of compositionality principles seems to be abundant in the physical chemistry of molecules, too. In contrast to older theories such as the valence shell electron pair repulsion theory (VSEPR), the molecular orbital theory describes the electrons in a molecule as delocalized; they are not confined to pairs of atoms, but are spread over the whole molecule. The central claim of the molecular orbital theory is that molecular orbitals are obtained from summing up atomic orbitals. More rigorously, each one-electron molecular orbital ϕ_i is expressed as a linear combination of atomic orbitals (LCAO): $\phi_i = c_{1i}\sigma_1 + c_{2i}\sigma_2 + c_{3i}\sigma_3 + \ldots + c_{ni}\sigma_n$, where the coefficients represent the weights of the contributions of each atomic orbital to the molecular orbital and are found using the Hartree-Fock method. The wavefunction for the molecule is then written as a product of one-electron wavefunctions. This is the molecular orbital approximation: the wavefunction of a multi-electron molecule is approximated as the product of individual molecular orbitals: $\Psi(r_1, r_2, \ldots r_n) = \Phi_1(r_1)\Phi_2(r_2)\ldots\Phi_n(r_n)$. The electron configuration of molecules is obtained from the same set of rules that yielded the electron configuration of multi-electron atoms.

In some sense, Humphreys is justified in thinking of the molecule non-compositionally, for a molecule is not simply the result of the spatial arrangement of atoms. If one descends one ontological level (e.g., from the level of the molecule to the level of atoms), the molecule cannot be described compositionally, in terms of separate but interacting atoms. However, if one descends *two* ontological levels (e.g., from the level of the molecule the level of nuclei and electrons), the molecule *can* be described in terms of separate but interacting components. What what looks like fusion at the *i*-level (molecular level) can be represented as composition at the *i*-2-level (level of electrons and nuclei). For example, in the case of a simple molecule such as the dihydrogen molecule, what looks like fusion between two hydrogen atoms could be understood as composition between two nuclei and two electrons.

14.8   Entanglement to the Rescue?

An argument that challenges this conclusion may in fact be available to the defender of non-compositionality. The argument is based on the remark that the electrons which participate in the covalent bond have opposite spins (are paired), and thus they are entangled (i.e., they form a singlet state, or a state in which their total spin is zero). If the entangled state is a *bona fide* case of fusion and hence it does not conform to the requirements of a compositional ontology, then the molecule must also be an example of fusion. On this view, the fact that the electrons participating in the covalent bond cease to possess separate states is sufficient grounds for concluding that the molecule is a non-separable whole which defies a compositional ontology. The defender of non-compositionality could argue that the covalent bond (and hence the molecule) owes its existence to the entanglement of the electrons constituting the bond. On this view, once two electrons belonging to different atoms have become entangled, a covalent bond occurs between the atoms and a new entity emerges: the molecule.

The problem with the argument above is that it does not give an accurate characterization of the origin and nature of the chemical bond. Chemical bonds are due to the interplay of four sets of forces: the attraction of each electron to the nucleus of its own atom, the attraction of each electron to the nucleus of the other atom, the electron-electron repulsion, and the nucleus-nucleus repulsion. The fact that the electrons participating in a covalent bond are paired is a consequence of their obeying the Pauli exclusion principle. However, the Pauli exclusion principle is not a force, but a constraint that the electrons must satisfy if a covalent bond is to be formed. Consider two hydrogen atoms whose electrons have parallel spins. If the atoms are brought together, the charge density from each electron is accumulated in the antibonding region (i.e., at the extremities of the system), rather than in the bonding region between the nuclei. Therefore, they will not form a dihydrogen molecule. The role of the Pauli exclusion principle is to veto those systems that cannot form a molecule by imposing a constraint on the spin of the electrons participating in the covalent bond. The Pauli exclusion principle tells us that only those hydrogen atoms whose electrons have opposite spins are eligible for forming a bond. The spin entanglement that can be found in a molecule does not play the role of a force holding the molecule together.[10]

In fact, there are molecules in which not all of the electrons are entangled, such as molecules with unpaired electrons or an open shell configuration. Although usually the unpaired electrons are found in the antibonding orbitals and they are expected to

