



Article scientifique

Article

2023

Published version

Open Access

This is the published version of the publication, made available in accordance with the publisher's policy.

---

## Chemical reduction and quantum interpretation: a case for thomistic emergence

---

Miller, Ryan Michaël

### How to cite

MILLER, Ryan Michaël. Chemical reduction and quantum interpretation: a case for thomistic emergence. In: Foundations of chemistry, 2023, vol. 25, n° 3, p. 405–417. doi: 10.1007/s10698-023-09479-6

This publication URL: <https://archive-ouverte.unige.ch/unige:180532>

Publication DOI: [10.1007/s10698-023-09479-6](https://doi.org/10.1007/s10698-023-09479-6)

© The author(s). This work is licensed under a Creative Commons Attribution (CC BY 4.0)

<https://creativecommons.org/licenses/by/4.0>



# Chemical reduction and quantum interpretation: A case for thomistic emergence

Ryan Miller<sup>1</sup>

Accepted: 13 August 2023 / Published online: 26 August 2023  
© The Author(s) 2023

## Abstract

The debate between ontological reductionists and emergentists in chemistry has revolved around quantum mechanics. What Franklin and Seifert (BJPS 2020) add to the long-running dispute is an attention to the measurement problem. They contend that all three realist interpretations of the quantum formalism capable of resolving the measurement problem also obviate any need for chemical emergence. I push their argument further, arguing that the realist interpretations of quantum mechanics actually subvert the basis for reduction as well, by undercutting the idea that fundamental physical particles are actual parts of molecules. With both reduction and traditional synchronic emergence pictures ruled out, the only option for realists about quantum chemistry is strong Thomistic emergence.

**Keywords** Chemical reduction · Chemical emergence · Interpretation of quantum mechanics · Measurement problem · Actually Present Elements · Thomistic emergence

## Introduction

Robin Hendry defines “the structure of a substance” as “the set of properties and relations which are preserved across all the conditions in which it can be said to exist” and argues that such “structures, and therefore the chemical substances and other materials to which they are essential, are emergent” (Hendry 2021b). Franklin and Seifert offer the rejoinder that the existence of chemical structure follows from resolving the measurement problem in quantum mechanics, and is therefore reducible to physics rather than emergent (Franklin and Seifert 2020). Similarly, Seifert suggests that chemical bonds can be reduced to “real patterns of interactions among subatomic particles” (Seifert, forthcoming), but such particles are localized in ways that give rise to such patterns as a result of decoherence or collapse of the wavefunction. I review the emergence debate in [The reduction-emergence debate in chemistry](#). In [A common assumption falsified](#), I argue that Franklin and Seifert undermine

---

✉ Ryan Miller  
Ryan.Miller@unige.ch

<sup>1</sup> University of Geneva, Geneva, Switzerland

Hendry in a way that strengthens rather than weakens the case for emergence—but a variety of emergence even stronger than the one Hendry envisions. In [The actually present elements principle](#) I show that Seifert’s arguments on behalf of reductionism share Hendry’s Actually Present Elements principle, which relies on the persistence of nuclear charge—born by physical particles—through chemical change. It is the persisting subatomic particles which are supposed to be localized by solutions to the measurement problem and thus ground chemical structure. In [Prospects for actually present elements in high-dimensional ontologies—Prospects for actually present elements in Bohmian mechanics](#), I suggest, however, that none of the three realist recipes for resolving the measurement problem (Maudlin 1995) canvassed by Franklin and Seifert (many worlds, objective collapse, and pilot waves) support the view that chemical properties and relations are preserved by actually present physical particles. In the absence of this principle, emergent chemical structure is vindicated in a much stronger way than Hendry expects, as only chemical entities are persistently available to be the bearers of such properties and relations.

## The reduction-emergence debate in chemistry

There has been extensive debate over the last thirty years, in these pages and others, over whether chemistry is reducible to quantum physics. We can here distinguish the epistemic reduction of chemical theories to physical ones, the ontological reduction of chemical powers (e.g. acidity and electronegativity),<sup>1</sup> properties, structures, and entities (e.g. orbitals and bonds) to the properties and entities of quantum physics, and the mereological reduction of complex chemical entities like molecules to fusions of fundamental particles. As the debate over epistemic reduction has become muddled (Scerri 1994, 2007b, 2016), and the mereological claim is broadly agreed upon (Scerri 2007a, 2012; Hendry 2012), attention has moved to the ontological controversy. On this issue, Hettema (2013, 2014) has defended the reductionist view while Olimpia Lombardi (Lombardi and Labarca 2005; Lombardi 2014) and Robin Hendry (2010, 2017, 2021b) argue for the emergentist position and Scerri (2012) counsels waiting for more empirical developments. Here I briefly canvas Hendry and Lombardi’s main arguments for ontological emergence in chemistry, then review a recent reductionist reply by Alex Franklin and Vanessa Seifert (2020) which draws on recent developments in the foundations and philosophy of physics on the interpretation of quantum mechanics.

