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Relational Quantum Mechanics, Causal Composition, and Molecular Structure

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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 concerns the relationship between QM and molecular structure, meaning the three-dimensional spatial relationships among the atomic centers in a molecule. 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

Molecules present a more challenging case. First, multi-particle atomic and molecular wave equations are generally computationally intractable, so various simplifying assumptions must be used. But when it comes to deriving molecular structure in particular, the conventional approach also appears to have an in-principle shortcoming. For example, hydrogen cyanide (HCN) is a triatomic molecule whose atoms are arranged linearly, with a hydrogen atom bonding to a central carbon atom and, on the opposite side, a (triple) bond with nitrogen. Its Schrödinger equation would need an appropriate Hamiltonian encompassing all of the constituent electrons and nuclei, and this opens up a wide array of possibilities for superposed positions (now including the nuclei as well as the electrons). Without solving the equation, we know there is a problem: the same

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.

constituents are present in another stable isomer, hydrogen isocyanide (HNC), which is a distinct chemical species (the hydrogen bonds to the nitrogen). Because of their different structures, the two isomers have different properties, including bond lengths, energies and dipole moments. Interestingly, these molecules are common in the interstellar medium, and the observability of their distinct spectra, along with their differential participation in various reactions, have made measuring their relative distributions useful in astrophysical investigations.⁴ However, they would be described by the same Schrödinger equation.

In practice, quantum models of molecules do not use Hamiltonians that group all the constituents together in this way. Instead, they separate the motions of the electrons from the (multiple) nuclei. 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. However, 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.⁵

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

⁴ See for example, Hacar, Bosman and van Dishoeck (2020).

⁵ 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.

cases of the measurement problem of quantum mechanics.”⁶ 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 view of the problem expands to encompass 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.⁷

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 addresses the measurement problem.⁸ 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

⁶ 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.

⁷ 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 distinction is criticized by Fortin and Lombardi (2021) as discussed below.

⁸ 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.

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).⁹ 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 observed.¹⁰ 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 Seifert 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

⁹ Other early references suggesting a role for external interactions include Primas (1975) and Claverie and Diner (1980).

¹⁰ See Bacciagaluppi (2020, section 2) and the discussion in Fortin, Lombardi, and Martínez González (2016), which focuses on the specific problem of optical isomerism.

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).¹¹ 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 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

¹¹ 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.

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 Robicheaux, 2016).¹² But progress on 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 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

¹² 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.

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 address the measurement problem, an interpretation needs to reconcile the quantum formalism with the fact that, upon measurement, we find definite quantities rather than superpositions (this is sometimes described as a “collapse of the wave function”). Frankin and Seifert (referencing Maudlin) describe how this is accomplished in each of the three interpretations they discuss.¹⁶

For introducing RQM specifically, it is helpful to examine an extension of the measurement problem: this is the so-called “Wigner’s friend” scenario (Wigner 1961/1967). To simplify the discussion, we can consider an experiment measuring electron spin along one spatial axis. The electron can be prepared so it is in a superposition of two possible states (labeled “up” or “down”), but only one of these will be realized upon measurement (each having a probability of 50%). Now picture two scientists involved in the experiment. The first, Alice, performs the spin measurement. This takes place in a sealed laboratory, and Alice’s friend Bob is positioned outside. Alice observes a definite outcome, as usual. Now, consider Bob’s perspective. If quantum mechanics is universally applicable, he should, in principle, be able to use it to formally model the lab and its contents. Everything in the lab would be part of a composite wave function, and its evolution over the time frame of the planned experiment would result in a superposition

¹⁶ Briefly, the Bohmian interpretation denies that the quantum formalism is complete, and supplements it. An ontology of particles with trajectories in 3D space is posited, and the wave function’s role is to guide the trajectories. Here, there is no collapse of the wave function: at all times the particle positions are determined. The probabilistic appearance of measurement outcomes is a due to our ignorance given the inaccessibility of the underlying dynamics. In the case of spontaneous collapse theories, the QM formalism is not supplemented but altered. A new, stochastic, dynamics is proposed to replace the Schrödinger equation. It includes new constants of nature that make wave function collapse more likely in certain conditions (and, of course, almost assured in those characterizing actual experimental contexts). The Everett interpretation denies that collapses occur: measurements only appear to find particular outcomes. All possible outcomes occur, but take place in mutually inaccessible “worlds.”

