This preprint has not undergone peer review or any post-submission improvements or corrections. The Version of Record of this article is published in *Foundations of Chemistry* and is available online at http://doi.org/10.1007/s10698-024-09513-1

Relational Quantum Mechanics, Causal Composition, and Molecular Structure

Stephen Esser

Franklin and Seifert (2021) argue that solving the measurement problem of quantum mechanics (QM) also answers a question central to the philosophy of chemistry: that of how to reconcile QM with the existence of definite molecular structures. This conclusion may appear premature, however, because interactions play a crucial role in shaping molecules, but we generally lack detailed models of how this is accomplished. Given this explanatory gap, simply choosing an interpretation of QM is insufficient, unless the interpretation also has relevant conceptual resources that address how spatially organized molecules are composed. This article seeks to close the gap, using the interpretation provided by relational quantum mechanics (RQM), along with a posited causal ontology. This framework, which entails the co-existence of multiple perspectives on systems within a single world, offers a path toward reconciling the quantum mechanical view of molecules with another conception more congenial to chemistry: that of molecules shaped by patterns of localizing interactions.

Introduction: One Problem or Two?

Quantum mechanics (QM) is famously the subject of interpretative difficulties (often summarized as the "measurement problem"). QM models of physical systems do not assign definite values to all of its quantities, but these can be realized when systems are measured. For example, if we are interested in the position of a moving particle, we describe it using a wave function (Ψ) and calculate its evolution in time using the Schrödinger equation. But the dynamics are not that of a particle moving in three-dimensional space. Here, Ψ is a function from possible positions to (complex) numbers.[1] This is often described as quantum superposition—the system being in a combination of possible configurations. It is only upon measurement that we can find

---

[1] For multi-particle systems, Ψ is defined in a multi-dimensional configuration space (3N dimensions where N is the number of particles in the system).

a particle in a location, with the formalism providing the probability of finding it in a given volume of space, derived from the square of the absolute value (or modulus) of Ψ.

Turning to the philosophy of chemistry literature, a long-standing debate has concerned the explanation of molecular structure. Modern chemistry uses QM models to calculate the value of molecular properties: one begins by estimating the molecular wave function and associated energies using the time-independent Schrödinger equation $\hat{H}\,\psi = E\psi$.[2] Conceptually, this may seem straightforward. The Hamiltonian for an atom or molecule will contain a kinetic energy operator and a potential energy operator that is based on the Coulomb attraction/repulsion among the particles. In the simple case of the hydrogen atom (where the nucleus is assumed to be stationary at the origin of the coordinate system), the calculated wave functions (called orbitals) indicate the position state of the electron: as in the case of the single particle, this is expressed in terms of complex-valued amplitudes over the possible position configurations. Also, as before, one can use the wave function (via the square of its absolute value) as the basis for calculating the probability of finding the electron in a given spatial volume around the nucleus.[3]

It turns out, however, that multi-particle atomic and molecular wave equations are generally computationally intractable, so various simplifying assumptions of some sort are used. When it comes to molecules, a crucial step is the separation of the motions of the multiple nuclei from the electrons. This move, called the Born-Oppenheimer approximation, calculates the electronic part of the wave function assuming the nuclei are stationary in a certain configuration in space. This configuration—the key ingredient for molecular structure—is not derived from within QM, but is added by the researcher, informed by experimental evidence. If we set aside this practice, and attempt to estimate wave functions without the Born-Oppenheimer approximation, one generally cannot recover the often highly asymmetric structures familiar to chemists.[4]

---

[2] I follow the convention of using the lower-case ψ for the time-independent equation, since it represents only the spatial dependence of Ψ after applying the separation of variables method to the time-dependent Schrödinger equation.

[3] For multi-electron atoms an approximate description of possible electronic states is built up from successive hydrogen-like orbitals of increasing energy. In this context, the wave function can be used to calculate the electron density distribution for the system: this gives the expected number of electrons one would find at a particular spatial location upon measurement.

[4] For a review of attempts to extract indications of molecular structure from "pre-Born-Oppenheimer" all-particle wave functions, see a review by Mátyus (2019). This work focuses on techniques based on an analysis of density distributions, an idea discussed by Claverie and Diner (1980). These methods can show some structural elements, but do not reveal sharp classical nuclear configurations.

To summarize: it is a general fact that quantum models don't feature particular values for quantities of interest, such as particle position. Despite this, we can locate the particle upon measurement. In the more complex case of molecules, there is a particular concern: a quantum mechanical model of an isolated system generally does not describe the spatial configuration of its atomic nuclei, a structure that is essential to explaining chemical phenomena. However, these structures are known via experiment. In both cases, there is a problem connecting QM models to certain definite values, importantly including spatial locations. Are these different versions of the same problem?

Franklin and Seifert (2021) argue that they are indeed: they explore three specific cases, together labeled the problems of molecular structure, and show how they can be construed as "special cases of the measurement problem of quantum mechanics."[5] The first involves optical isomers (enantiomers); these are chiral molecules always found to be left or right "handed," even as the wave function describes a superposition (Hund's paradox). The second case generalizes to the more general class of isomers, where multiple molecules have the same number of nuclei and electrons (and hence would be treated identically as isolated systems in a pre-Born Oppenheimer analysis), but exhibit (in experimental contexts) distinct structures with very different chemical properties. The third case is the most general of all: viewing the problem in terms of symmetry breaking. The ground state solution of the Schrödinger equation for a collection of nuclei and electrons (again, without the Born Oppenheimer approximation) has symmetry properties that are generally absent in various (spatially structured) molecules.[6]

Next, Franklin and Seifert examine how solving the measurement problem would serve to also address these three problems of molecular structure. They do this by utilizing three well-known interpretations of QM: the Everett (many-worlds) approach, Bohmian mechanics, and spontaneous collapse theories. In each case, the authors discuss how the interpretation generally

---

[5] As the authors acknowledge, there have been previous discussions linking these issues. I focus on Franklin and Seifert's article since it provides a focused discussion of the relationship between several versions of the problem of molecular structure as well as multiple possible solutions to the measurement problem. While they also discuss some implications of their conclusions for the philosophical debate regarding the reducibility of chemistry to physics, the present article will not directly address this topic.

