The Irreducibility of Chemistry to Everettian Quantum Mechanics

Abstract

The question of whether chemical structure is reducible to Everettian Quantum Mechanics (EQM) should be of interest to philosophers of chemistry and philosophers of physics alike. Among the three realist interpretations of quantum mechanics, EQM resolves the measurement problem by claiming that measurements (now interpreted as instances of decoherence) have indeterminate outcomes absolutely speaking, but determinate outcomes relative to emergent worlds (Maudlin, 1995). Philosophers who wish to be sensitive to the practice of quantum chemistry (e.g. Scerri, 2016) should be interested in EQM because Franklin and Seifert (2020) claim that resolving the measurement problem also resolves the reducibility of chemical structure, and EQM is the interpretation which involves no mathematical structure beyond that used by practicing scientists. Philosophers interested in the quantum interpretation debate should be interested in the reducibility of chemistry because chemical structure is precisely the kind of determinate three-dimensional fact which EQM should be able to ground if it is to be empirically coherent (see Allori, 2023). The prospects for reduction of chemical structure are poor if it cannot succeed in EQM; the prospects for EQM as a guide to ontology are poor if it cannot reduce chemical structure.

Unfortunately for proponents of chemical reduction and EQM, there are three serious barriers to the reduction of chemistry to EQM. The first concern is that quantum treatments of chemical structure rely on the Born-Oppenheimer approximation, which holds nuclear locations fixed while minimizing the energy of the electronic configuration (Hendry, 2022), but this approximation is not licensed by EQM. The Born-Oppenheimer approximation relies on nuclei and molecular orbitals being simultaneously present, but in the three-dimensional ontology following from the Everett interpretation these only emerge at different energy scales and are not simultaneously present (Miller, 2023). The second concern is that the emergent worlds of EQM are supposed to be decoherent at the macro-scale (A. Wilson, 2020), but the recent development of superchemistry suggests that chemical reactions can occur in coherent states (Zhang et al., 2023). The third concern is that emergent worlds are only pragmatic pseudo-processes (Wallace, 2012b), but this means EQM trades realist physics for mere instrumentalism about chemistry. Absent a commitment to chemical realism, reduction is an empty promise. The prospects for reduction of chemical structure to EQM are therefore poor.

The Ontological Reducibility of Chemistry

Whether the ontology of chemistry (e.g., atoms, bonds, and molecules) forms a distinct layer of reality or is reducible to quantum physics has been a central concern for philosophers of chemistry. Standardly a distinction is made between epistemic/theoretical, ontological, and mereological reduction (Hendry & Needham, 2007). Mereological reduction of chemical to physical entities—the view that molecules just are fusions of fundamental particles in certain states—is the weakest claim and correspondingly has the broadest support (e.g. Le Poidevin, 2005; Hendry, 2012; Scerri, 2012). Ontological reduction adds the further claim that the properties of those fusions can be analyzed entirely in terms of the properties of their parts—i.e., that they lack emergent properties or downward causal powers. This view has more mixed support, with Alex Franklin and Vanessa Seifert (2020) presenting a novel argument in favor, Eric Scerri (2016) seeing a hopeful possibility not yet fully established, and Robin Hendry (2012) dismissing it as a baseless hope. The epistemic-theoretical claim—that physical theories and laws plus appropriate bridge-laws or approximations make chemical theories and laws strictly redundant as mere pragmatic simplifications—is the strongest and generally dismissed by philosophers of chemistry (e.g. Scerri, 1991b, 1994).

Of course, if chemical theorization is strictly redundant, then so are the entities described by those theories, so epistemic reduction implies ontological reduction, and if chemical properties are ontologically reducible then surely chemical entities can be no more than mereological fusions, so ontological reduction implies mereological reduction. The reverse is not true: mereological reduction without ontological reduction is what is what David Chalmers (2008) calls strong emergence, and ontological reduction without epistemic reduction is what he refers to as weak emergence.[1] In this paper I will grant the consensus on the (present) failure of epistemic reduction and focus on the ontological reduction claim.