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 ways of treating interaction. In the absence of any interaction, a system evolves in time as described by the Schrödinger equation. But interactions are handled in two distinct 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 composite system may be in a superposition of states where no definite values for a given quantity can be ascribed.

Each interpretation of QM would address this extension of the measurement problem in its own fashion: for instance, they may deny that one of the two types of interaction exists (Bohmian mechanics and Everett discard measurement collapses) or attempt to unite the two in a new formalism (spontaneous collapse theories). RQM, introduced by Rovelli (Rovelli 1996), addresses it in a unique way. It posits that a physical interaction is a measurement-style event, manifesting definite quantities.¹⁷ However, this is only true from the perspective of systems directly involved in the interaction. These participating systems merely become entangled from the perspective of a “third-party” system not directly involved. 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 only manifest 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

¹⁷ For additional background, see Laudisa and Rovelli (2021). For discussion of some recent debates, see Di Biagio and Rovelli (2022).

perspective of a third party such as Bob. RQM does not solve the measurement problem by altering the textbook formulation of QM, but specifies that the quantum formalism describing a system (e.g. wave function and Schrödinger equation) is always describing it relative to a reference system.¹⁹ This reference system, in most textbook cases, would be understood as that of an observer/experimental apparatus that has interacted with the system in the past (i.e. preparing the system for measurement) but has not yet interacted again (i.e. performed measurement). When the measurement is performed (and an outcome realized), this again must be understood as relative to the reference system participating in the interaction.

The next crucial part of the 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 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

¹⁹ A recent article discussing how RQM handles the measurement problem (including in the context of Maudlin's trilemma) is Oldofredi (2023).

happened.²¹ But it remains the case that the co-existence of such different perspectives on systems is the primary “cost” of resolving the measurement problem.²²

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 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-

²¹ 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.

²² Philosophical critiques of RQM include Brown (2009), van Fraassen (2010) and Ruyant (2018).

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.

The goal is to provide an interpretation that does not merely show that the existence of familiar molecular structures is compatible with QM, but to go further to show why we should expect that a quantum physical world will include these structures. To further this goal, it will be helpful to propose some additional ontological elements to define what it is that (relational) quantum descriptions represent.

A Causal Ontology for RQM

Interpretations of QM sometimes include explicit proposals regarding ontology.²³ 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 interaction 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)

²³ While Bohmian mechanics typically posits particles with definite positions in 3D space, supporters of the Everett and spontaneous collapse interpretations have diverse approaches to questions about ontology (for an argument that these interpretations should include a so-called “primitive ontology” in 3D space, see Allori, 2013.) One difference between RQM and other interpretations such as Bohm/Everett that is relevant to ontology concerns the role of “the wave function of the universe”. In the case of Bohmian mechanics, for example, the particles, considered by themselves, are inert: they don’t have momentum, energy, or spin. These quantities appear to be manifest in experiments due to the way the entire collection of particles is guided by the universal wave function. In RQM, there is no universal wave function (since all wave functions are only defined relative to a distinct system). An ontology where systems bear causally potent properties is a better fit, as in the proposal below.

This implies there is no basis for assigning ontological features (such as properties) to a system in the absence of interaction. Unfortunately, this picture offers limited resources for understanding topics such as the composition and structure of larger systems. However, it is possible to suggest alternative ontologies that are consistent with RQM, and several have been proposed.²⁴ 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 Dorato explains, 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”).²⁵ 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. According to this view, we take a realist stance toward non-interacting systems, characterized by their dispositional profile, as well as about the interaction events. A difference between the two stances is that the former cannot be taken to be localized in three-dimensional space: only the measurement-like interaction events can be localized.

To expand further upon Dorato’s suggestion, we can note that this picture of evolving 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

²⁴ See discussion in Oldofredi (2023).

²⁵ 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).

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 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.²⁷ So, now our ontology can be summarized this way: quantum systems (between interactions) are propagating causal processes; quantum states represent their dispositional profile; and interactions are causal production events where the probabilistic dispositions of participating systems are made manifest (altering the dispositional profiles of the participating systems). Note that this picture captures something of the old idea of wave-particle duality, with propagating causal processes bearing non-localized potentials, only having particle-like definite features and locations in the context of interaction.