[6] The authors explain that not all types of symmetry breaking would fall under the category of interest for connecting the problem of molecular structure to that of quantum measurement. Some (such as organically produced sugar molecules) result from identifiable external factors. This latter discussion is criticized by Fortin and Lombardi (2021) as discussed below.

addresses the measurement problem.[7] This is followed by a brief exposition explaining how the framework would address the problems of molecular structure: why, for example, a QM model of a molecule would describe it in a symmetric superposition, while, on the other hand, an actual observation would reveal a determinate asymmetric structure.

So, are Franklin and Seifert correct that the problems of molecular structure are "special cases" of the measurement problem? This is an ambitious claim that appears only partially supported by their discussion. This discussion bolsters the thesis that solving the measurement problem is necessary for a complete understanding of the relationship between QM models and our observations of spatial structure. However, the situation seems very different from that of showing how various QM interpretations account for observation of, say, the location or spin of a single particle. The authors' account of how the interpretations address molecular structure is comparatively incomplete.

The Crucial Role of Interactions

Experimental chemists generally do not analyze molecules in isolation, while many quantum mechanical models, on the other hand, do treat physical systems as isolated (Seifert 2022). Given this, discussions of the problem of molecular structure have often invoked the importance of considering interactions. Woolley and Sutcliffe, for instance, have long suggested that environmental interactions, variously characterized, may play a role (Woolley 1978, Woolley 1991; Sutcliffe and Wooley 2022).[8] It has been suggested that decoherence theory, an approach to analyzing system-environment interaction within QM, might be an important tool for addressing structure. In one example of such an effort, Trost and Hornberger (2009) model a decoherence mechanism for suppressing superposition between left-handed and right-handed configuration states in the Hund's paradox case (using a background environment of gas particles). While philosophers of chemistry have expressed optimism about the potential of decoherence to address the challenge of structure (Scerri 2011), a consensus appears to have emerged that decoherence alone will not solve the problem of how definite outcomes are

---

[7] The authors use Maudlin's (1995) discussion of the measurement problem to organize their discussion. Maudlin's framework will be used below when introducing RQM.

[8] Other early references suggesting a role for external interactions include Primas (1975) and Claverie and Diner (1980).

observed.[9] But perhaps the conjunction of combining an appeal to decohering interactions with an interpretation of QM can be more fruitful.

Indeed, when discussing the three interpretations of QM, Franklin and Siefert point out how the issue of interaction enters into the account of structure. For instance, the Everett interpretation would imply no collapse to particular outcomes: instead, there is an evolving wave function for the universe that encompasses all outcomes: this would encompass various possible structures for a molecule (and versions of the chemists who observe them). But decoherence is assigned a key role in explicating the interpretation, as environmental or measurement interactions suppress interference effects between parts (branches) of the wave function that are taken to approximate independent "worlds." An experimental observation of a particular molecular structure takes place in one of these individual branches/worlds.

But this explanation is only schematic (as it is in the discussion of the other two QM interpretations considered).[10] We would like to know more about how decohering interactions are responsible for the specific structures we observe (in our world). Franklin and Seifert allow that "a complete analysis of how quantum mechanics describes the structure of non-isolated molecules also requires considering the particular environment in which the molecule is considered (25)."

Understanding the role of interactions in more detail might allow one to address the critique of Fortin and Lombardi (2021), who argue that Franklin and Siefert's central claim is "too optimistic (380)." One issue Fortin and Lombardi raise is that of the "preferred basis" problem: in a number of interpretations, it may be explained why measurement appears to reveal a definite outcome for some quantity, but there is a further question about why this quantity is picked out from the many possibilities offered by the system under study. Often, as in contemporary

---

[9] See Bacciagaluppi (2020, section 2) and the discussion in Fortin, Lombardi, and Martínez González (2016), which focuses on the specific problem of optical isomerism.

[10] In the case of Bohmian mechanics, one adds to the wave function an ontology of particles which always have determinate positions (sometimes said to be "guided" by the wave function). While an isolated system in superposition will feature determinate particle positions, they would generally not be in configurations matching chemical structures. But decoherence is presumed to result in the concentration of the particles in components of the wave function that are associated with structures we observe. Spontaneous collapse theories differ in that they modify QM dynamics, so that an isolated system in superposition will stochastically assume a particular structure (collapses are assumed to take place in the position basis). Here decoherence does not play a leading role, although environmental and measurement interactions play an indirect role in triggering collapse: the probability of collapse is linked to size, and interactions thus create larger entangled systems much more likely to collapse.

discussions of the Everett interpretation, the explanation is entrusted to decoherence: it is expected that environmental interactions will suppress interference effects involving the preferred set of states (Bacciagaluppi 2020). In particular, there is an expectation that the position basis will often be preferred, although this depends on the details of the interaction being modeled. But this solution arguably offers limited understanding for a problem such as that of structural isomers, where we would like to know why only some particular asymmetric configurations are picked out. As Fortin and Lombardi stress, the wave function encompasses "all the mathematically possible nuclear configurations, *with the same probability* (387, emphasis original)." They also raise the question of how asymmetric configurations remain stable, since in the quantum dynamics there is no reason for particular structure to be maintained through time (absent more information about a stabilizing mechanism, such as may result from environmental interaction). Lastly, Fortin and Lombardi raise another interesting point with regard to Franklin and Siefert's discussion of symmetry breaking. Franklin and Seifert argue only some types are instances of the measurement problem, while others are not. In the latter case, they point to the asymmetric chirality of sugar molecules in organic systems being the product of environmental asymmetries. Fortin and Lombardi point out that "then the problem is moved one step back because now the asymmetry of the environmental molecules cries for an explanation (391)."

To summarize: even after we pick out a favorite solution to the QM measurement problem, we are looking to environmental interactions to play a substantial role in an explanation of molecular structure, but in most cases, we have been given few details about how this is accomplished.