### Hendry and Lombardi’s emergentist argument

Lombardi (2014) takes molecular shape as the central issue relating the ontologies of chemistry and physics. Lombardi notes that molecules have characteristic structures, understood as relative angles and distances between their nuclei, which do not follow from any exact solution of the wavefunction of the particles. Instead, these nuclear locations are assumed at the outset in the Born-Oppenheimer approximation, which treats the nuclei as infinitely massive relative to the electrons, and hence holds nuclear positions fixed while solving the electronic wavefunction computationally. Lombardi identifies two difficulties with using the Born-Oppenheimer approximation to justify the reduction of molecular structure to quan-

<sup>1</sup> These are called powers because they are supposed to explain dispositions (Friend and Kimpton-Nye 2023).

tum mechanics: it presumes the chemical fact (shape) that it sets out to explain, and it relies on the eigenstate-eigenvalue link to fix the total energy of the stationary state, which she earlier found objectionably description-dependent (Lombardi and Castagnino 2010).

Hendry (2021b) offers a more detailed version of this argument. First, he clarifies that structure should not be understood with regard to a naïve macro-understanding of “shape” or “arrangement” but rather as the essential bonding and geometric properties of a molecule, which are dynamic and hence scale-relative. Second, Hendry claims that essential molecular properties are emergent because they are multiply realizable<sup>2</sup> and only obtain when fundamental particles are trapped in a potential well by their mutual physical interaction. Hendry (2017) also elaborates on Lombardi’s first concern about using the Born-Oppenheimer approximation to argue for reduction. Isomers such as ethanol and dimethyl ether have different structures (essential bonding and geometric properties) and different Born-Oppenheimer equations, Hendry notes, but identical Schrödinger equations since they have identical constituents. Since knowledge of the differing structures arises in chemistry and the Born-Oppenheimer approximation relies on them to regard each isomer as falling within a potential well, the Born-Oppenheimer approximation cannot succeed at reducing chemistry to physics. Chemical structure is thus best regarded as ontologically emergent.

### Franklin and Seifert’s reductionist rejoinder

The key concern for the ontological emergence of chemistry, according to Hendry and Lombardi, is whether chemical structure is reducible to quantum mechanics. Franklin and Seifert (2020) distinguish this concern into three closely related problems. The first is Hund’s paradox that chiral molecules are always observed in one of their two optical isomers even though their potential energy well corresponds to the superposition of the two isomer structures. The second formulation is the closest to that given by Hendry: the resultant Hamiltonian given by the Schrödinger equation is insufficient to determine the configurational Hamiltonian given by the Born-Oppenheimer approximation, so quantum physics cannot in principle reveal the chemical structure of isomers. Franklin and Seifert’s third formulation extends the first two cases to molecules that are not isomers. Here they follow Hendry (2010) in noting that resultant Hamiltonians (and hence the potential wells defining molecular structure) should be spherically symmetrical, so *all* asymmetrical molecular structure is provided quantum mechanically *only* by configurational Hamiltonians given by the Born-Oppenheimer approximation.

Nonetheless Franklin and Seifert (2020) point out that strictly speaking, the resultant Hamiltonian says not that the *actual* state of the particles governed by the wavefunction will be spherically symmetrical, but rather that the *set of possible states* is spherically symmetrical. The transition of a quantum system between a set of possible states and the actually found state is a matter of measurement, so Franklin and Seifert argue that the three closely related problems of molecular structure are instances of the quantum measurement problem. Maudlin (1995)’s trilemma characterizes the measurement problem, in turn, as three mutually-incompatible assumptions about quantum systems: that the wave-function always evolves in accord with the Schrödinger equation, that measurements have determinate outcomes, and that the wave-function of a system is complete. These three assumptions

<sup>2</sup> For a definition of multiple-realizability and its importance for the emergence-reduction debate, see Fodor (1974, 1997).

all seem to be in play in the puzzle about molecular structure: the (symmetrical superposition) wave-function is supposed to completely describe the molecular structure and evolve according to the Schrödinger equation, yet molecules are always found with determinate structures rather than in superpositions, which is especially evident for optical isomers.

The importance of Franklin and Seifert (2020)'s characterization of emergent molecular structure as an instance of the measurement problem is that the measurement problem has three realist<sup>3</sup> solutions *within physics* that do not necessitate positing novel chemical powers. Each solution amounts to denying one of the assumptions of Maudlin's trilemma:

- Ghirardi-Rimini-Weber (GRW) objective-collapse theorists deny that the wave-function always evolves in accordance with the Schrödinger equation (multiplying it by a Gaussian of width  $\sigma$  at rate  $\lambda$ ),
- Everettian (EQM) many-worlds theorists deny that measurements have determinate outcomes (outcomes are only determinate relative to observers in decoherent worlds), and
- de Broglie-Bohm (DBB) pilot-wave theorists deny the completeness of the wave-function (supplementing it with a guidance equation).

Franklin and Seifert then argue that each of these realist solutions to the measurement problem in quantum mechanics has the resources to resolve the puzzle of molecular structure without chemical emergence. According to GRW, a macro-quantity of a chemical substance or an individual molecule entangled with a macro-size measuring apparatus has a high probability of collapse within a vanishingly small amount of time, and such a collapse breaks the symmetry of the wave-function yielding a determinate chemical structure. In Everettian quantum mechanics, environmentally-induced decoherence ensures that macro-quantities of chemical substances or individual molecules entangled with macro-size measurement apparatus will have determinate structure relative to observers who share their decoherent world. In Bohmian mechanics, environmentally-induced decoherence ensures that macro-quantities of chemical substances or individual molecules entangled with macro-size measurement apparatus will contain fundamental particles with the classical trajectories required to maintain determinate chemical structures. In each case, isolated molecules may lack determinate structures, but isolated molecules are neither directly observed nor the objects of chemical laws which regard molar quantities of substances. Each realist solution to the measurement problem may be regarded as envisaging certain emergent behavior as the result of wave-function collapse or decoherence, but that behavior will be emergent at the strictly physical level rather than implying uniquely chemical structures and powers, thereby blocking the Lombardi/Hendry argument for chemical emergence.

