

# The Problem of Molecular Structure Just Is The Measurement Problem

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## Abstract

Whether or not quantum physics can account for molecular structure is a matter of considerable controversy. Three of the problems raised in this regard are the problems of molecular structure. We argue that these problems are just special cases of the measurement problem of quantum mechanics: insofar as the measurement problem is solved, the problems of molecular structure are resolved as well. In addition, we explore one consequence of our argument: that claims about the reduction or emergence of molecular structure cannot be settled independently of the choice of a particular resolution to the measurement problem. Specifically, we consider how three standard putative solutions to the measurement problem inform our understanding of a molecule in isolation, as well as of chemistry's relation to quantum physics.

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## **1 Introduction**

Molecular structure is central to chemistry; identifying the structure of a molecule is often required for the explanation of chemical, physical, and biological phenomena. Philosophers who are interested in understanding the relation of chemistry to quantum physics have examined in detail whether and how successfully quantum mechanics describes molecular structure.<sup>1</sup>

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<sup>1</sup>In particular, questions about molecular structure have attracted considerable attention in the philosophy of chemistry. This may be explained by the fact that the relation of

Three problems have been raised, all of which cast doubt on the capacity of quantum physics to determine molecular structure: we call these ‘problems of molecular structure’.<sup>2</sup> The first problem is standardly referred to as Hund’s paradox; it concerns the quantum mechanical explanation of handedness (chirality) of enantiomers. The second problem concerns the failure of resultant Hamiltonians to determine the structure of isomers. The third problem is the most general and concerns symmetry breaking for molecules with observed asymmetric structures.

We argue that all three problems are special cases of the measurement problem of quantum mechanics. Therefore, insofar as the measurement problem is solved, these three problems of molecular structure are resolved as well.

Importantly, this implies that any philosophical claim about molecular structure is at least contingent on, if not determined by, the choice of a particular resolution to the measurement problem. In fact, we argue that under certain interpretations of quantum mechanics, isolated molecules lack determinate structure.

Note that we do not purport to solve all the problems that are raised in the literature with respect to chemistry’s relation to quantum physics. Nor do we provide a complete defence of the reducibility of chemistry. However, the problems of molecular structure have been central in the investigation of chemistry’s relation to quantum physics and are often invoked against the reduction of chemistry. Therefore, by arguing that these problems are special cases of the measurement problem, we offer a new way to address relevant anti-reductionist worries.

On a more general note, we agree with Lombardi and Castagnino ([2010]) that foundational problems in quantum mechanics are often overlooked in the philosophy of chemistry. In this spirit, we examine how the measurement problem informs one’s understanding of molecular structure and of chemistry’s relation to quantum physics.

In section 2 we present the problems of molecular structure together

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chemistry with quantum physics has been viewed as the cornerstone for establishing the philosophy of chemistry as an independent discipline within philosophy of science (for an overview see for example (Baird et al. [2011]) and (Scerri [2008])).

<sup>2</sup>While there are other related issues in the literature (for example Chang [2015] and González et al. [2019]), these three seem to us to be the most problematic, and are the only ones that will be discussed here.

with the responses to these problems in the current literature. In section 3 we present Maudlin's ([1995]) trilemma as a way of expressing the measurement problem of quantum mechanics, and show how each of the problems of molecular structure satisfy each lemma, thus allowing the inconsistency to be derived in the same way as in Maudlin's original version. In section 4 we argue that three of the most discussed putative solutions to the measurement problem (namely the Everett interpretation, de Broglie-Bohm theory, and spontaneous collapse theories) resolve the problems of molecular structure. In this section we also consider how each solution to the measurement problem informs our understanding of the structure of isolated molecules, and of chemistry's relation to quantum physics.

## 2 The Problems of Molecular Structure

Three apparently distinct features of the quantum mechanical description of molecular structure have been regarded as posing problems for the relation between chemistry and quantum physics. In this section we present these problems as well as the existing putative solutions to them.