Certainly, decoherence analyses relevant to the questions of molecular structure will continue to be forthcoming. A detailed review is beyond the scope of this article, but recent years have seen further study of chiral molecules showing how environmental interactions can effectively suppress interference (Bahrami, Shafiee, and Bassi, 2012). Other work, based on scattering models, shows how photon gas and particle environments can generally induce decoherence in systems with rotational degrees of freedom (Zhong and Robicheax, 2016).[11] But progress on

---

[11] In a pair of interesting recent articles, Mátyus and Cassam-Chenaï (Mátyus and Cassam-Chenaï, 2021, and Cassam-Chenaï and Mátyus, 2021) examine the mechanism of decoherence *within* an isolated molecule, that is, considering the electrons as an environment surrounding the nuclei. In the case of estimates calculated for light elements, they find a modest suppression of interference (10% or less), but speculate that in molecules with larger nuclei the suppression effect would be greater.

modelling molecules of interest in realistic environments continues to be limited by substantial practical challenges.

Given this state of affairs, to label the problems of molecular structure “special cases of the measurement problem” seems to require assuming that, while environmental interactions play a key role, the absence of detailed accounts of this role is not an in-principle obstacle to reaching this conclusion. However, the remaining explanatory gap offers room for skeptics to argue otherwise, as Hendry (2022) does in a recent critique:

> A more specific worry is that it is rather implausible to think that the general issues raised by the interpretation of quantum mechanics are all there is to the problem of molecular structure. Those general interpretative issues arise independently of any specific assumptions about the physical composition of a quantum system…it is implausible that we can answer the question of how molecules have determinate structures without taking into account the very important information that they are systems of electrons and nuclei interacting in a rather specific way (Hendry, 2022, 162).

In the absence of more detailed QM models, closing this explanatory gap requires an interpretative framework that can better address the specific challenge of molecular structure.

Relational Quantum Mechanics and the Co-existence of Multiple Perspectives

To introduce RQM, we will follow Maudlin’s (1995) use of the example of electron spin to discuss the measurement problem. The wave function is represented as a vector in the basis corresponding to spin, with its evolution modeled using the Schrödinger equation. Along any axis (x, y, and z), there is an observable (e.g. “z-spin”) with only two possible determinate values, labelled informally “up” and “down”. If an electron is prepared with a determinate spin value of, say, z-up, then, upon subsequent measurement, the composite system consisting of the electron and an appropriate z-spin measuring device will evolve so the device’s pointer will move from the “READY” position to “UP.” As expected, an experimenter will observe the outcome as an UP result. However, if an electron is prepared with either spin value in the x direction, then it will not have a determinate value in the *z* direction. It will be in a superposition state with regard to *z*-spin.[12] Its state in the *x*-spin basis may be represented as a sum (or difference) of vectors, e.g.:

$$|x - \mathrm{up} > = \left(\frac{1}{\sqrt{2}}\right) |z - \mathrm{up} > + \left(\frac{1}{\sqrt{2}}\right) |z - \mathrm{down} >$$

Since the electron's spin has neither a determinate value of up nor down in the *z* direction, the composite system including the electron and measuring device evolves into a superposition:

$$\left(\frac{1}{\sqrt{2}}\right) |z - \mathrm{up} > \otimes \left(\frac{1}{\sqrt{2}}\right) |\mathrm{UP} > + \left(\frac{1}{\sqrt{2}}\right) |z - \mathrm{down} > \otimes \left(\frac{1}{\sqrt{2}}\right) |\mathrm{DOWN} >$$

However, an observer will instead find the pointer to be either "UP" or "DOWN." The only connection between the QM representation and the observation is a probabilistic prediction derived from taking the squared absolute value of the vector components (or amplitudes) associated with each possible value. In this case, we can predict the outcome of measuring the particle as either spin up or spin down to be $|(1/\sqrt{2})|^2 = 50\%$.

A central puzzle is the fact that we never observe a superposition, but instead always observe a determinate outcome with the calculated probabilities. The system no longer evolves according to the Schrödinger equation. Instead, we have a "collapse" to a particular value.

Maudlin presents the problem in terms of a trilemma:[13]

> 1.A The wave-function of a system is *complete,* i.e. the wave-function specifies (directly or indirectly) all of the physical properties of a system.
>
> 1.B The wave-function always evolves in accord with a linear dynamical equation (e.g. the Schrödinger equation).

---

[12] Here, "*z*-spin" and "*x*-spin" are observables that are incompatible and subject to the uncertainty principle.

[13] He calls this the "problem of outcomes" (Maudlin, 1995, 7).

> 1.C Measurements of, e.g., the spin of an electron always (or at least usually) have determinate outcomes, i.e., at the end of the measurement the measuring device is either in a state which indicates spin up (and not down) or spin down (and not up). (Maudlin, 1995, 7, emphasis original)

If the first two statements are true, then our measurements or observations should be of superpositions, inconsistent with the truth of the third statement. Maudlin (and Franklin and Seifert) discuss how several interpretations of QM resolve the trilemma by rejecting one of the statements.[14]

For discussing RQM specifically, another aspect of the problem will be especially instructive: this involves the so-called "Wigner's friend" scenario (Wigner 1961/1967). Picture two scientists running an experiment: Alice performs the *z*-spin measurement as above. This takes place in a sealed laboratory, and Alice's friend Bob is positioned outside. Alice observes an outcome as usual. From the friend's perspective, however, a quantum description of the situation in the lab would describe a composite system evolving in a superposition representing the two possible outcomes—but now it is a superposition that also includes two versions of *Alice*. It is only upon "measuring" the lab (opening the door, perhaps) that this composite wave function collapses. Until then, we have two incompatible accounts of the experiment: Alice's from inside the lab (definite outcome) and that of Bob on the outside (no definite outcome).

This scenario highlights the inconsistency arising from the presence of what appears to be two completely different kinds of interaction. In the absence of any interaction, a system evolves in time as described by the Schrödinger equation. But interactions are handled in two different ways. On the one hand, we have a measurement. On the other hand, we can also describe an interaction between two systems not subject to measurement. In the first kind of interaction, a definite value of a system's physical quantity is found (we say the wave function of the system collapses). In the second kind of interaction, we represent two (or more) systems, previously considered isolated, as now correlated in a composite system (they become entangled). In this second case the system goes on to evolve as does any isolated system. And, as such, the

---

[14] Briefly: Bohmian mechanics denies the first statement, since QM must be supplemented with information about a particle configuration; Spontaneous collapse theories deny the second statement, modifying quantum dynamics; Everett interpretations deny the third statement, seeking to describe QM without determinate measurement outcomes.

composite system may be in a superposition of states where no definite values for a given quantity can be ascribed.