Of course, in the context of RQM, we have to also incorporate the presence of multiple perspectives in causal network. The interaction events only feature manifestations of definite values from the perspective of participating systems/causal processes (the internal perspective), while from the external perspective, the participants continue in uninterrupted propagation. Their dispositions are correlated, but not manifested in definite quantities, from this third-party standpoint.

²⁷ In response to criticism, Salmon dropped the mark-transmission account in favor of definitions that relied on transmission and exchange of conserved quantities. In both versions of the theory, he sought to define causal influences 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. Another difference is that Salmon's definitions implied that processes follow definite trajectories in spacetime, inconsistent with QM.

The final supplement to Salmon’s approach relates to the question of composition. Here, we posit that coherent entities at a larger scale arise from patterns of interactions among a set of smaller-scale processes. We can call these *composite* causal processes. 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.²⁸

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).²⁹ And while he describes how different theoretical concerns lead us to utilize a variety of analytical 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

²⁸ 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.

²⁹ 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).”

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.³⁰ 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.

While there are certainly many more details that can be debated, we now have ontological elements that correspond to the systems we are interested in. Electrons and nuclei represent elementary causal processes whose interactions form composites: atoms and molecules. This framework will aid our discussion of how RQM can address the explanatory gap in the relationship between QM and molecular structure.

Converging Perspectives on Molecular Composition and Structure

Recalling the discussion of the Wigner's friend scenario, we know that every interaction per RQM can be viewed from two perspectives. The internal perspective is that of the participating systems themselves. The interaction is a measurement-like event, revealing definite values for quantities such as spatial position or spin. Using our ontology, the two systems are causal processes participating in a causal event: a mutual manifestation of their relative dispositions to interact. From the external perspective, the same event, according to the quantum description, is represented as giving rise to entanglement. There is now a composite system that continues to evolve according to the Schrödinger equation. Its wave function, per RQM, is defined relative to an external reference system. This wave function would only collapse if the external system subsequently interacts with the composite, thereby becoming a direct participant. From the

³⁰ 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.

ontological framework, the wave function of the propagating composite process represents its dispositions toward such possible further interactions.

Quantum descriptions of systems (i.e. wave functions and Schrödinger equations) always represent the external perspective on a system. If we infer that these systems are involved in various (unobserved) interactions, then we can use extensions of QM to construct models of these more complex entanglements, using tools such as the decoherence framework. But RQM tells us that all of these interactions have an internal perspective as well, featuring measurement-like events, and this is something we need to hold in mind as we consider the case of atoms and molecules.

A quantum model of the atom incorporates the constituent electrons and nuclei and relevant forces among them (of course, a more realistic account would also acknowledge interactions with outside systems). Drawing on our ontology, the atom is a composite causal process. As such, it is composed via a pattern of repeated interactions among its sub-processes. But now it is clear we lose something important if we only acknowledge the external perspective. If we infer what is happening from the internal perspective of the constituents, we can envision the presence of ongoing, discrete measurement-like interaction events across time. Like any interaction events viewed from the perspective of direct participants, these would feature manifestation of definite outcomes. If we assume that at least some of these ongoing events involve position localization, then this inferred internal perspective is characterized by a pattern of spatial manifestations of the subatomic particles.³¹

When atoms, in turn, manifest certain dispositions to form a new, larger, composite—a molecule—they enter into a new pattern of interactions involving the combined atomic nuclei/electrons. In realistic environments, the evolution of this pattern is undoubtedly influenced by incessant interactions with outside systems as well. While inaccessible from the external

³¹ Unlike some interpretations, RQM does not stipulate a preferred basis. If a basis is not defined by an experimental context or otherwise favored by environmental factors, then it may be unclear for a given interaction what basis will prevail. The assumption in the discussion is that we can infer there are a great many ongoing interactions among microscopic systems happening from the internal perspective, and at least some of these correspond to the position basis.

perspective, there is again an internal perspective (or collection of perspectives) on these systems that involves ongoing patterns of discrete realization outcomes, including localization events.³² If the interaction pattern of constituents is responsible for composing a particular molecule (as our ontology envisions), then we would expect the localization events associated with the pattern to trace out its characteristic molecular structure in space. When we do directly interact with molecular systems, then we, of course, encounter them as entities that are spatially organized—the internal and external perspectives converge.