Before doing so, it is crucial to define molecular structure. Standardly, molecular structure refers to the spatial arrangement of the atoms that constitute a molecule.<sup>3</sup> It is a collective term in the sense that it is identified by specifying a number of different properties, such as the types and number of chemical bonds, the angles and lengths of chemical bonds, dipole moment and chirality.

While one might fruitfully engage with the question of which set of properties are required for a complete specification of molecular structure, we do not have space to address that question. The three problems examined here are more fundamental: can quantum mechanics determine any of the properties that are invoked in the specification of molecular structure?

Each problem of molecular structure concerns distinct but overlapping sets of molecules. Hund's paradox is the most specific problem in that it only concerns chiral molecules. The problem of resultant Hamiltonians concerns isomers (that is chiral and non-chiral isomers), though the problem may generalise to other kinds of molecules. Lastly, the problem of symmetry breaking is the most general, and concerns any molecule that

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<sup>3</sup>This is also referred to as the shape or geometry of a molecule.

has been observed with a non-symmetric structure even though its *ab initio* Hamiltonian is symmetric.

Note that the current literature is not very clear about whether and how closely these problems are related. On the one hand, the literature standardly distinguishes them; as can be seen from the relevant references, the discussion of these problems does not usually overlap. However, it is also the case that when one of the three problems is examined, then one of the two other problems is often discussed (see for example Woolley [1988], pp. 58-72; Sutcliffe and Woolley [2012], p. 416; Fortin et al. [2016]). By considering all three together and by arguing that each is just a special case of the measurement problem, we offer a clear and novel account of the relations between these three problems. We go on to assess the previously unacknowledged implications of the identification of these problems for the ontology of chemistry.

One possible diagnosis for the failure explicitly to identify such problems as special cases of the measurement problem is that they are presented in different ways, using different technical and conceptual languages. This is also partly responsible for the small overlap between the literatures on philosophy of chemistry and philosophy of physics.<sup>4</sup> It's our hope that our work will help to remedy this unfortunate lack of communication.

Lastly, we should stress that our analysis of the problems of molecular structure by no means exhausts the discussion of how chemistry relates to quantum physics, nor does it settle all aspects of the debate about reduction and emergence in chemistry. Related problems which we do not discuss include, for example, those raised in (Chang [2015]; González et al. [2019]) who argue that assuming fixed nuclear positions in the quantum mechanical description of molecules is problematic for reduction because it contravenes Heisenberg's uncertainty principle. While we believe that such issues are likely addressed by considering putative solutions to the measurement problem, we believe that such discussion is best left to a separate paper. In any case, even though our account does not establish reductionism for chemistry, we demonstrate that a significant set of hurdles to reductionism can be overcome.

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<sup>4</sup>Note that Fortin et al. ([2017, 2018]) do relate these problems by examining how some of the problems of molecular structure are resolved by, respectively, Bohmian mechanics and the Modal Hamiltonian Interpretation.

## 2.1 Enantiomers and Hund's Paradox

Friedrich Hund ([1927]) formulated a paradox concerning chiral molecules.<sup>5</sup> A molecule is chiral when it has the geometric property of not being superimposable on its mirror image (IUPAC [2014], p. 269). The term 'enantiomer' refers to each molecule of any pair of chiral molecules (also referred to as the right- and left-handed enantiomers, or optical isomers).

The paradox stems from the fact that a chiral molecule is always observed as either right-handed or left-handed despite the fact that, according to the quantum mechanical description of an isolated chiral molecule:

- i. the two enantiomeric structures are not energy eigenstates of the symmetric resultant Hamiltonian (Bahrami and Shafiee [2011a], p. 1); and instead,
- ii. the molecule's energy ground state corresponds to the symmetric superposition of the two enantiomeric structures (Trost and Hornberger [2009], p. 1).

On the assumption that molecules can be successfully described using quantum mechanics, and that the quantum mechanical analysis should, thus, predict the observed molecular structure, Hund's paradox is that molecules with definite chirality are observed while the quantum mechanical description is chirally symmetric.