Introduced by Rovelli (Rovelli 1996), RQM resolves this inconsistency by stipulating that a physical interaction is a measurement-style event.[15] However, this is only true for those systems directly involved: the systems are merely entangled from the standpoint of other "third-party" systems. The appearance of two sorts of interaction arises from a difference in perspective. Interaction events do have outcomes, but particular values of the physical quantities are manifest only relative to the interaction partner(s) involved. We accept the prima facie lesson of the Wigner's friend scenario: the direct participant (Alice) observes a definite outcome, while the systems involved are entangled from the perspective of a third party such as Bob.

With regard to the trilemma, RQM does not reject any of the three statements, but modifies them to specify their relational nature.[16] The first statement remains true, as long as we stipulate that the wave function specifies the physical properties of a system relative to a reference system. The second statement must be supplemented to note that the dynamics also describe a system with reference to another system (to be clear, it should also add that this applies in the absence of their direct interaction). The third statement must add a stipulation that definite outcomes are realized relative to a measuring (directly interacting) system.

An important part of this interpretation is that all physical systems are treated the same way. While examples may feature human observers and macroscopic measurement devices, there is nothing special about them: all systems will (mutually) manifest definite values for quantities when they directly interact with each other. At the same time, systems cannot generally be ascribed such definite values from the perspective of other systems in the absence of a direct interaction.

This relational quality, and the attendant loss of the usual, classical, "view from nowhere," is the unintuitive or revisionary aspect of RQM. Note that its relational aspect is more than a merely epistemological distinction: It isn't just that Bob doesn't know what happened in the lab: for him

---

[15] For additional background, see Laudisa and Rovelli (2021). For discussion of some recent debates, see Di Biagio and Rovelli (2022).

[16] A recent article discussing how RQM handles the measurement problem (including in the context of Maudlin's trilemma) is Oldofredi (2023).

it did not happen, and the unobserved system remains in superposition. Of course, the thought experiment idealizes from some practical realities. First, even from Bob's perspective, interference effects involving macro-level superpositions would be suppressed by environmental decoherence within the lab. More to the point, a perfect sealing of the lab is also an idealization, and realistically, a shared environment will ensure that Bob and Alice will agree about what happened.[17] But it remains the case that the co-existence of such different perspectives on systems is the primary "cost" of resolving the measurement problem.[18]

At this point in the discussion, we have added another QM interpretation to those included by Franklin and Seifert, and we can sketch how the different perspectives implied by RQM would handle the problems of molecular structure as "special cases." QM models of isolated molecules describe them with electrons and nuclei in a superposition, evolving according to the Schrödinger equation with no determinate molecular structure. This is akin to Bob's view, which we can label the external perspective. When chemists experimentally interact with molecules, definite values are revealed (Alice's view: call this the internal perspective). As in the case of some other interpretations, an important role in shaping molecular structure from the external perspective would be assigned to decohering interactions. As in the earlier discussion, we can only assume that the remaining puzzles surrounding molecular structure are ones that will be made clearer if and when we have more detailed quantum mechanical analyses that include realistic depictions of their internal and external environments.

But so far, we have arguably not moved the discussion forward. As discussed, the fact that so much is left to be explained opens up room for skeptics to argue that solving the measurement problem is not a panacea when it comes to the problems of molecular structure. Even for those that think it plays an important or even the crucial role, there seems to be little reason to think

---

[17] Recently, several thought-experiments have been proposed that extend Wigner's friend-style scenarios (involving multiple observers and experiments) in order to derive results that appear to lead to genuine disagreement between observers about outcomes (e.g. Frauchiger and Renner, 2018). This literature is still subject to active debate, and the details won't be discussed here. Even though these scenarios are idealized, it may be thought worrisome that QM under some interpretations (including RQM) may not provide guarantees of agreement. Recently, Adlam and Rovelli (2023) proposed an addition to RQM's principles, postulating the existence of so-called "cross-perspective links." Briefly, the idea is that any outcome observed by Alice should have a physical effect on her, creating a record of the information. Then, unless it is destroyed by subsequent interactions, an appropriate subsequent measurement of Alice by Bob should in principle be capable of measuring the physical variable encoding the information, with the result matching that of Alice's original measurement.

[18] Philosophical critiques of RQM include Brown (2009), van Fraassen (2010) and Ruyant (2018).

one's choice among QM interpretations would have much to do with the particular concerns in the philosophy of chemistry.

However, we will proceed to explore how adopting RQM's stipulation of multiple perspectives within a single world can offer additional insights. The starting point is to note that, even from the external perspective, one can infer that other systems are involved in ongoing measurement-like interaction events from their internal perspectives. For atoms and molecules this would include interactions among their constituents as well as with other systems in their environment. Then, one can envision these inferred interactions playing a role in composing and shaping a molecule that complements the external perspective described by QM models.

To help do this, however, it will be useful to propose some additional ontological elements to help define what it is that (relational) quantum descriptions represent.

A Causal Ontology for RQM

In its original conception, RQM was taken to imply an ontology of events—the discrete measurement-like interactions between systems:

> The world is therefore described by RQM as an evolving network of sparse relative events, described by punctual relative values of physical variables. (Laudisa and Rovelli, 2021)

In contrast to the events, Rovelli has taken a deflationary or instrumental view of quantum states themselves, saying they merely encode predictive information about a system or systems (from the perspective of a given reference system) derived from prior interactions:

> In RQM, the quantum state is not a representation of reality: it is always a relative state and is only a mathematical tool used to predict probabilities of events *relative to a given system*. (Di Biagio and Rovelli, 2022, 62, emphasis original)

This implies there is no basis for assigning ontological features (such as properties) to a system in the absence of interaction. For present purposes, this sparse picture offers limited raw material for understanding topics such as composition and structure. However, it is possible to suggest alternative ontologies that are consistent with RQM, and several have been proposed.[19] Dorato (2016) suggests that non-interacting systems can be characterized as having dispositions:

> In other words, such systems S have intrinsic dispositions to correlate with other systems/observers O, which *manifest* themselves as the possession of definite properties q relative to those Os. (Dorato, 2016, 239; emphasis original)

As he points out, referencing ideas due to philosopher C.B. Martin, such manifestations only occur as mutual manifestations involving dispositions characterizing two or more systems (which Martin calls “reciprocal disposition partners”).[20] The wave function may be taken to represent, then, dispositions of a system that apply to potential manifestations in an interaction with a specified reference system. Likewise, the Schrödinger equation may be taken to represent the evolution of the system and its dispositions between such interactions.[21]

This picture of propagating systems and their interactions is a close fit with the account of causal structure introduced by Salmon (1984). Salmon describes a causal network intended to underpin explanations in the sciences. His basic entity or object is labeled a causal process, and there are two dimensions of causation: propagation and production. Propagation refers to the evolution of a causal process in the absence of interaction, while production refers to the change that causal processes undergo when an interaction occurs. As described by Ladyman and Ross:

> The metaphysic suggested by process views is effectively one in which the entire universe is a graph of real processes, where the edges are uninterrupted processes, and the vertices the interactions between them (Ladyman and Ross, 2007, 263).