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[10]The so-called "exchange force" or "exchange interaction" which decreases the expectation value of the distance between two electrons (or fermions, more generally) with identical quantum numbers when their wave functions overlap is not a true force and should not be confused with the exchange forces produced by the exchange of force carriers, such as the electromagnetic force produced between two electrons by the exchange of a photon, or the strong force between two quarks produced by the exchange of a gluon.
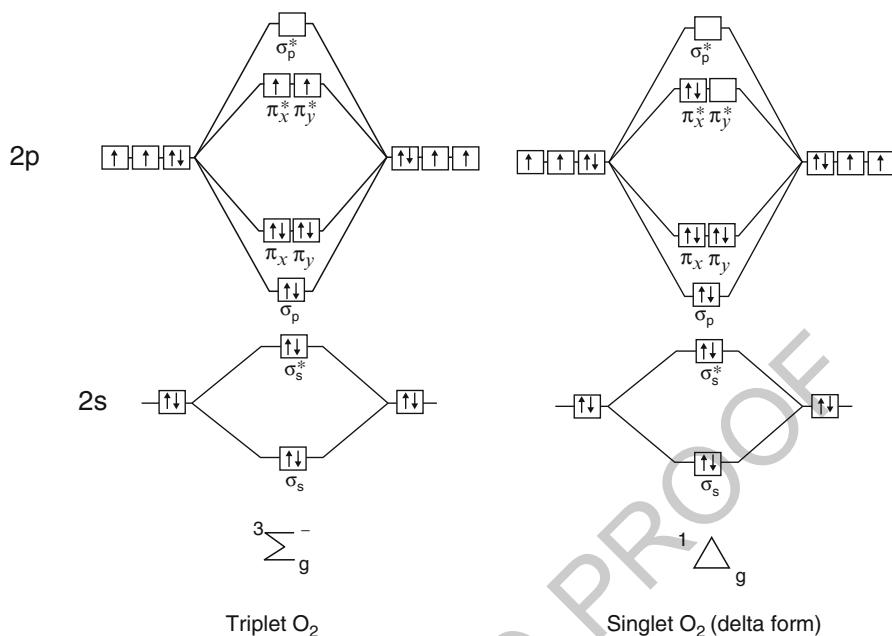
Fig. 14.2 Triplet O_2 vs. singlet O_2

lower the bond order and thus decrease the bond energy, there are cases such as the oxygen molecule, O_2, in which the unpaired electrons actually increase the strength of the bond. The ground state of the oxygen molecule is also known as the triplet oxygen because the total spin of the molecule is 1: the electrons occupy two different $2p\pi^*$ molecular orbitals singly and, according to Hund's rule, their spins are parallel (this can also be deduced empirically, from oxygen's paramagnetism) (See Fig. 14.2 below). The triplet oxygen is known to be more stable than the singlet oxygen – a diamagnetic form in which the electrons are paired in the same $2p\pi^*$ orbital (Wiberg et al., 2001, p. 476).[11] Another example is that of the molecular hydrogen ion, H_2^+, in which there is no entanglement since there is only one electron. The bond holding together the dihydrogen cation is described as a "one-electron bond", and has a formal bond order of $\frac{1}{2}$ (Pauling and Wilson, 1963, p. 362). For this simple system the Schrödinger equation can be solved accurately and the calculations show clearly that the molecular entity possesses a bound state, i.e., it possesses a ground state whose energy is less than that of a hydrogen atom and a free electron. In the case of dilithium, the binding energy is greater for the one-electron Li_2^+ than for the two-electron Li_2, although in the Li_2^+ there is no entanglement involved in bonding, while in the Li_2 there is (James, 1935).

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[11]The specific form referenced here is $O_2a^1\Delta_g$.

These examples show that the connection between the chemical bond and entanglement is not as strong as the argument that is available to Humphreys may assume it to be. They show that (i) the chemical bonding of some molecular entities is possible even in the absence of entanglement, as in the case of the one-electron bonds, and (ii) the chemical bond of some molecules is actually stronger if not all electrons are entangled.

14.9 Conclusion

Humphreys' fusion emergence is an elegant solution to the exclusion problem, but it is not without its difficulties. There are a couple of general concerns. First, there is the worry that Humphreys' division of labor between properties may be an ad hoc response to the problem of basal loss if we don't have independent justification for why the dichotomy between the properties that are able to undergo fusion and those that are not should overlap with the dichotomy between the properties that are not essential in the functioning of the system and those that are. Second, the notion of a physical operation plays a crucial role in Humphreys' emergentist account, but it is not clear what this operation means, and how it is implemented at the physical level.

There are also more specific concerns which regard Humphreys' core example of fusion emergence. In developing this example, Humphreys assumes a deep contrast between ionic and covalent bonding that is not warranted by physical chemistry. It is not clear how the the fuzzy boundary between ionic and covalent bonding maps onto the discrete boundary between a compositional and a non-compositional ontology.

Finally, Humphreys' claim that chemistry gives us reasons to reject a compositional ontology is problematic. While it is true that the molecule can be described as the fusion of atoms, if one thinks of the molecule not as a collection of atoms but as a collection of electrons and nuclei, what looks like fusion between two atoms could perhaps be described as composition of electrons and nuclei. In fact, chemistry is full of compositional principles: in the molecular orbital theory, each one-electron molecular orbital is expressed as a linear combination of atomic orbitals; the orbital approximation gives us a way of learning about the wavefunction of a multi-electron atom or molecule on the basis of the wavefunctions of the individual electrons; and the Aufbau principle gives us explicit rules of composition for obtaining the electronic structure of atoms and molecules. Given the effectiveness of these rules and principles and the fact that they are compositional *par excellence*, it is premature to conclude that the entities forming the subject matter of chemistry cannot be accommodated within the framework of a compositional ontology.

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