In more detail, the paradox is formulated in the context of a model of the chirality of an isolated molecule where the two observed states are represented as follows:

$|L\rangle$  represents the state of the molecule that corresponds to the left-handed enantiomer

$|R\rangle$  represents the state of the molecule that corresponds to the right-handed enantiomer

Each state is related to a wavefunction which is effectively localised in one of the two wells (see figure 1). These states have definite chirality, do not have definite parity, and are degenerate in energy (Berlin et al. [1996], p.

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<sup>5</sup>See (Berlin et al. [1996]; Trost and Hornberger [2009]; Bahrami and Shafiee [2011a]; Bahrami and Shafiee [2011b]; Bahrami et al. [2012]; Fortin et al. [2018]).

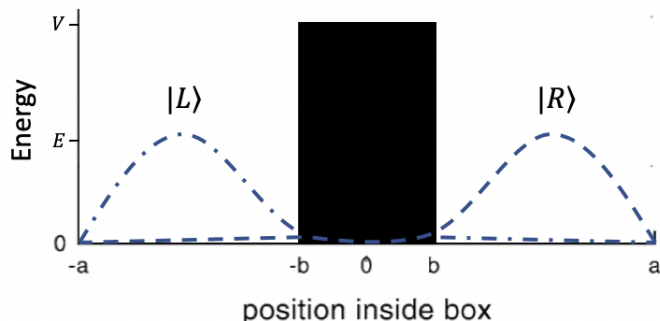


Figure 1: The model of an isolated chiral molecule in terms of a one-dimensional symmetrical double-well system. The barrier of height  $V$  is between  $b$  and  $-b$ . The two enantiomers are described by the  $|L\rangle$  and  $|R\rangle$  states of the molecular system. They have the same energy  $E$  and are not in energy eigenstates due to quantum tunnelling.

333). However, they are not energy eigenstates of the system because, for a finite barrier, their respective wavefunctions overlap.<sup>6</sup> Due to this overlap, the energy eigenstates of the molecule are symmetric and antisymmetric combinations of the two chiral states, namely;

$$|+\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle) \quad (1)$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|L\rangle - |R\rangle) \quad (2)$$

State  $|+\rangle$  corresponds to the energetic ground state of the molecule, whereas state  $|-\rangle$  is its first energetic excited state (Fischer and Mittelstaedt [1990], p. 412). The ground state  $|+\rangle$  does not have definite chirality; instead it corresponds to the symmetric superposition of the right- and left-handed molecules. By contrast, chiral molecules are always observed to have definite chirality; that is, they are found either in  $|L\rangle$  or  $|R\rangle$ . This is the paradox.

Various responses to Hund's Paradox have been proposed. First, Hund explained the observation of one enantiomer, instead of a superposition of two enantiomeric structures, by the 'possibly very long tunnelling time from a left-handed configuration state  $|L\rangle$  to a right-handed one  $|R\rangle$ ' (Trost

<sup>6</sup>This is also specified by stating that the two wavefunctions are quasi-localised in each of the respective wells (Fischer and Mittelstaedt [1990], p. 413).

and Hornberger [2009], p. 1). Other accounts suggest that environmental decoherence resolves the paradox and specify which particular structure a chiral molecule will take under particular environmental conditions (for example Trost and Hornberger [2009] and Bahrami et al. [2012]).<sup>7</sup>

A specific interpretation of quantum mechanics has also been claimed to resolve the paradox; namely the Modal Hamiltonian Interpretation (MHI) (Fortin et al. [2016; 2018]). Lastly, it has been claimed that the ‘correct’ ground state of an isolated chiral molecule is not of definite parity because there is a ‘small parity-violating energy shift’ to one of the two enantiomers which, if taken into account, results in a ground state corresponding to an ‘unequal’ superposition of the two chiral states (MacDermott and Hegstrom [2004], pp. 56-57; see also Bahrami and Shafiee [2011a;2011b]). In this context, if one takes into account environmental effects, this different ground state purportedly explains the empirical identification of a molecule’s chiral structure in a way that is consistent with its quantum mechanical description.<sup>8</sup>