Salmon’s original account defined production as the introduction of a change or “mark” to the characteristics (or “structure”) of a process, with the distinguishing characteristic of a

---

[19] See discussion in Oldofredi (2023).

[20] See Martin (2008). Note that since these manifestations have a probabilistic aspect to them, the dispositions might also be referred to as propensities. There is a tradition of interpreting QM using the notion of propensities, going back at least to Heisenberg (1958); some of these are surveyed and critiqued by Suárez (2007).

[21] For familiar reasons, the dispositions cannot be taken to be localized in spacetime. Only the measurement-like interaction events can have spacetime locations.

propagating process being its capability of "transmitting" the mark between interactions (Salmon, 1984, 147-156). If we modify Salmon's original account using the dispositional framework, then causal processes are characterized by a propagating bundle of dispositions between interactions, while production refers to the mutual manifestations of dispositions in interaction events.[22]

The relational twist is, of course, another modification, introducing the presence of multiple perspectives on this causal network. Only the events in which a process takes part feature manifestations of definite values (the internal perspective). From an external perspective, processes continue in uninterrupted propagation.

Finally, we can add to the causal network a simple conception of composition, positing that coherent entities at a larger scale arise from patterns of interactions among a set of smaller-scale processes. In the Salmon-style framework, we can call these *composit*e causal processes. Their higher scale causal features can be assessed by analyzing the constituting patterns at the lower scale. In particular, when a group of processes interact more frequently with each other than with "outsiders," then it can form a composite.[23]

This idea is familiar from other discussions of causal composition (in mainly macroscopic contexts). For instance, as part of his discussion of analyzing complex systems, Wimsatt explores the idea of decomposition based on interactions, i.e., breaking down a system into subsystems based on the relative strength of intra vs extra-system interactions. (Wimsatt, 2007, 184).[24] And while he describes how different theoretical concerns lead us to utilize a variety of analytical

---

[22] In response to criticism, Salmon changed his view and dropped the mark-transmission account in favor of definitions that relied on transmission and exchange of conserved quantities. In both versions of the account, he sought to define causal influences in in a way friendly to a traditional empiricism, in contrast to relying on dispositions (or other notions of unreduced causal power or influence) as in the present discussion.

[23] Salmon (1984) outlines a pertinent distinction between etiological explanations and constitutive explanations. Etiological explanations trace the relevant preceding processes and interactions leading up to a phenomenon. A constitutive explanation, on the other hand, is one that cites the interactions and processes that compose the phenomenon. However, neither Salmon nor others who have offered causal process theories provide a detailed account of constitution/composition.

[24] As Wimsatt mentions, related ideas are found in Herbert Simon's account of complex systems. Simon discusses the role interactions play in forming hierarchies, describing hypothetical systems where there are no interactions between parts as "decomposable," and then developing the notion of "*nearly decomposable* systems, in which the interactions among the subsystems are weak but not negligible (Simon, 1996, 197, emphasis original)."

strategies, Wimsatt makes it clear that such patterns of causal connections are the ultimate basis for understanding complex systems:

> Ontologically, one could take the primary working matter of the world to be causal relationships, which are connected to one another in a variety of ways—and together make up patterns of causal networks…Under some conditions, these networks are organized into larger patterns that comprise *levels of organization* (Wimsatt, 2007, 200, emphasis original).

Wimsatt explains that levels of organization are "compositional levels", characterized by hierarchical part-whole relations (201). This notion of composition includes not just the idea of parts, but of parts engaged in certain patterns of causal interactions, consistent with the approach to composite causal processes suggested above.

To summarize: a composite causal process consists of a number of sub-processes with dispositions toward interacting at a greater frequency with each other than with other processes.[25] Just like any causal process, a composite process carries its own dispositions: the particular pattern of interacting sub-processes accounts for how composite processes will themselves interact with their environment. We can then also envision how such interactions can further impact the character of the composite entity.

For present purposes, electrons and nuclei are the elementary causal processes whose interaction patterns form composites: atoms and molecules. This framework will aid our interpretation of RQM's internal perspective on these systems. The next section develops these ideas in relation to views about the ontological status of electron density, then concludes by assessing implications for the debates over molecular structure.

Density and the Internal Perspective on Molecules

---

[25] In physical terms (the external perspective), this differential may be measured by varying strength of forces, but in this causal account, the raw material of composition is the frequency of discrete interactions.

While calculating wave functions is the starting point for analysis in quantum chemistry, the electron density distribution (usually labeled ρ) also plays a featured role. Recall that the probability of finding a particle in a given volume of space in a measurement is calculated from the absolute value (or modulus) squared of the appropriate wave function, or, equivalently, the product of the wave function and its complex conjugate (denoted by ψ*). For an atom with a single electron (in the time-independent case), the probability of finding the electron in given infinitesimal volume of space $r + dr$ is given by: [26]

$$\psi * \psi dr$$

(where r represents the three space coordinates with the origin on the stationary nucleus as well as the spin coordinate). For a multi-electron system (given a certain arrangement of nuclei[27]), the similar expression:

$$\psi * (1, 2, \ldots, N)\psi(1, 2, \ldots, N)dr_i$$

gives the probability of finding the first electron between $r_1 + dr_1$, and the second electron between $r_2 + dr_2$, …, and the *N*th electron between r_N and dr_N. If we are interested only in finding the probability of finding a particular electron in a particular location, then one must integrate over all possible positions for the rest of the electrons:

$$p_1 r_1 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} \psi * (1, 2, \ldots, N)\psi(1, 2, \ldots, N)dr_2 dr_3 \ldots dr_N$$

but since electrons are indistinguishable, the probability of finding any electron in the same volume is the same. So, by multiplying this value by the number of electrons in the system we can find the probability for finding any of the *N* electrons at a particular location:[28]

---

[26] The notation in this discussion follows that of Veszprémi and Fehér (1999).