### Lombardi and Hendry's replies

Hendry and Lombardi have both responded to Franklin and Seifert's reductionist rejoinder. Hendry (2022) levels four criticisms: that Franklin and Seifert fail to consider interpretations which violate the "completeness" assumption of the trilemma (and might vindicate

<sup>3</sup> This focus on the three realist interpretations of quantum mechanics following from Maudlin's trilemma characterization of the measurement problem is important both because realist interpretations are the most natural basis for ontological disputes and because they avoid the issues inherent to orthodox quantum mechanics discussed by Lombardi (Lombardi and Castagnino 2010; González et al. 2019).

emergence), that they do not discuss whether GRW wave-function collapse depends on the environment, that the physical meaning of isomeric superpositions is unclear, and that Franklin and Seifert do not explain how to prepare such superpositions. The responses to Hendry's first, second, and fourth criticisms seem to me trivial. Bohmian mechanics is the realist interpretation which violates completeness and it is discussed by Franklin and Seifert in the same detail as the others.<sup>4</sup> GRW wave-function collapse does depend on the environment (Maudlin 2019; Tumulka 2021). Preparing a superposition of two isomers is done by running a chemical synthesis that can produce either isomer and isolating the product without measurement (just as in the Schrödinger's Cat experiment that Hendry considers adequately specified).<sup>5</sup> This leaves only the more serious problem of how to give physical meaning to superpositions of isomers, which is more disputed among philosophers of physics. Nonetheless there is a leading answer for each interpretation: for Bohmians this is an epistemic uncertainty about which isomer was synthesized (Fortin et al. 2017), for Everettians this is a centered chance of which isomer obtains in our world (Wilhelm 2022), and for GRW theorists this is simply a brief period where there is no fact of the matter about which isomer obtains (Tumulka 2018).

Fortin and Lombardi (2021), meanwhile, make a more fundamental argument which places multiple-realizability at the center of the issue. A measurement of, say, a molecule's electric dipole moment does not settle the molecule's chemical structure because many structures could yield the same dipole. This is true, but ignores the actual mechanics by which each interpretation solves the measurement problem. All measurements can be reduced to the position basis, and the process of measuring the molecule's electric dipole will entangle the large ensemble of the measuring device with the positions of the molecular nuclei, leading to resolution of the nuclear positions by either collapse or decoherence (Maudlin 2019). Quantum measurements are only independent if the degrees of freedom measured are independent, and the relationship between dipole and structure is only underdetermined rather than independent. Thus the act of measuring the dipole is sufficient to constrain the structure within the probabilistic framework of each realist interpretation, even though dipole is multiply realizable and does not logically constrain the structure. Fortin and Lombardi also gesture towards earlier work (Fortin et al. 2016) where they argue that solely decoherence-based proposals like EQM don't solve the measurement problem, because they don't provide a relevant basis for interpreting the quantum statistics. This argument fails to engage more recent versions of decoherence theory, namely the work by Wallace (2012) which reinterprets quantum statistics in decision-theoretic terms and has convinced many eminent former skeptics of Everettian probability like Maudlin (2019).<sup>6</sup>

I do not suppose, of course, that my brief sallies have settled these issues. As Hendry (2022) is at pains to point out, there is much work to do in making each of the three realist interpretations of quantum mechanics plausible. Each of the interpretations has physical and philosophical weaknesses, which is precisely why the debate has not yet been settled

<sup>4</sup> Furthermore, Fortin et al. (2017) provide an extensive discussion of how to characterize chemistry in Bohmian terms.

<sup>5</sup> Practically it may be difficult to produce such one molecule of product, just as it was once impossible to produce just one electron at a time for double-slit experiments, but this is not an obstacle in principle, and laser stimulated methods to overcome to activation barrier may work in practice.

<sup>6</sup> In fact Fortin et al. (2016) rely on the work of Bacciagaluppi, who has more recently expressed great appreciation for Wallace's achievement (Bacciagaluppi & Ismael, 2015).

and all three interpretations remain. Even if Franklin and Seifert are right, serious claims of the ontological reduction of chemistry to physics remain unproven until that work is done. Nonetheless, Franklin and Seifert have significantly tilted the deck against Lombardi and Hendry's arguments for chemical emergence by following Scerri's plea to lean on newer developments in the foundations of physics. The quantum interpretation research program is unfinished, and may involve emergence, but Hendry and Lombardi have given us no reason to suppose that such emergence will be distinctively *chemical*.