## 2.2 Isomers and the Inability of Resultant Hamiltonians to Determine Molecular Structure

Chemists and philosophers have drawn attention to the fact that quantum mechanics describes molecular structure by employing the so-called configurational Hamiltonian for the solution of the molecular Schrödinger equation.<sup>9</sup> Configurational Hamiltonians are defined in contrast to resultant Hamiltonians. A Hamiltonian is called resultant when it takes into account all and only the physical properties of the entities that comprise the molecule, down to the level of nuclei and electrons (Hendry [2010a], pp. 210-211). On the other hand, configurational Hamiltonians impose certain

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<sup>7</sup>Different kinds of environmental effects have been examined in the literature, such as the effect of interactions with phonons of optically inactive solids below a particular temperature (Berlin et al. [1996], p. 1), the effect of intermolecular interactions and blackbody radiation (Bahrami et al. [2012]), and the effect of collisions with a background gas (Trost and Hornberger [2009]; Bahrami and Shafiee [2011b]).

<sup>8</sup>This putative solution to Hund’s paradox will not work because even if there is an ‘unequal’ superposition of the two chiral states, the ground state would still correspond to a superposition.

<sup>9</sup>See (Woolley and Sutcliffe [1977]), (Woolley [1978]), (Woolley [1998]), (Bishop and Atmanspacher [2006]), (Hendry [2006]), (Hendry [2010a]), (Hendry [2010b]), (Scerri [2011]), (Sutcliffe and Woolley [2012]), (Primas [2013]), (Hendry [2017]), (Hetteema [2017]). To avoid confusion, we use Hendry’s terminology to present the problem.



restrictions on the behaviour of these particles, by registering structural information from chemistry.

There are two main questions that can be raised with respect to the shift from resultant to configurational Hamiltonians. First, there is the issue of how the description provided by the resultant Hamiltonian relates to our observations of molecular structure (we call this the in-principle problem). Why does the resultant Hamiltonian not determine the observed structure of particular molecules? Are there in-principle reasons for the resultant Hamiltonian's inability to determine molecular structure? Secondly, there is the issue of how one shifts from resultant to configurational Hamiltonians (we call this the in-practice problem). What sort of assumptions and approximations are made when employing configurational Hamiltonians? How are these assumptions justified? An answer to the former set of questions explains why one raises the latter: the inability of resultant Hamiltonians to determine structure in a way consonant to observations leads to the use of configurational Hamiltonians. Nevertheless, an answer to the former does not suffice to provide a complete answer to the latter. That is, explaining the inability of resultant Hamiltonians to determine structure does not fully account for the nature and justification of the assumptions made during the construction of configurational Hamiltonians.

Unfortunately, the literature does not distinguish between these two sets of questions. By separating these questions and offering a response to the in-principle questions, we provide a clear and novel way of understanding the overall problem with resultant and configurational Hamiltonians. We argue that the apparent in-principle inability of resultant Hamiltonians to determine observed structure is a special case of the measurement problem, and that it is resolved by putative resolutions of the measurement problem. Therefore, our proposal greatly impacts how one understands the shift from resultant to configurational Hamiltonians. Nevertheless, it does not offer a complete answer to the entire problem as we do not address the in-practice issues (see for example Seifert [2020]).

Let us explain the in-principle problem by means of an example.<sup>10</sup> In a putative bottom-up derivation one is expected to start with a collection of nuclei and electrons, which may be represented by the chemical formula  $C_8H_8$ . Our endpoint is the observed molecular structure of ethenylbenzene (also known as styrene), which is represented as  $C_6H_5CH=CH_2$ . The question is how we get from an unstructured collection of nuclei and electrons

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<sup>10</sup>This example is also discussed in (Woolley [1988]).

to a given molecule with a particular arrangement of individual atoms.