The main argument in favor of strong emergence for chemical entities and properties is given by Hendry (2006, 2010, 2012, 2017, 2019, 2021, 2022). In its strongest form, it runs as follows: quantum mechanics cannot generate molecular structure from the list of physical components of the molecule, but structure is essential to molecular identity and chemical properties, therefore molecules and chemical properties are strongly emergent. The argument can be made in either a more practical or a more theoretical form. Practically speaking, approximate molecular structure is an input to quantum chemical calculations about bond angles and lengths. The Born-Oppenheimer approximation takes these nuclear locations as fixed when calculating electronic energies, which are minimized in calculating stable states. Theoretically speaking, a completely *ab initio* wavefunction generated by the Schrodinger equation will always be radially symmetrical, which real molecules generally are not. Asymmetries are introduced by constraining the solution—but for molecules in gas phase that can only be done by assuming structure. These issues are especially clear in the case of stereo isomers—differently structured (inversely handed) molecules with different properties but the same physical components, hence the same *ab initio* wavefunctions.

The strongest argument in favor of ontological reduction is given by Franklin and Seifert (2020). They point out that *all* quantum mechanical results are symmetrical without imposed structure, not just chemical ones. The Schrodinger equation always evolves linearly, giving rise to the famous "measurement problem" embodied in the Schrodinger's Cat thought experiment, where the cat's wavefunction is symmetric between |live> and |dead> states, yet the outcome of measurement is exclusively one state or the other. The fact that molecules are always found in a particular isomer rather than a symmetric state is just an instance of the measurement problem, and quantum mechanics must be interpreted to solve the measurement problem if it is to be consistent on its own terms, since it pertains to the outcome of purely physical experiments (Maudlin, 2019). Fortin and Lombardi (2016; 2017, 2021) and Hendry (2022) may be skeptical of whether the measurement problem can be solved in a compelling way, but their skepticism is not broadly shared among philosophers of physics, as major progress has been made in the last decade by all three realist interpretations of quantum mechanics (Maudlin, 2019). While I do not have the space to examine this dispute in detail here,[2] it is worth at least granting *arguendo* that decoherence solves the measurement problem in Everettian many worlds (Wallace, 2010, 2012a) and Bohmian pilot wave (Romano, 2023) mechanics. The burden is therefore on ontological emergentists to respond to Franklin and Seifert's argument.

[1] Jessica Wilson (2021) argues that weak emergence, too, can have metaphysical force.
[2] For background on decoherence, see (Bacciagaluppi, 2020; Schlosshauer, 2007, 2009; Joos, 2009).

As Scerri (1991a, 1998) and Seifert (2022) remind us, these are not merely idle questions for philosophers. They have implications for the funding of long-term research initiatives (will quantum methods come to predominate in every area of chemistry?), particular research directions (e.g., should quantum chemists study decoherence theory?), and especially chemical education (should the classical or quantum models be taught as approximations?). The ontological reduction (or emergence) of chemistry to quantum mechanics is worth investigating.

The Ontology of Everettian Quantum Mechanics

Scerri (2016) and Hendry (2022) both rightly insist that the ontological reduction question should be investigated with respect to the details of chemical and physical theory and practice, rather than in an overly abstract or airy manner. Hendry levies the particular demands that Franklin and Seifert propose a method for preparing superposed molecular structures and a physical mechanism for symmetry-breaking. Yet this is precisely what Seifert does: she claims that single molecules in isolation lack structure and that environmental decoherence is the physical mechanism for symmetry-breaking (Seifert, 2019, 2020). Nor are such proposals limited to the philosopher's armchair, as laser chemistry allows single-molecule synthesis (Bloembergen & Zewail, 1984; Nuernberger et al., 2010)[3] and induced symmetry-breaking (Shapiro & Brumer, 1997; Assion et al., 1998) including the observation of unstable transition states (Polanyi & Zewail, 1995). The question at hand is thus whether we can give an adequate theoretical account of these processes in a purely *ab initio* manner.

While Franklin and Seifert (2020) discuss all three realist interpretations of quantum mechanics, I will focus on the Everettian many-world interpretation here because it is the closest to physical practice Wallace (2020), without the new (and inevitably somewhat toy model) mathematics of Bohmian pilot-wave or GRW objective-collapse interpretations. This is not to deny that such interpretations have their advantages, but if Franklin and Seifert's argument works anywhere it should be on its strongest ground in Everettian quantum mechanics, which is better equipped to model the complex interactions and real life laboratory situations where reduction seems most plausible (Scerri, 2016).