## A common assumption falsified

### The actually present elements principle

I nonetheless suggest that in casting doubt on Hendry and Lombardi's motivations for emergence, Franklin and Seifert have opened the door to an even stronger form of chemical emergence than that envisaged by Lombardi and Hendry. The reason is that the realist forms of quantum interpretation canvassed by Franklin and Seifert cast doubt on a principle shared by all of the players in the debate: that fundamental particles are actually present in molecules. Scerri (2007a, 2012) considers this mereological assumption "uncontroversial." Franklin and Seifert (2020)'s arguments all consider indeterminacy only with regard to "structure," "configuration," or "arrangement." In the Everettian interpretation, Franklin and Seifert take molecules to be in superpositions of "atomic spatial configurations," i.e. the relative positions of nuclei by angle and distance. In their discussion of Bohmian mechanics, Franklin and Seifert (2020) are even more explicit: "The resultant Hamiltonian describes a quantum wavefunction that is in a superposition of enantiomers, isomers, and inversions of *some collection of atoms* [emphasis added]" and the consequence of non-classical trajectories before decoherence is supposed to be that the particles "will not be located in the relative positions predicted by chemists." Even in GRW, they characterize the uncollapsed state as a superposition of *structure* and the collapsed state as determining that structure, where structure has been defined throughout as relative nuclear position. In each case the mereology is taken as fixed, and the physical quantum measurement process is only supposed to alter the angles and distances between nuclei. If the quantum measurement process itself is a matter of objective physical reality, then so is the molecular structure.

Robin Hendry provides more background on this shared assumption. Hendry (2012) explicitly holds the mereological assumption that just as higher-level entities have molecular parts and molecules have atomic parts, "according to chemical theory itself, the parts of chemical entities are studied by physics." Hendry (2021a) justifies this view by reflection on the metaphysical stature of what he calls the "Actually Present Elements principle" (APE) that chemical elements are, *pace* Aristotle (Wood and Weisberg 2004), actually present in their compounds. While APE is on its face about the relation between chemical compounds and elements—molecules and atoms—Hendry's discussion also implicates the compositional relationship between chemical entities and the particles of fundamental physics. "Modern chemistry clearly vindicates APE," says Hendry (2021a), as "elements survive in their compounds because nuclear charge, the elemental property by which chemistry has individuated the elements since 1923, is preserved across chemical change." Nuclear charge may be a way of individuating chemical elements, but physicists account for that charge,

and indeed the binding together of nuclei, in terms of the up and down quarks of the Standard Model and their strong force interactions. Indeed, like Feynman et al. (2015), Hendry (2020) embraces this mereological heuristic as a legacy of atomism.<sup>7</sup> Hendry's brand of emergence embraces novel chemical powers by way of downward causation and the rejection of physical causal closure (Hendry 2006), not by way of questioning the actual presence of fundamental physical particles as parts of chemical entities.

While I think that Franklin and Seifert's analysis of chemical structure in terms of the measurement problem serves as an effective reductionist rejoinder to Hendry's emergentism about structure, I take it that all three realist interpretations of quantum mechanics shed considerable doubt on the Actually Present Elements principle. If fundamental particles are not even present in molecules, however, then chemical structure clearly cannot even supervene on the positions of those particles, let alone be determined by their mutual physical interactions. That leaves chemistry emergent in a strong sense, indeed.

### Prospects for actually present elements in high-dimensional ontologies

While Franklin and Seifert (2020) limit their engagement with realist quantum mechanics to the three dynamical *interpretations*, we must go beyond dynamics to ontology. Talk of mere "interpretations" is somewhat misleading, as each interpretation requires unique ontological posits to support its unique mathematical structures. One important question which cuts across all three dynamical interpretations is whether the fundamental ontology should be considered as existing in our familiar 3/4-dimensional spacetime (Allori 2015; Allori et al. 2014) or in the higher-dimensional configuration space corresponding to the wave-function (Ney 2021). The high-dimensional options are  $S_0$  (Ney's wave-function realism for EQM),  $GRW_0$  (a collapsing wave-function with no further ontology—the original proposal of Ghirardi et al. (1986), and the marvelous point (a single particle following the Bohmian guidance equation in high-dimensional configuration space as proposed by Albert [1996]). None of these high-dimensional proposals are friendly to the Actually Present Elements principle, since they do not envisage a world of fundamental particles moving in space as presumed by Hendry. Albert (1996)'s marvelous point ontology for Bohmian mechanics treats both particles and molecules as mere dynamical *projections* into three-dimensional space, rather than as concrete objects, let alone as parts.  $GRW_0$  offers no three-dimensional ontology at all, which has led to its status as a paradoxical and somewhat deprecated proposal (Tumulka 2018). Ney (2021)'s  $S_0$  proposal is the most promising, since she does think that some part-hood relation holds between the wave-function, physical particles, and macro-objects.  $S_0$  and APE would still be an awkward pairing, however. First, Ney grants that in her system particles would only be parts *to-a-degree*, weakening Hendry's strong mereological actualism. Second, even that claim is dubious since by the locational principle of Expansivity wholes are where their parts are (Calosi 2018) and Ney's wave-function cannot exist in the four-dimensional space of molecules and particles. Neither the reductionist nor the emergentist position about chemistry is readily explicable in Ney's universe since the wave-function drives all of the dynamics with no real role for physical particles to determine chemical structures or for chemical structures to exert downward causation on physical particles.

The so-called "primitive" ontologies for each realist interpretation of quantum mechanics, which posit fundamental entities in 4D spacetime, are more promising for the Actually

<sup>7</sup> In fairness, with certain reservations (Needham and Hendry 2018).