Identifying styrene's structure is particularly important as there are other ways in which the same number and type of atoms can be connected that result in different molecular structures and thus distinct molecules (such as cubane, xylylene, and barrelene). Describing styrene quantum mechanically requires identifying the wavefunctions that represent the states of styrene. To identify them, one solves the time-independent non-relativistic Schrödinger equation (henceforth Schrödinger equation). In general, the Schrödinger equation for an isolated molecule provides an infinite number of solutions (that is, wavefunctions) each of which corresponds to different stationary states of the molecule. An isolated molecule in its ground state is represented by the wavefunction that has the minimum total energy.

As noted above, the resultant Hamiltonian operator should include all the factors that determine the energy of the molecule.<sup>11</sup> However, because of the mathematical complexity involved in employing the resultant Hamiltonian, molecules are usually examined within the framework of the Born-Oppenheimer approximation (henceforth BO approximation).<sup>12</sup> The BO approximation is a '[r]epresentation of the complete wavefunction as a product of an electronic and a nuclear part  $\psi(r, R) = \psi_e(r, R)\psi_N(R)$ ' (IUPAC [2014], p. 179). The BO approximation is also referred to as the adiabatic approximation, and its validity is 'founded on the fact that the ratio of electronic to nuclear mass [...] is sufficiently small and the nuclei, as compared to the rapidly moving electrons, appear to be fixed' (ibid.). Peter Atkins explains the importance of the BO approximation to the quantum mechanical description of a molecule:

The practical effect of the approximation is that it is possible to simplify both the discussion and the calculation of molecular electronic structures. Instead of having to treat all the particles in the molecule on an equal footing, it is possible, according to the approximation, to set the nuclei into a frozen conformation, and then to calculate the electronic energy and distribution cor-

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<sup>11</sup>Note that the resultant Hamiltonian disregards, among other things, the effects of the weak and strong force on the behaviour of a molecule's particles. This aspect of the resultant Hamiltonian is not taken into account in any of the existing formulations of the problem so it is disregarded here as well.

<sup>12</sup>The resultant Hamiltonian has been employed only for small systems, like the hydrogen atom (Hendry [2010a], p. 212).

responding to it. (Atkins [1974], p. 29)

After applying the BO approximation one can, in principle, formulate quantum descriptions for all the possible fixed positions of the nuclei. Each assignment of positions to nuclei corresponds to different quantum states of the system and, in general, to different values of the total energy,  $E$ , of the molecule. However, in practice this process is not followed. By having prior knowledge of the system that is under examination (in this case, by knowing the chemical and structural properties of styrene) only particular configurations are considered when constructing the Hamiltonian operator in order to identify the molecule's ground state. This method of constructing the Hamiltonian, which involves assuming that nuclei hold fixed and specific positions, corresponds to identifying the so-called configurational Hamiltonian.<sup>13</sup>

The problem with the transition from the resultant to the configurational Hamiltonian is that molecular structure cannot be identified unless one first applies the BO approximation; this is taken as evidence that the resultant Hamiltonian does not determine the molecule's structure. As (Hendry [2006], p. 185) states, a quantum mechanical explanation of molecular structure 'is conditioned on determinate nuclear positions'. In the case of styrene, for example, one cannot identify its structure by taking into account all and only the physical interactions of the particles that comprise styrene. In addition, one needs to assume that the nuclei are fixed in space in a particular configuration.

The choice of styrene for the presentation of this problem is not arbitrary. Styrene is an isomer and it is in virtue of being an isomer that the inability of resultant Hamiltonians to determine molecular structure is particularly stark (see Woolley [1998], p. 11; Hendry [2010a], p. 213).<sup>14</sup> Isomers are sets of molecules which have the same number and types of atoms but whose atoms are connected differently in each molecule.<sup>15</sup> As such, distinct isomers are described by the same resultant Hamiltonian, and thus

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<sup>13</sup>Applying the BO approximation is most often not sufficient for the solution of the Schrödinger equation. In addition, different computational methods are employed which involve making additional assumptions (see for example the Valence Bond and Molecular Orbital Approaches.)