Before continuing, it is instructive to compare this conception of spatial localizations to some interpretations of atomic and molecular electron density (usually labeled ρ) that have been offered. 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 (equivalently, the product of the wave function and its complex conjugate). This idea can be extended to a multi-particle atom or molecule: one can derive from the electronic wave function the probability of finding any of the N electrons at a particular location. The density ρ is a function that assigns this expected number of electrons to points in 3D space.³³

In addition to being defined as the expectation value for probabilistically predicting the location of electrons upon measurement, 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.

³² When atoms form a molecule, the new compositional interaction 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. The latter 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.

³³ For the derivation of ρ and related discussion, see Veszprémi and Fehér (1999), pp. 173-4.

Also, 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 can be derived directly from ρ .³⁴ Another research program based on electron density is the quantum theory of atoms in molecules (QTAIM), developed by R.F.W. Bader and others.³⁵ 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.

The usefulness of electron density in these research contexts may seem surprising if we only think of it as fulfilling its statistical predictive role. 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.³⁶ 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.³⁷ For our purposes, the most interesting

³⁴ 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 (Hohenberg-Kohn theorems).

³⁵ Bader (1990); Gillespie and Popelier (2001, Chs.6-7) provides an introduction.

³⁶ 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 .

³⁷ 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

suggestion proposes that electrons briefly occupy (even in the absence of measurement) a succession of positions in 3D space that, upon time-averaging, fill out a pattern equivalent to the density.³⁸

The present proposal is interesting to compare to this notion, in that it also infers the existence of localization events—in this case they accompany the interactions that compose an atom or molecule viewed from RQM’s internal perspective. Upon a closer look, however, this is a superficial similarity, and the electron density cannot be taken to be a (time-extended) representation of these events in the RQM-based account. First, it is worth recalling that the usual calculation of ρ derives from wave functions that use the Born-Oppenheimer approximation, so this doesn’t properly address the context of molecular composition. But more importantly, the wave function, per RQM, models the system from the external perspective. Therefore, the ρ derived from this wave function does as well, and should continue to be interpreted in its traditional predictive role. It also should also be emphasized that positing the presence of localization events, while important for explaining structure, needs to be justified by a larger interpretative account of a molecule. In the present proposal, localization is something that accompanies the pattern of interacting constituents/sub-processes that is responsible for molecular composition. In addition to the interaction events themselves, this pattern also includes the dispositions of the propagating subprocesses between interactions. The entire pattern endows the molecule, as a composite causal process, with its own dispositions to interact (corresponding to its physical and chemical properties).

Returning to our main discussion, the goal is to offer an interpretation of QM that goes further than others in addressing the problems of molecular structure. The challenge exists because, while any interpretation that solves the measurement problem offers a story that links the QM formalism to the existence of (at least apparent) spatial locations, molecules represent a

method can be interpreted to reflect classical electrostatics involving the interaction between the electron density and the nuclei.

³⁸ 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. See Sebens (2021) for discussion of other interpretive possibilities for charge density, including some in the context of Bohmian mechanics, Everett-style interpretations, and spontaneous collapse theories.

particularly challenging case. As discussed, QM models of molecules would need to include much more realistic descriptions of internal and external interactions to provide an adequate representation that doesn't rely on the Born-Oppenheimer approximation. Given the absence of such models at present, there continues to be room for skepticism that interpretations offered to solve the measurement problem really address the specific case of molecular structure. Arguably, these interpretations offer little more than a consistency check by allowing that familiar molecular structures are possibilities.

The present interpretation does better, because it offers an account of how complex composite systems are generally formed and why this activity is naturally accompanied by spatial structure. While the discussion of composition and structure from so-called internal perspectives is unavoidably informal and qualitative, it offers a complementary and intuitive picture to accompany the development of more realistic quantum physical models of these systems. These internal and external perspectives on systems co-exist in one world, and therefore will conform to one another.

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. The interpretation depends on a particular account of causal composition, and this is extended to the microscopic domain, where it posits a role for frequent measurement-like interactions in the formation and maintenance of relatively stable atomic and molecular systems. However, there are reasons to think the framework is reasonable. The account of composition follows a well-known approach to analyzing complex systems. At the same time, one of the distinctive features of RQM is its even-handed treatment of all physical systems. Compared to some interpretations, it undermines presumptions of sharp discontinuities in nature between the macroscopic and microscopic realms. This clears the way toward offering a unified view of how patterns of interaction, featuring spatial localization, form composites 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) can 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.

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