Present Elements principle and warrant a more extended look. For the GRW objective-collapse dynamics there are two,  $GRW_m$  which posits a matter-density field (Egg and Esfeld 2014) and  $GRW_f$  which posits only an event ontology of so-called “flashes” in spacetime (Bassi and Ghirardi 2007; Tumulka 2006, 2009, 2021). For EQM there is the  $S_m$  spacetime state realism of Wallace and Timpson (2010), and for Bohmian mechanics there is the familiar many-particle ontology (Fortin et al. 2017; Gisin 2018; Lazarovici 2020). Each of these will be reviewed in turn.

### Prospects for actually present elements in GRW

Neither primitive ontology for GRW supports the Actually Present Elements principle. In the matter-density ontology  $GRW_m$ , the only concrete physical entity is a single continuous matter-density field extending through all of spacetime (Egg and Esfeld 2014). This is a patently “stuffy” ontology, without any entities to participate in discrete configurations, or to bear properties like charge or spin. Its peaks may distinguish hydrogen and oxygen, but they will not distinguish  $^{14}\text{C}$  and  $^{14}\text{N}$ , crucial to chemical structure. Chemical laws may supervene on the dynamics of the theory, but they will neither emerge from nor reduce to its mereological structure. In any case,  $GRW_m$  has been largely superseded by  $GRW_f$  for good physical reasons (Wallace 2014; McQueen 2015).

The situation in  $GRW_f$ , the relativistic flash ontology, is even worse. A particle in a nucleus will not undergo spontaneous collapse more than once every hundred thousand years (Feldmann and Tumulka 2012). Insofar as the nucleus is entangled with a large ensemble of particles in a chemical substance, or with a macroscopic measuring apparatus, its *possible* flash locations will be highly constrained by the bounds on the wave-function created by the other flashes in the entangled system (Maudlin 2019; Tumulka 2021). These environmentally induced constraints will, as Franklin and Seifert note, determine what relative position the nucleus *can* have, and hence what molecular structures it *can* take part in. Yet, strictly speaking, the nuclear particle only has a spacetime location at *incredibly* sparse times—so sparse that no two nuclear particles of a molecule are ever likely to experience flashes in temporal proximity to one another. Without cotemporal flashes, there are no nuclear positions in spacetime for chemical structures to supervene on (the wave-function exists in high-dimensional configuration-space, not spacetime), and there can be no spatial parthood relationship between molecules and fundamental particles. The Actually Present Elements principle is seriously undermined by GRW.

### Prospects for actually present elements in EQM

In Wallace and Timpson (2010)’s spacetime state ontology for Everettian quantum mechanics, by contrast, particles have a more natural place since “a single particle (which usually won’t be localized in some particular region) will be represented by an entangled state composed of a superposition of states each differing from the vacuum only in a small region.” As in Franklin and Seifert’s general account of EQM, emergent localization is secured by decoherent quasi-classical histories, and this process works in the same way for individual particles, isolated molecules, and the large systems characteristic of chemical substances and measuring devices. Yet Wallace and Timpson (2010) remind us that:

This brings home the point that the true state of a spatial region is very far from being directly accessible to any realistic agent. An observer in region  $A$  (present in the quasi-classical situation encoded by  $\hat{P}_A^i$ , say) might very well speak of *the* state of  $A$  being  $\hat{P}_A^i$  and *the* state of  $B$  as being  $\hat{P}_B^i$ , but these would be emergent and approximate notions (somewhat akin to Everett's original 'relative states'). The true, ontologically primary, state of  $A$  would still be  $\hat{P}_A$ .

If chemical structures are to supervene on the relative locations of nuclei, then these must both have quasi-classical histories secured by decoherence. But what decoheres depends on the energy levels of our measurements. At the energy levels used for x-ray diffraction, molecular structure appears but nuclear particles themselves do not. Meanwhile at the energies needed to resolve fundamental particles by deep inelastic scattering, even nucleons are destroyed (Bellac 2011). Entities only exist at particular locations in EQM when they have decoherent histories, and what decoheres depends in an ineliminable way on the energy scale of our measurements. This ontology profoundly validates Hendry (2021b)'s claim that reality is scale-relative. What it undermines, however, is the view that every scale of reality is simultaneously present: molecular structure and nuclear particles cannot decohere concurrently since their energy scales are so different. If molecular structure and nuclear particles are not concomitant, though, the former cannot supervene on the latter. When there are molecules there are no actually present nuclear particles, and when there are actually present nuclear particles, there are no chemically structured molecules. EQM is thus no more supportive than GRW of the Actually Present Elements principle.