The basic claim of Everettian quantum mechanics is that wavefunctions are symmetrical with respect to the global state—the Schrodinger equation of the universe evolves linearly without collapse and all possible experimental outcomes occur—but definite outcomes occur with respect to *worlds* and their occupants. Measurement is thus understood as the branching of worlds, which in contemporary versions of Everettianism is ascribed to decoherence rather than any particular experimental action or human mental state (Wallace, 2003a). What distinguishes worlds is their relative causal isolation (due to decoherence) up to some chosen fineness of grain. The branching of worlds, in turn, can be understood either as fission—where worlds split and the Born rule is an expectation value of the future (Deutsch, 1999; Wallace, 2003b, 2012b) or as divergence—where previously qualitatively identical worlds begin to differ and the Born rule is a centered chance (A. Wilson, 2020; Wilhelm, 2022, 2023).

The ontological reduction of chemical entities and properties is an important proving-ground for the ontology of Everettian quantum mechanics. Everettians tend to posit a Hilbert-space vector (Carroll & Singh, 2019), a wavefunction (P. J. Lewis, 2004, 2016; Albert, 2013; Ney, 2021, 2023), or a spacetime state (Wallace & Timpson, 2010) as their sole fundamental ontology. If Everettianism is to be empirically adequate, macro-objects like chemical substances should be reducible to that fundamental ontology (Maudlin, 2010; Ney, 2013, 2015, 2020; Allori, 2023). An interpretation of

[3] For background on laser chemistry, see (Laforge et al., 2023).

quantum mechanics which cannot plausibly reduce chemical entities and properties is implausible in its pretensions to be a complete theory of physical reality (Maudlin, 2007; Albert, 2015). Philosophers of physics with strong physicalist and Everettian sympathies should thus be as interested in the question of the ontological reducibility of chemistry as philosophers of chemistry and practicing quantum chemists. Much is at stake, but three important barriers remain.

The Mereological Barrier

As noted in the first section, ontological reduction presumes mereological reduction: if chemical properties can be identified with physical ones, then chemical entities must be mere fusions of physical entities, which are the bearers of physical properties.[4] As I have previously argued, however, mereological reduction is problematic for Everettians (Miller, 2023). The ontological innocence of composition means the whole is present whenever and wherever the parts are and vice versa[5] which implies that mereological reduction requires compresence of parts and wholes with respect to times and worlds. If the parts are not present at a time when the whole is present, then the whole cannot be reduced to the parts at that time—and therefore must not be a mere fusion of those parts. Furthermore, the chemical whole and its physical parts must belong to the same Everettian world. This is because Everettians adopt the Lewisian device of using “actual” to refer to the index world (Wallace, 2002; A. Wilson, 2020), lest it fail to be the case that experiments have determinate actual results. If the physical parts do not belong to the same Everettian world as the whole, then they are not actually present and cannot be the bearers of the actual properties measured by the chemist. This is what Hendry (2020) calls the “actually present elements principle” and it is uncontroversial in the literature, relied on by both emergentists and reductionists (e.g. Le Poidevin, 2005; Hendry & Needham, 2007; Scerri, 2007, 2012; Franklin & Seifert, 2020).

The difficulty is that Everettian quantum mechanics precludes mereological reduction of chemical entities. The fundamental ontology for Everettians is either the wavefunction or the spacetime state, and the particles of the Standard Model are patterns in this state (Albert, 2013; Wallace & Timpson, 2010). For mereological reduction to occur, the chemical patterns would need physical subpatterns,[6] the way a painting is built up from brushstrokes, and both the painting as a whole and individual brushstrokes are identified by patterns of color and texture in the paint. Patterns only exist in Everettian worlds when physical decoherence processes secure relative causal isolation, however, and the scale of decoherence depends on the energy scale of the experiment (Wallace, 2012b). The X-Rays used for molecular structure determination in diffraction experiments have wavelengths on the order of 10^{-11}m while nuclei have radii on the order of 10^{-14}m. Thus worlds where molecular structure is actual at a given time and place lack any pattern for nucleons at that time and place, while regions of spacetime probed at the energy levels required to resolve nuclei would actually

[4] This is David Lewis’s Weak Composition-as-Identity (D. K. Lewis, 1991; Hawley, 2014; Varzi, 2014). If composition is not ontologically innocent, then there can be no identity of wholes with their parts, and thus no mereological reduction, or ontological reduction at all (only eliminativism, which requires). The alternative, I suppose, is that chemical entities could be parts of physical ones, but this both runs counter to the practice of quantum chemistry and would tend to make chemical entities the fundamental ones—the slogan is that composition is ontologically innocent, not that decomposition is. Even in approaches where the physical whole is fundamental, like Schaffer (2010; Ismael & Schaffer, 2020), chemical entities are usually treated as derivative fusions of microphysical parts.