[27] For the purposes of the following passages, we will assume that the molecular wave functions and associated electron densities are derived from the usual post-Born-Oppenheimer models.

[28] This is not a probability density function, since it sums to *N* rather than one. If one integrates the expression over the entire space, one will recover the number of electrons, as expected.

$$\rho(r_1) = N\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty}\psi*(1,2,\ldots,N)\psi(1,2,\ldots,N)dr_2\,dr_3\ldots dr_N$$

In this way, the electron density ρ(r) can be defined at each point.

While this is the counterpart of the expectation value used to probabilistically predict the outcome of a measurement for any quantum system (the Born rule), the electron density plays other roles in quantum chemistry. First, alongside diagrams depicting wave functions/orbitals, it is a popular way to visually depict atoms and molecules in textbooks. Because it is a function assigning (real) numbers to points in 3D space, it offers a more intuitive basis for pictures of shape or structure, e.g. using 2-D dot-density, cloud or contour diagrams. In addition to using estimated wave functions to calculate ρ, techniques such as X-ray crystallography also offer a way to construct images of ρ for actual molecules. Such images may give rise to a temptation to think that ρ represents molecules as spatial objects, despite the density's statistical interpretation (see discussion below).

More importantly, electron density frequently assumes a direct role in quantum chemical analysis. Density Functional Theory (DFT) uses ρ instead of ψ as a starting point to estimate electronic properties. This relies on the fact that it can be demonstrated that ground state energy and other properties cam be derived directly from ρ (Hohenberg-Kohn theorems). This degree of informational equivalence between ψ and its associated density is clearly not generally true for quantum systems, but in this case the existence of a minimum energy solution allows for the result to be mathematically established.

Another research program based on electron density is the quantum theory of atoms in molecules (QTAIM), developed by R.F.W. Bader and others.[29] This approach begins with an analysis of the topological features of ρ. The electron density for an isolated molecule shows concentration near the nuclei, diminishing as you move outward, but a close examination shows other details (such as gradients and critical points). These features are then linked to a variety of chemical concepts, including bonding. One of QTAIM's principles, relevant to the discussion below, is that such

---

[29] Bader (1990); Gillespie and Popelier (2001, Chs.6-7) provides an introduction.

topological features may be used to pick out atomic systems and their interactive relationships within the molecule.[30] This contrasts with quantum models that treat molecules as a composite of nuclei and electrons, without an explicit role for atomic systems as such within molecules.

The usefulness of electron density in these research contexts may seem surprising if we only think of it as fulfilling its statistical (Born rule) role, that is, as a predictive tool for hypothetical measurements. And indeed, there is a history of attempts to interpret it in another way: as a representation of charge density—an actual distribution of electric charge in three-dimensional space (multiplying density times the charge of an electron). This idea was present in Schrödinger's early quantum articles, but then largely abandoned. Obstacles to the idea include the fact that, for multi-electron systems, the wave function is defined in a high-dimensional configuration space, and there exists information about these systems that can be derived from the wave function but not the density.[31] Despite this, the idea that charge density is something real has had its defenders, Bader being a notable case:

> The charge density provides a description of the distribution of charge throughout real space and is the bridge between the concept of state functions in Hilbert space and the physical model of matter in real space. (Bader, 1990, 169)

Recently, Sebens (2021) has reviewed motivations for the charge density idea and offered an assessment of some possible ways to justify it.[32] One idea would rely on electrons occupying (even in the absence of measurement) a succession of positions that, upon time-averaging, fill out a pattern equivalent to the density.[33] Sebens also describes a compromise (between what he calls the "Born role" and "Schrödinger role") that sees charge density as real and spread out in

---

[30] The density can also play a role in measuring intra-molecular forces via the Hellmann-Feynman theorem.

[31] Gao (2018) discusses this history, and describes several shortcomings associated with the idea, including Born's criticism that the quadrupole moment cannot be expressed as a function of ρ.

[32] In addition to discussing DFT, Sebens (2021) highlights the role density can be seen to play in more traditional approximation methods. For instance, important components of the Hamiltonian created using the Hartree-Fock method can be interpreted to reflect classical electrostatics involving the interaction between the electron density and the nuclei.

[33] Gao (2018) presents a view like this. He concludes while one cannot say ρ is real in the sense of being distributed in space at an instant, one can say it "effectively" exists, distributed as a series of localized point charges taking the form of "ergodic motion" of a localized particle, such that its average value over time comprises an effective charge density.

space except when we measure it, at which time it contracts to a point representing the expected number of electrons. With the first idea, one would need add to QM a dynamical theory of charged particles moving in three-dimensional space, while in the second case, charge density might perhaps be added directly as a posit of "primitive ontology" to accompany an interpretation of QM that provides a solution to the measurement problem.[34]

A strength of RQM is that it can make sense of the motivations for attributing reality to charge density in three-D space, but without modifying or supplementing quantum theory. From the external perspective, the electron density plays its standard (Born) role. Strictly speaking, we cannot view any particular ρ (derived from a calculation of ψ) as representing internal perspectives of molecular systems or their constituents. But when making (fallible) inferences about what is happening from these perspectives, we find the picture includes something akin to one of the ideas suggested to justify the existence of charge density.

Recall that every interaction event is measurement-like from the internal perspectives of the participating systems, and we can infer such events occur frequently in a typical busy environment. We further assume that many of these would feature manifestation of quantities in the position basis (localizing interactions). When applied to the case of molecular electrons, this suggests a view of charge density with some similarity to the first (dynamic) idea discussed above: that of a time-extended averaging of a series of localized appearances of charged particles—except now it is stipulated that it is the discrete but frequent interactions among systems that are responsible for a series of electron localizations.