### Prospects for actually present elements in Bohmian mechanics

Bohmian mechanics may seem like the saving grace for the Actually Present Elements principle. After all, de Broglie-Bohm pilot-wave theory guarantees that nucleons and electrons are always present with classical positions, and molecular structure obtains when such particles arranged in the right way. Franklin and Seifert (2020) draw our attention to the "surreal" non-classical trajectories that Bohmian particles exhibit before decoherence, but both they and Fortin et al. (2017) assume that such particles "preserve their identity as components of a composite system." This severely understates just how non-classical Bohmian particle trajectories must be, though, in order to reproduce the data of quantum mechanics. Bohmian particles deviate from their classical trajectories on the order of *millimeters* (Mahler et al. 2016) while molecular radii are on the order of *picometers*. This wild discrepancy prevents any plausible identification of particular nuclei or electrons as belonging to a certain molecule prior to decoherence. Decoherence does not merely arrange disorderly quantum particles into classical chemical structures; it must actively assemble the physical constituents needed to compose the molecule in the first place. Bohmian particles may have *some* definite location prior to decoherence, unlike their Everettian or objective-collapse counterparts, but that location does not correspond to any particular molecule. As in the other two interpretations, there are no actually present physical particles from which chemical structure can emerge or to which chemical structure can be reduced. Hendry (2022) is willing to allow that quantum systems can intermittently constitute molecules, but here there is no general assurance that *a* quantum system exists. Unlike the other two interpretations, however, Bohmian mechanics does vindicate the Actually Present Elements principle while

molecular structure is decohered. Yet in the tunneling isomer cases discussed by Hendry and Franklin and Seifert, quantum behavior is still evident, which means that Bohmian trajectories must still be non-classical, and there is little guarantee in such situations that Bohmian trajectory deviations will remain on the picometer scale. So even when molecular structure is believed to exist chemically—just resonant between two structures—Bohmian mechanics cannot guarantee sufficiently localized fundamental physical particles to play the role of Actually Present Elements.

## Conclusion: Thomistic emergence

Franklin and Seifert (2020) urge us to take the realist interpretations of quantum mechanics seriously, and thus see the emergence of molecular structure as a form of the strictly physical measurement problem rather than a non-reductive chemical phenomenon. Taking those realist interpretations seriously, however, means taking their ontologies seriously, and those ontologies do not vindicate the Actually Present Elements principle by which chemical structure is supposed to *either* emerge from *or* reduce to the mutual interactions of physical particles. Yet being realist about quantum mechanics should not dissuade us from being realists about chemistry. Avogadro's number has a perfectly good role in connecting molar chemical substances to counts of molecules and atoms (Sarikaya 2013), which underwrites a realist view of those chemical entities. If chemical entities are persistently present, though, despite the lack of physical entities to serve as their Actually Present Elements, then molecules must be emergent in a way that does not necessitate their having concrete separable parts. This is just the Thomistic view of emergence championed by Patrick Toner (2008, 2011). While much work remains to be done in developing such views, the emergence of chemical structure should count in their favor since none of the three realist interpretations of quantum mechanics provide the persistent physical parts relied on by more mainstream accounts of emergence.

**Funding** Open access funding provided by University of Geneva. Research funding was provided by the Swiss National Science Foundation under Doc.CH grant number 207186.

**Open Access** This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

## References

- Albert, D.Z.: Elementary Quantum Metaphysics. In J. T. Cushing, A. Fine, & S. Goldstein (Eds.), *Bohmian Mechanics and Quantum Theory: An Appraisal* (Vol. 184). Springer Netherlands. <http://link.springer.com/> (1996). <https://doi.org/10.1007/978-94-015-8715-0>
- Allori, V.: Primitive ontology in a Nutshell. *Int. J. Quantum Found.* **1**(3), 107–122 (2015)