[5] Technically this also requires a near-universally accepted formal principle of location, Expansivity (Calosi, 2020, 2022).

[6] The alternative, that chemical patterns are parts of the overall pattern, is precluded because four-dimensional chemical entities cannot be parts of the wavefunction (Calosi, 2022) nor the spacetime state (Wallace & Timpson, 2010).

destroy molecular structure (Bellac, 2011). No experiment can decohere molecular structure and nucleonic positions simultaneously, so they cannot be compresent in the same world, and the former cannot be mereologically reduced to the latter. If mereological reduction fails, so does ontological reduction—only eliminativism is left, and it is subject to the criticisms of the last section on chemical realism.

The Decoherence Barrier

A second barrier for the ontological reduction of chemistry to Everettian quantum mechanics is found not in the lack of adequate decoherence for physical particles, but for chemical structures themselves. Chemists appeal to chemical structure in their explanations of chemical properties, especially reactivity (Hendry & Needham, 2007). Perhaps isolated molecules lack structures (Seifert, 2020), since they are by definition not engaging in chemical reactions or physical experiments which chemists would explain with structure. The permanence or essential aspect of structure may thereby be idealizations. But if molecules lack structure while they are undergoing chemical reactions, then an anti-realist rather than reductionist attitude has been adopted, because the chemical explanation in terms of structure lacks any grounding in chemical ontology. Everettian quantum mechanics, however, cannot be the reduction base for chemical structure during all chemical reactions.

Some additional elaboration on the relationship between worlds and decoherence in Everettian quantum mechanics will help to shine light on this decoherence requirement. According to contemporary Everettians like David Wallace (2012b) and Alastair Wilson (2020), worlds exist not only with different definite outcomes but with different fineness of grain. Decoherence is a continuous process, so there are no special measurement points at which worlds branch or diverge. Rather, worlds branch or diverge when human pragmatic thresholds for definiteness of outcome are exceeded. Definite states are those which appear fixed in scientific explanations. If humans care only about extremely macro-scale processes, then they will inhabit coarse-grained worlds which exhibit a great deal of quantum behavior at the micro-scale below their threshold of care. On the other hand, humans who care about relatively micro-scale processes will inhabit more fine-grained worlds which thereby necessarily exhibit less quantum behavior. Thus contemporary Everettians move Copenhagen concepts of measurement into the pragmatic realm.

This account is problematic for contemporary quantum chemistry. On the one hand, chemical structures are supposed to serve as explanans in chemical reactions. If those chemical structures are definite due to quantum decoherence processes as Franklin and Seifert (2020) suggest, then we must be living in a quite fine-grained world. The recent development of superchemistry—whereby reactions occur in coherent states (Zhang et al., 2023)—suggests that we must live in a coarser-grained world, however, where chemical realities are not always definite, even during reactions. How can an Everettian world be fine-grained enough for definite chemical structures to decohere, yet coarse-grained enough that the very existence of the reagents or products is not yet definite? This is obviously a contradiction, but then Everettians cannot invoke decoherence to ontologically reduce the structures that chemists rely on to explain reactivity. Simply put, Everettians have no way to invoke both the quantum and classical elements simultaneously in the way that quantum chemical explanations do, and thereby lack any means to ontologically reduce quantum chemistry. Perhaps Everettians could appeal to pragmatic differences in fineness of grain between chemists appealing to quantum coherence explanations for superchemistry and those appealing to quantum decoherence explanations for structure, but that leads to the anti-realism criticized in the next section.

The Realism Barrier

The final difficulty for ontological reduction of chemistry to Everettian quantum mechanics is that such reductions should be realist about chemistry in a way that Everettians cannot be. A great deal of Everettianism's allure is that it offers a realist account of quantum mechanics (unlike the Copenhagen view of measurement) and indeed one that reads the existing highly successful scientific formalism in a realist way (unlike Bohmian or collapse accounts which add new elements to the formalism and regard the existing widely used one as only a model). Any attempted ontological reduction of chemistry to Everettian quantum mechanics owes chemistry the same courtesy, as a well-developed highly-accurate and fruitful empirical natural science in its own right. Perhaps folk theories of mind are appropriate for more eliminativist treatment (e.g. Churchland, 1981), but chemical accounts in terms of moles of reagents with certain structures have extreme predictive success. It is one thing to treat those explanans eliminatively as part of a successful epistemic reduction where the lower-level physical theory correctly reproduces all of the predictions of the reduced theory (as in the reduction of Newtonian mechanics to general relativity), but in the case of chemistry no such theoretical reduction is in view, as discussed in the first section. Properly ontological reduction, on the other hand, has no grounds for eliminating the reduced theory, and must instead attempt to identify the entities and properties of the reduced theory with entities and properties of the reducing theory, or fusions thereof. A successful ontological reduction of chemistry to Everettian quantum mechanics would thereby maintain realism about chemical structures and molarities.