Having made this connection with density, we can make a fuller sketch of how atoms and then molecules are shaped from this internal perspective. We will start by discussing composition, using the causal ontology introduced above. As a composite causal process, an atom is composed by a pattern of interactions among its subprocesses (nuclei and electrons), with its evolution also shaped by further interactions involving external systems. Here it is important to note that the

---

[34] See Sebens (2021) for further discussion of interpretive possibilities, including some in the context of Bohmian mechanics, Everett-style interpretations, and spontaneous collapse theories. Several authors have argued that an account of primitive ontology in 3D space is generally needed to accompany interpretations of QM (see Allori, 2013).

localizing events we have been discussing, while crucial for understanding for manifestations of spatial shape, are not all there is to the atom: it is the entire pattern of interacting sub-atomic processes (including their propagations between interactions) that is responsible for an atom's constitution, endowing it with its own dispositions to interact.[35]

When atoms, in turn, manifest certain dispositions to form a new composite (molecule), they create a new interaction pattern. This pattern can be viewed in two ways. At a coarse-grained level, the molecule consists of interacting atomic systems, while a fine-grained analysis sees a new pattern of interactions involving the combined atomic nuclei/electrons. Notably, as suggested by the picture provided by densities, this new pattern involves an alteration of the prior atomic patterns (reflecting bonding and other, ongoing interatomic interactions), but a large part of the pattern that characterizes the atoms in other contexts is preserved in the molecule.

To fill out an explanation of molecular composition, we would need to add to this picture a discussion of how specific interactions with systems in the external environment shape the final patterns composing the molecule, and perhaps also serve to stabilize it. In realistic environments, such environmental interactions would occur incessantly. As in the earlier discussion, we can infer that this is a crucial ingredient. Further, we can now see that from the internal perspective of these systems, all of the resulting patterns would be expected to include localizing events that trace out characteristic molecular structures in three-dimensional space.

While this discussion of molecular composition and structure from RQM's internal perspectives is unavoidably informal and qualitative, it offers a complementary and intuitive picture to accompany the familiar physical models of these systems. It can thereby bolster our confidence that, despite the present lack of realistic detailed models, quantum mechanics can indeed account for molecular structure. This is because, given RQM, the internal and external perspectives co-exist in one world, and therefore will conform to one another. The two perspectives converge

---

[35] We can draw the following parallel. Just as the density does not include all of the information in the wave function (external perspective), the interaction events among sub-processes are a subset of what constitutes a composite causal process—one needs to also take into account their propagation between interactions (internal perspective).

whenever a modeled system is observed, and given the framework presented here, it is not surprising that our observations of molecules find them to be spatially structured.

This contrasts to the situation described earlier, where invoking solutions to the measurement problem still left an explanatory gap, leaving room for skeptics to question Franklin and Seifert's thesis that the problems of molecular structure were special cases of the measurement problem. The main issue is arguably that the solutions to the measurement problem Franklin and Seifert discuss do not provide enough additional interpretative resources to envision how structures are formed. The work of this article is to introduce a framework that can accomplish this task.

Possible objections to the present discussion are worth noting. While responding to objections to the basic principles of RQM are beyond the scope of this article, one might object to the additional ontology and to the specific assumptions made about unobservable interactions among microscopic systems. Specific worries about the latter may include whether one can assume frequent occurrence of measurement-like interactions (featuring outcomes in the position basis), while also assuming that their existence is consistent with the formation and maintenance of relatively stable atomic and molecular systems. However, there are reasons to think the inferred picture is reasonable: RQM entails the existence of multiple perspectives, but compared to some interpretations it undermines presumptions of sharp discontinuities in nature between the macroscopic and microscopic realms. This clears the way to employ a plausible account of composition and spatial localization across scales.

Conclusion

When we interact with molecules, they have a characteristic definite spatial structure, one that is not evident from QM models. Choosing a solution to the measurement problem of QM seems necessary to make progress: at a minimum, these solutions offer an account of how definite outcomes (for properties such as position) exist in our experience. However, more is needed in order to explain molecular structures, particularly given the evident importance of interactions in accounting for their formation. RQM, with the addition of a causal ontology, offers the needed resources to improve our understanding. First, via its multiple perspectives, RQM allows us to reconcile the representations of quantum mechanics with the definite outcomes we observe. But beyond this, RQM is also distinctive in that it that allows us to infer that measurement-like interactions featuring definite outcomes are ubiquitous in our world. With the addition of a complementary causal ontology, the interpretation can be used to frame an account of how patterns of interactions will lead to composite systems like molecules, with spatially organized structures.

References

Adlam, E., Rovelli, C.: Information is physical: cross-perspective links in relational quantum mechanics. Philos. Phys. **1**, 4 (2023). https://doi.org/10.31389/pop.8

Allori, V.: Primitive ontology and the structure of fundamental physical theories. In Ney, A., Albert, D. Z. (eds.) The Wave Function, pp. 58-75. Oxford, Oxford University Press (2013)

Bacciagaluppi, G.: The role of decoherence in quantum mechanics. In: Zalta, E. N. (ed) The Stanford Encyclopedia of Philosophy (Fall 2020 Edition) (2020). https://plato.stanford.edu/archives/fall2020/entries/qm-decoherence/

Bader, R. F.: Atoms in Molecules: A Quantum Theory. Oxford, Clarendon Press (1990)

Bahrami, M., Shafiee, A., and Bassi, A.: Decoherence effects on superpositions of chiral states in a chiral molecule. Phys. Chem. Chem. Phys. **14**, 9214–9218 (2012). https://doi.org/10.1039/C2CP40920H

Brown, M. J.: Relational quantum mechanics and the determinacy problem. Br. J. Philos. Sci. **60**, 679-695 (2009). https://doi.org/10.1093/bjps/axp017

Cassam-Chenaï, P., Mátyus, E.: Electrons as an environment for nuclei within molecules: a quantitative assessment of their contribution to a classical-like molecular structure. Theor. Chem. Acc. **140**, 159 (2021). https://doi.org/10.1007/s00214-021-02857-3

Claverie, P., Diner, S.: The concept of molecular structure in quantum theory: interpretation problems. Isr. J. Chem. **19,** 54-81 (1980). https://doi.org/10.1002/ijch.198000006

Di Biagio, A., Rovelli, C.: Relational quantum mechanics is about facts, not states: a reply to Pienaar and Brukner. Found. Phys. **52**, 62 (2022). https://doi.org/10.1007/s10701-022-00579-5