<sup>14</sup>For example, Hendry explains this problem by invoking as an example the case of ethanol and methoxymethane which are distinct isomers with the same chemical formula (Hendry [2010a], p. 214).

<sup>15</sup>Note that chiral molecules (namely the type of molecules that have been the center of concern in Hund's paradox; see 2.1) are considered as a particular type of isomers. That

the Schrödinger equation has the same form. It is not possible to use the resultant Hamiltonian to distinguish molecules which only differ in terms of their isomerism; including styrene from cubane, xylylene and other distinct molecules which are composed of 8 carbon atoms and 8 hydrogen atoms:

If all molecules were described by the ground state of their associated Hamiltonian with full symmetry, no such isomers would exist as distinct species, since they would simply correspond to equally probable nuclear configurations of the same 'complete' eigenstate. (Claverie and Diner [1980], p. 59)

One way to understand this observation is that the ground state wavefunction of the resultant Hamiltonian corresponds to a superposition of all the different isomers. On the other hand, only individual isomers are directly observed.

The problem just outlined has been invoked in support of various epistemic and metaphysical views about the nature of molecular structure, as well as about the relation between chemistry and quantum mechanics. Specifically, the problem has been interpreted as an instance of the failure of the Nagelian reduction of chemistry to quantum mechanics, as well as of reductive and non-reductive physicalism.<sup>16</sup> This problem is also taken to support various forms of emergence (for example Bishop and Atmanspacher [2006] and Hendry [2010a]). Hendry argues that the resultant Hamiltonian is, in principle, unable to describe the structure of the system because molecular structure strongly emerges from quantum mechanics.

A potential reductionist, however, might argue that the problem can be explained by the epistemic difficulties involved in solving the Schrödinger equation with the resultant Hamiltonian. In this context, the use of configurational Hamiltonians is justified on the grounds that it 'makes only a small difference to the calculated energy of the molecule' (Hendry [2010a], p. 213).<sup>17</sup> Furthermore, Scerri ([2011], p. 25) argues that this situation is an

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is, all chiral molecules are isomers but not all isomers are chiral. There are other types of isomers such as diastereomers and constitutional isomers.

<sup>16</sup>Nagelian reduction requires the derivation or deduction of chemistry from quantum mechanics. While there are different accounts of physicalism in the philosophy of science, physicalism (whether reductive or non-reductive) is broadly understood here as the 'ontological position according to which the physical facts determine all the facts' (Hendry [1999], p. 118).

<sup>17</sup>This position is rejected by Hendry [2006], pp. 183-184 who refers to it as the 'proxy

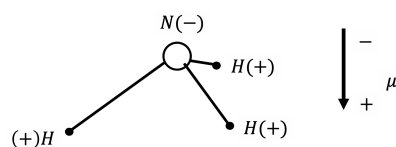
instance of the ‘problem of the collapse of the wavefunction’ which can be resolved by appeal to decoherence. Given this, he argues that the problem does not have any implications on one’s metaphysical views about chemistry’s relation to quantum mechanics or about molecular structure, since the symmetry breaking that occurs by employing the BO approximation is a ‘theoretical rather than an ontological issue’.<sup>18</sup> Lastly, Primas ([2013]) argues that the use of configurational Hamiltonians is explained by the putative fact that quantum mechanics is incomplete or false.

### 2.3 Symmetry Breaking

In the previous two subsections we considered problems which are standardly considered in the philosophy of chemistry literature. In both cases, the problem involved a difference between the molecular structure that could be derived from quantum physics, and the structure observed in experiments. The subject matter of this section can be similarly characterised but is less often considered as a ‘problem of molecular structure’. Nonetheless we include it because, as we will argue, it bears a strong analogy to the problems outlined above, and it may likewise be understood as an instance of the measurement problem.