Unfortunately contemporary Everettians who treat worlds as mere pragmatic pseudo-processes (Wallace, 2012b) or context-dependent vague predicates (A. Wilson, 2020) are ill-placed to maintain realism about chemical claims. According to the Everettian reductionist, molecules are determinate non-fundamental entities which thus only exist within worlds. Whether a certain molecular structure is present, and hence how many moles of a certain substance there actually are, depends on the grain of the world we inhabit. If the grain is coarse, only outcomes with major macro-scale consequences count as determinate, and it will count as indeterminate what structures (and hence what moles of what substances) exist in say gas phase. If the grain is fine, then more micro-scale outcomes count as determinate, and it will be true to say that there are more decohered molecular structures present, and hence more moles of a certain substance. Chemical facts will depend on pragmatic choices about coarse-graining of worlds. But this is counter to realism about chemistry. Chemists measure their reagents and invoke stoichiometry to evaluate the molarities of various products. After the measurable energy transfer in an exothermic or endothermic reaction is complete, measurements confirm what products were synthesized, they do not themselves synthesize the products. Placing chemical entities within Everettian worlds has come at the cost of realism about those chemical entities.

Nor can the Everettian provide any justification for this irrealist stance towards chemistry without invoking ontological reduction as an a priori dogma. Realism about chemical entities is justified by the same track record of experimental success that justifies Everettian realism about the wavefunction. Certainly we can agree that chemical entities are non-fundamental in the sense that they depend on physical processes with broader applicability, but this should not imply that they are arbitrary or of no ontological concern—that is what the eliminativist has the burden to demonstrate. Unless Everettians can provide a realist account of chemical entities, their stance amounts to a hopeful eliminativism about chemistry rather than a hard-headed ontological reductionism.

Conclusion

Reductionism about chemistry comes in different strengths: mereological (chemical entities are fusions of physical ones), ontological (chemical entities can be identified with physical ones), and empistemic/theoretical (chemical entities can be completely accounted for by physical theories). Since most parties take the first for granted and find the third implausible, the dispute has focused on ontological reduction. Since such reduction depends on resolving quantum indeterminacy (Franklin & Seifert, 2020), proponents should take the contemporary Everettian decoherence approach to resolving such indeterminacy as a serious test case. If reduction is implausible on the best developed realist interpretation of quantum mechanics, then it is implausible tout court. In the other direction, contemporary Everettians like David Wallace and Alastair Wilson who consider the theory a complete guide to fundamental reality should take the ontological reduction of chemistry as a test case. If chemical realities are likely to exhibit some form of strong emergence, then Everettian quantum mechanics does not offer a complete account of the state of the world.

As we have seen, there are three serious barriers to optimism about the ontological reduction of chemistry to Everettian quantum mechanics. First, even mereological reduction may not hold due to the difference in scales of decoherence between molecular structures and fundamental physical particles. Second, relying on decoherence to reduce chemical structures undercuts the possibility of chemical explanations for reactions which occur in coherent states, so-called superchemistry. Third, placing chemical entities solely within pragmatically defined worlds undercuts realism about chemistry, which is motivated by the same experimental successes which motivate Everettian realism about quantum mechanics. These barriers are so fundamental to the structure of Everettian quantum mechanics as a physical theory that they make it unlikely that any related theory could serve to ontologically reduce chemistry. This should be especially worrying for proponents of reduction, since Everettianism is more likely than Bohmian or objective-collapse theories to serve as an interpretation of quantum gravity, the next major threshold development in physical theory.[7] The hope of ontological reduction for chemistry therefore seems unmotivated.

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[7] In brief, extant theories of quantum gravity treat quantum phenomena as fundamental but spacetime as emergent—due to the structure of the Wheeler-DeWitt equation (Wüthrich, 2019) whereas Bohmian and objective-collapse theories rely on spacetime to formulate quantum phenomena.

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