- Allori, V., Goldstein, S., Tumulka, R., Zanghi, N.: Predictions and primitive ontology in Quantum Foundations: A study of examples. *Br. J. Philos. Sci.* **65**(2), 323–352 (2014). <https://doi.org/10.1093/bjps/axs048>
- Bacciagaluppi, G., Ismael, J.: Review of *The Emergent Multiverse* [Review of *Review of The Emergent Multiverse*, by D. Wallace]. *Philosophy of Science*, **82**(1), 129–148. (2015). <https://doi.org/10.1086/679037>
- Bassi, A., Ghirardi, G.: The Conway-Kochen argument and relativistic GRW Models. *Found. Phys.* **37**(2), 169–185 (2007). <https://doi.org/10.1007/s10701-006-9097-1>
- Bellac, M.L.: *Quantum Physics*. Cambridge University Press (2011)
- Calosi, C.: Quantum monism: An assessment. *Philos. Stud.* **175**(12), 3217–3236 (2018). <https://doi.org/10.1007/s11098-017-1002-6>
- Egg, M., Esfeld, M.: Primitive ontology and quantum state in the GRW matter density theory. *Synthese.* **192**(10), 3229–3245 (2014). <https://doi.org/10.1007/s11229-014-0590-3>
- Feldmann, W., Tumulka, R.: Parameter diagrams of the GRW and CSL theories of wavefunction collapse. *J. Phys. A: Math. Theor.* **45**(6), 065304 (2012). <https://doi.org/10.1088/1751-8113/45/6/065304>
- Feynman, R.P., Leighton, R.B., Sands, M.: *The Feynman Lectures on Physics: Mainly Mechanics, Radiation, and Heat*. New Millennium, vol. 1. Basic Books (2015)
- Fodor, J.A.: Special sciences (or: The disunity of science as a working hypothesis). *Synthese.* **28**(2), 97–115 (1974). <https://doi.org/10.1007/BF00485230>
- Fodor, J.A.: Special Sciences: Still Autonomous after all these years. *Philosophical Perspect.* **11**, 149–163 (1997)
- Fortin, S., Lombardi, O.: Is the problem of molecular structure just the quantum measurement problem? *Found. Chem.* **23**(3), 379–395 (2021). <https://doi.org/10.1007/s10698-021-09402-x>
- Fortin, S., Lombardi, O., Martínez González, J.C.: Isomerism and decoherence. *Found. Chem.* **18**(3), 225–240 (2016). <https://doi.org/10.1007/s10698-016-9251-6>
- Fortin, S., Lombardi, O., González, J.C.M.: The relationship between chemistry and physics from the perspective of Bohmian mechanics. *Found. Chem.* **19**(1), 43–59 (2017). <https://doi.org/10.1007/s10698-017-9277-4>
- Franklin, A., Seifert, V.A.: The Problem of Molecular structure just is the Measurement Problem. *Br. J. Philos. Sci.* (2020). <https://doi.org/10.1086/715148>
- Friend, T., Kimpton-Nye, S.: *Dispositions and Powers*. Cambridge University Press. (2023). <https://www.cambridge.org/core/elements/dispositions-and-powers/B5E3BD78798365332743236ED9913C34>
- Ghirardi, G.C., Rimini, A., Weber, T.: Unified dynamics for microscopic and macroscopic systems. *Phys. Rev. D.* **34**(2), 470–491 (1986). <https://doi.org/10.1103/PhysRevD.34.470>
- Gisin, N.: Why Bohmian mechanics? One- and two-time position measurements, Bell Inequalities, Philosophy, and physics. *Entropy.* **20**(2) (2018). Article 2 <https://doi.org/10.3390/e20020105>
- González, J.C.M., Fortin, S., Lombardi, O.: Why molecular structure cannot be strictly reduced to quantum mechanics. *Found. Chem.* **21**(1), 31–45 (2019). <https://doi.org/10.1007/s10698-018-9310-2>
- Hendry, R.F.: Is There Downward Causation in Chemistry? In D. Baird, E. Scerri, L. McIntyre, R. S. Cohen, J. Renn, K. Gavroglu, & L. Divarci (Eds.), *Philosophy Of Chemistry* (Vol. 242, pp. 173–189). Springer Netherlands. (2006). <http://link.springer.com/content/r22x546p656g1362/abstract/>
- Hendry, R.F.: Ontological reduction and molecular structure. *Studies in history and philosophy of Science Part B: Studies. History and Philosophy of Modern Physics.* **41**(2), 183–191 (2010). <https://doi.org/10.1016/j.shpsb.2010.03.005>
- Hendry, R.F.: Reduction, Emergence and Physicalism. In A. I. Woody, R. F. Hendry, & P. Needham (Eds.), *Philosophy of Chemistry* (pp. 367–386). North-Holland. (2012). <http://www.sciencedirect.com/science/article/pii/B978044451675650027X>
- Hendry, R.F.: Prospects for strong emergence in Chemistry. In: *Philosophical and Scientific Perspectives on Downward Causation*. Routledge (2017)
- Hendry, R.F.: Trusting atoms. In U. Zilioli (Ed.), *Atomism in Philosophy: A History from Antiquity to the Present* (pp. 470–488). Bloomsbury Academic. (2020). <https://doi.org/10.5040/9781350107526>
- Hendry, R.F.: Elements and (first) principles in chemistry. *Synthese.* **198**(14), 3391–3411 (2021a). <https://doi.org/10.1007/s11229-019-02312-8>
- Hendry, R.F.: Structure, scale and emergence. *Stud. History Philos. Sci. Part A.* **85**, 44–53 (2021b). <https://doi.org/10.1016/j.shpsa.2020.08.006>
- Hendry, R.F.: Quantum Mechanics and Molecular Structure. In O. Lombardi, J. C. Martínez González, & S. Fortin (Eds.), *Philosophical Perspectives in Quantum Chemistry* (pp. 147–172). Springer International Publishing. (2022). [https://doi.org/10.1007/978-3-030-98373-4\\_7](https://doi.org/10.1007/978-3-030-98373-4_7)
- Hettema, H.: Austere quantum mechanics as a reductive basis for chemistry. *Found. Chem.* **15**(3), 311–326 (2013). <https://doi.org/10.1007/s10698-012-9173-x>
- Hettema, H.: Linking chemistry with physics: A reply to Lombardi. *Found. Chem.* **16**(3), 193–200 (2014). <https://doi.org/10.1007/s10698-014-9200-1>