The issue is most famously raised by Anderson ([1972], p. 394):

The chemists will tell you that ammonia ‘is’ a triangular pyramid



with the nitrogen negatively charged and the hydrogens positively charged, so that it has an electric dipole moment ( $\mu$ ), negative toward the apex of the pyramid [...] no stationary state of a system (that is, one which does not change in time)

defence’ of reduction (see also Hettema [2017], p. 54).

<sup>18</sup>We agree with Scerri that the problem comes down to the measurement problem, however we disagree that decoherence resolves this (see Bacciagaluppi [2016]), and that this renders the problem merely a theoretical one – different candidate resolutions of the measurement problem imply radically different ontologies; see section 4.

has an electric dipole moment. If ammonia starts out from the above unsymmetrical state, it will not stay in it very long. By means of quantum mechanical tunneling, the nitrogen can leak through the triangle of hydrogens to the other side [...] A truly stationary state can only be an equal superposition of the unsymmetrical pyramid and its inverse.

The issue explored by Anderson is that quantum mechanics predicts that molecules should have certain symmetry properties, which the molecules are observed to violate. In the particular example raised, Anderson asks how it is that ammonia exhibits an electric dipole, with a preferred direction, when the quantum mechanical description is rotationally symmetric – a description with no preferred direction and no dipole moment.

A notable feature of this case is that the prediction and observation of tunnelling between the two orientations requires that we take the symmetric superposition state seriously as a representative of the quantum system. However, any particular observation is always of an asymmetric system with a particular orientation. As such, the problem of mismatch between the two descriptions is especially compelling in this context.

Interestingly, the problem of symmetry breaking has also been examined in the context of resultant Hamiltonians' inability to determine molecular structure. Specifically, Hendry, Sutcliffe and Woolley argue that the problem of correctly determining molecular structure via resultant Hamiltonians extends to molecules which are not isomers but exhibit non-symmetric structure (Hendry [2010b], p. 186; Sutcliffe and Woolley [2012], p. 409). This is the case for example with hydrogen chloride which exhibits a non-symmetric structure due to its non-zero net electric dipole moment (Hendry [2010a], p. 213).<sup>19</sup> Similarly to the quantum mechanical description of isomers, the resultant Hamiltonian will not describe molecules with asymmetric structure. This is because it predicts that the net dipole moment of hydrogen chloride is zero which, in turn, is explained by the fact that 'arbitrary solutions to the Coulombic Schrödinger equations should be spherically symmetrical' (Hendry [2010a], p. 213).<sup>20</sup> However, such asymmetries play an important role in specifying molecular structure and chem-

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<sup>19</sup>Electric dipole moment is 'a quantitative measure of the degree of charge separation in a molecule' (Ebbing and Gammon [2010], p. 384). It is often invoked for specifying molecular structure and a molecule's chemical behaviour (such as its reactivity).

<sup>20</sup>Hendry defines 'Coulombic Schrödinger equations' as those equations which employ resultant Hamiltonians.

ical behaviour. Therefore, one inserts information regarding such asymmetries into the configurational Hamiltonian in order to construct an accurate description of asymmetric molecules.

Note that Anderson's account of symmetry breaking is hardly mentioned in the literature on the problems considered in sections 2.1-2.2 above, though a notable exception is Claverie and Diner ([1980]). This is surprising not only because the examples invoked by both problems are almost identical, but because Anderson's paper is widely known and cited in the philosophy of emergence. As a consequence, the standard way of setting up this problem, which we follow here, involves considerations of symmetry breaking rather than the Hamiltonians employed by chemists.