Dorato, M.: Rovelli's relational quantum mechanics, anti-monism, and quantum becoming. In: A. Marmodoro, A. and Yates, D. (eds.) The Metaphysics of Relations, pp. 235-262. Oxford, Oxford University Press (2016). https://doi.org/10.1093/acprof:oso/9780198735878.003.0014

Fortin, S., Lombardi, O.: Is the problem of molecular structure just the quantum measurement problem? Found. Chem. **23**, 379–395 (2021). https://doi.org/10.1007/s10698-021-09402-x

Fortin, S., Lombardi, O., and Martínez González, J. C.: Isomerism and decoherence. Found. Chem. **18**, 225–240 (2016). https://doi.org/10.1007/s10698-016-9251-6

Franklin, A., Seifert, V.: The problem of molecular structure just is the measurement problem. Br. J. Philos. Sci. (2021). https://doi.org/10.1086/715148

Frauchiger, D., Renner, R.: Quantum theory cannot consistently describe the use of itself. Nat. Commun. **9**, 3711 (2018). https://doi.org/10.1038/s41467-018-05739-8

Gao, S.: Is an electron a charge cloud? A reexamination of Schrödinger's charge density hypothesis. Found. Sci. **23**, 145–157 (2018). https://doi.org/10.1007/s10699-017-9521-3

Gillespie, R. J., Popelier, P. L.: Chemical Bonding and Molecular Geometry. New York, Oxford University Press (2001)

Heisenberg, W.: Physics and Philosophy. New York, Harper and Brothers (1958)

Hendry, R.F.: Quantum mechanics and molecular structure. In: Lombardi, O., Martínez González, J.C., Fortin, S. (eds.) Philosophical Perspectives in Quantum Chemistry, pp. 147-172. Springer, Cham. (2022) https://doi.org/10.1007/978-3-030-98373-4_7

Ladyman, J., Ross, D.: Everything Must Go. Oxford, Oxford University Press (2007)

Laudisa, F., Rovelli, C.: Relational quantum mechanics. In: Zalta, E.N. (ed) The Stanford Encyclopedia of Philosophy (Winter 2021 Edition) (2021). https://plato.stanford.edu/archives/win2021/entries/qm-relational/

Martin, C.: The Mind in Nature. Oxford, Oxford University Press (2008)

Mátyus, E.: Pre-Born–Oppenheimer molecular structure theory. Mol. Phys. **117**, 590-609 (2019). https://doi.org/10.1080/00268976.2018.1530461

Mátyus, E., Cassam-Chenaï, P.: Orientational decoherence within molecules and emergence of the molecular shape. J. Chem. Phys. **154**, 024114 (2021). https://doi.org/10.1063/5.0036568

Maudlin, T.: Three measurement problems. Topoi **14**, 7–15 (1995)

Oldofredi, A.: The Relational Dissolution of the Quantum Measurement Problems. Found. Phys. **53**, 10 (2023). https://doi.org/10.1007/s10701-022-00652-z

Primas, H.: Pattern Recognition in Molecular Quantum Mechanics. Theoret. Chim. Acta **39**, 127-148 (1975)

Rovelli, C.: Relational quantum mechanics. Int. J. Theor. Phys. **35**, 1637-1677 (1996)

Ruyant, Q.: Can we make sense of relational quantum mechanics? Found. Phys. **48**, 440–455 (2018). https://doi.org/10.1007/s10701-018-0156-1

Salmon, W. C.: Scientific Explanation and the Causal Structure of the World. Princeton, Princeton University Press (1984)

Scerri, E.R.: Editorial 37. Found. Chem. **13**, 1–7 (2011). https://doi.org/10.1007/s10698-011-9107-z

Sebens, C.T.: Electron charge density: a clue from quantum chemistry for quantum foundations. Found. Phys. **51**, 75 (2021). https://doi.org/10.1007/s10701-021-00480-7

Seifert, V.A.: Do molecules have structure in isolation? How models can provide the answer. In: Lombardi, O., Martínez González, J.C., Fortin, S. (eds) Philosophical Perspectives in Quantum Chemistry, pp. 125-143. Springer, Cham. (2022). https://doi.org/10.1007/978-3-030-98373-4_6

Simon, H. A.: The Sciences of the Artificial (3rd ed.). Cambridge, MIT Press (1996).

Suárez, M.: Quantum propensities. Stud. Hist. Philos. Sci. B - Stud. Hist. Philos. Mod. Phys. **38**, 418-438 (2007). https://doi.org/10.1016/j.shpsb.2006.12.003

Sutcliffe, B., Woolley, R.G.: Is chemistry really founded in quantum mechanics? In: Lombardi, O., Martínez González, J.C., Fortin, S. (eds) Philosophical Perspectives in Quantum Chemistry, pp. 173-202. Springer, Cham. (2022) https://doi.org/10.1007/978-3-030-98373-4_8

Trost, J., Hornberger, K.: Hund's paradox and the collisional stabilization of chiral molecules. Phys. Rev. Lett. **103**, 023202 (2009). https://doi.org/10.1103/PhysRevLett.103.023202

van Fraassen, B.: Rovelli's world. Found. Phys. **40**, 390-417. (2010). https://doi.org/10.1007/s10701-009-9326-5

Veszprémi, T., Fehér, M.: Quantum Chemistry: Fundamentals to Applications. Dordrecht, Kluwer (1999)

Wimsatt, W. C.: Re-Engineering Philosophy for Limited Beings. Cambridge, Harvard University Press (2007)

Woolley, R.G.: Must a molecule have a shape? J. Am. Chem. Soc. **100**, 1073-1078 (1978)

Woolley, R.G.: Quantum chemistry beyond the Born-Oppenheimer Approximation. J. Mol. Struct. **230**, 17-46 (1991). https://doi.org/10.1016/0166-1280(91)85170-C

Zhong, C., Robicheaux, F.: Decoherence of rotational degrees of freedom. Phys. Rev. A **94**, 052109 (2016). https://link.aps.org/doi/10.1103/PhysRevA.94.052109

Wigner, E.: Remarks on the mind-body problem. In Good, I.J. (ed.) The Scientist Speculates, pp. 284-302. Heinemann, London (1961); Reprinted in Wigner, E.: Symmetries and Reflections, pp. 171-184. Indiana University Press, Bloomington (1967)