- Lazarovici, D.: Position measurements and the empirical status of particles in Bohmian mechanics. *Philos. Sci.* **87**(3), 409–424 (2020). <https://doi.org/10.1086/709412>
- Lombardi, O.: Linking chemistry with physics: Arguments and counterarguments. *Found. Chem.* **16**(3), 181–192 (2014). <https://doi.org/10.1007/s10698-013-9197-x>
- Lombardi, O., Castagnino, M.: Matters are not so clear on the physical side. *Found. Chem.* **12**(2), 159–166 (2010). <https://doi.org/10.1007/s10698-010-9090-9>
- Lombardi, O., Labarca, M.: The ontological autonomy of the Chemical World. *Found. Chem.* **7**(2), 125–148 (2005). <https://doi.org/10.1007/s10698-004-0980-6>
- Mahler, D.H., Rozema, L., Fisher, K., Vermeiden, L., Resch, K.J., Wiseman, H.M., Steinberg, A.: Experimental nonlocal and surreal bohmian trajectories. *Sci. Adv.* **2**(2), e1501466 (2016). <https://doi.org/10.1126/sciadv.1501466>
- Maudlin, T.: Three measurement problems. *Topoi.* **14**(1), 7–15 (1995). <https://doi.org/10.1007/BF00763473>
- Maudlin, T.: *Philosophy of Physics: Quantum Theory*. Princeton University Press (2019)
- McQueen, K.J.: Four tails problems for dynamical collapse theories. *Stud. History Philos. Sci. Part B: Stud. History Philos. Mod. Phys.* **49**, 10–18 (2015). <https://doi.org/10.1016/j.shpsb.2014.12.001>
- Needham, P., Hendry, R.F.: Aspects of the Concept of Potentiality in Chemistry. In K. Engelhard & M. Quante (Eds.), *Handbook of Potentiality* (pp. 375–400). Springer Netherlands. (2018). [https://doi.org/10.1007/978-94-024-1287-1\\_15](https://doi.org/10.1007/978-94-024-1287-1_15)
- Ney, A.: *The World in the Wave Function: A Metaphysics for Quantum Physics*. Oxford University Press (2021)
- Sarikaya, M.: A view about the short histories of the mole and Avogadro's number. *Found. Chem.* **15**(1), 79–91 (2013). <https://doi.org/10.1007/s10698-011-9128-7>
- Scerri, E.R.: Has Chemistry Been at Least Approximately Reduced to Quantum Mechanics? *PSA: Proceedings of the Biennial Meeting of the Philosophy of Science Association 1994, One*, 160–170. (1994)
- Scerri, E.R.: Reduction and emergence in Chemistry—Two recent approaches. *Philos. Sci.* **74**(5), 920–931 (2007a). <https://doi.org/10.1086/525633>
- Scerri, E.R.: The ambiguity of reduction. *HYLE—International J. Philos. Chem.* **13**(2), 67–81 (2007b)
- Scerri, E.R.: Top-down Causation regarding the Chemistry–Physics Interface: A sceptical view. *Interface Focus.* **2**(1), 20–25 (2012). <https://doi.org/10.1098/rsfs.2011.0061>
- Scerri, E.R.: The changing views of a philosopher of chemistry on the question of reduction. In: Scerri, E.R., Fisher, G. (eds.) *Essays in the Philosophy of Chemistry*. Oxford University Press (2016)
- Seifert, V.A.: (forthcoming). The Chemical Bond is a Real Pattern. *Philosophy of Science*. <http://philsci-archive.pitt.edu/20333/>
- Toner, P.: Emergent substance. *Philos. Stud.* **141**(3), 281–297 (2008). <https://doi.org/10.1007/s11098-007-9160-6>
- Toner, P.: Independence accounts of substance and substantial parts. *Philos. Stud.* **155**(1), 37–43 (2011). <https://doi.org/10.1007/s11098-010-9521-4>
- Tumulka, R.: A relativistic version of the Ghirardi–Rimini–Weber Model. *J. Stat. Phys.* **125**(4), 821–840 (2006). <https://doi.org/10.1007/s10955-006-9227-3>
- Tumulka, R.: The point processes of the grw theory of wave function collapse. *Rev. Math. Phys.* **21**(02), 155–227 (2009). <https://doi.org/10.1142/S0129055X09003608>
- Tumulka, R.: Paradoxes and primitive ontology in collapse theories of Quantum mechanics. In: Gao, S. (ed.) *Collapse of the Wave Function: Models, Ontology, Origin, and Implications*. Cambridge University Press (2018). <https://doi.org/10.1017/9781316995457>
- Tumulka, R.: A Relativistic GRW Flash Process with Interaction. In V. Allori, A. Bassi, D. Dürr, & N. Zanghi (Eds.), *Do Wave Functions Jump?: Perspectives on the Work of GianCarlo Ghirardi* (pp. 321–347). Springer International Publishing. (2021). [https://doi.org/10.1007/978-3-030-46777-7\\_23](https://doi.org/10.1007/978-3-030-46777-7_23)
- Wallace, D.: *The Emergent Multiverse: Quantum Theory According to the Everett Interpretation*, 1st edn. Oxford University Press (2012)
- Wallace, D.: Life and death in the tails of the GRW wave function. *ArXiv:[Quant-Ph]*. (2014). <https://doi.org/10.48550/arXiv.1407.4746>
- Wallace, D., Timpson, C.G.: Quantum mechanics on spacetime I: Spacetime state realism. *Br. J. Philos. Sci.* **61**(4), 697–727 (2010). <https://doi.org/10.1093/bjps/axq010>
- Wilhelm, I.: Centering the Everett Interpretation. *Philosophical Q.* **72**(4), 1019–1039 (2022). <https://doi.org/10.1093/pq/pqab068>
- Wood, R., Weisberg, M.: Interpreting Aristotle on mixture: Problems about elemental composition from Philoponus to Cooper. *Stud. History Philos. Sci. Part A.* **35**(4), 681–706 (2004). <https://doi.org/10.1016/j.shpsa.2004.02.002>

---

Springer Nature or its licensor (e.g. a society or other partner) holds exclusive rights to this article under a publishing agreement with the author(s) or other rightsholder(s); author self-archiving of the accepted manuscript version of this article is solely governed by the terms of such publishing agreement and applicable law.