Specifically, in the recent philosophy literature Margaret Morrison argues that symmetry breaking is incompatible with reduction:

symmetry breaking [...] provides the dynamical explanation of emergent phenomena, but the specific microphysical details are irrelevant; how the symmetry is broken is not part of the account. In that sense the emergent phenomenon is not reducible to its microphysical constituents, yet both retain full physical status. (Morrison [2012], p. 156)

Morrison further claims that symmetry breaking imposes a top-down order on the world and that no bottom-up mechanism for symmetry breaking is provided. As such, her response to Anderson's argument would be to claim that the net electric dipole moment of ammonia is not given by any quantum mechanical story; instead, the symmetry breaking acts as a top-down constraint on the molecule.<sup>21</sup>

James Fraser ([2016]) outlines two different categories of response to arguments of this form: first, one might consider the symmetry to be hidden rather than broken – Fraser argues that certain systems may be such that they exhibit an overall symmetry, but for finite time periods are found in one or other asymmetric state; second, the symmetry may be broken by an asymmetric perturbation. Both these options may undermine Morrison's arguments. Which option applies to Anderson's example?

In fact, the categories of Fraser's taxonomy each refers to different cases discussed by Anderson. Given that the ammonia molecule has a rela-

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<sup>21</sup>This argument has a lot in common with claims due to Hendry ([2010a]).

tively high inversion frequency, the symmetry breaking falls under Fraser's first category. On sufficiently long timescales the molecule seems to retain the underlying symmetry because we have an equal chance of finding its dipole oriented in either direction. Importantly, however, this observation does not solve the more general worry concerning why ammonia molecules have a dipole moment at all when quantum mechanics predicts that it should be found in a symmetric superposition of its inversions with no consequent dipole. That is, a mechanism for symmetry breaking has not yet been offered. This point is developed in the next section where we claim that this problem is a special case of the measurement problem.

In certain other cases mentioned by Anderson, observed asymmetries are the consequences of asymmetric perturbations, as in Fraser's second category. Specifically, this concerns the example with sugar (Anderson [1972], p. 394): 'Every sugar molecule made by a living organism is spiral in the same sense, and they never invert, either by quantum mechanical tunneling or even under thermal agitation at normal temperature [...] If, on the other hand, we synthesize our sugar molecules by a chemical reaction more or less in thermal equilibrium, we will find that there are not, on the average, more left- or right-handed ones or vice versa.'

This difference between biologically produced sugar and artificially synthesized sugar suggests that not all asymmetry in molecular configurations is the product of quantum mechanical symmetry breaking. Unlike with the case of ammonia, the uniformity among biologically produced sugar is presumably the consequence of some asymmetry in biological sugar production mechanisms.<sup>22</sup>

The distinction between the two categories of symmetry breaking is important for our ends. It is not the case that all discovered molecular symmetry breaking finds its source in the measurement problem. However, as we argue in the next section, a significant class of molecular symmetry breaking is, nonetheless, ascribed to whatever physical goings-on lead to the resolution of the measurement problem.

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<sup>22</sup>Such mechanisms would account for the inapplicability of the symmetric resultant Hamiltonian without any resort to the measurement problem.



### 3 The Measurement Problem

In this section, we'll present the measurement problem of quantum mechanics in terms of Maudlin's trilemma. We'll then show how each of the problems of molecular structure falls foul of the trilemma. As such, we claim, the problems of molecular structure just are special cases of the measurement problem. In the next section, we'll demonstrate that three mainstream resolutions of the measurement problem also resolve the problems of molecular structure. Therefore, in this section and the next we demonstrate both that the problems of molecular structure have the same form and that they have the same array of putative resolutions as the measurement problem.

One of the most influential presentations of the measurement problem is found in (Maudlin [1995]) where the measurement problem is called 'the problem of outcomes'. Following this formulation, the measurement problem amounts to the incompatibility of the following statements:

- 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 [time-dependent] Schrödinger equation).
- 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], p. 7)

The inconsistency of this trilemma is a consequence of the linearity of the Schrödinger equation, which implies that any sum of solutions is itself a solution. This fact underlies the superposition principle – that sums of states are also candidate physical states. No less important is the fact that superpositions in the basis of observable quantities play a crucial role in explaining the results of interference.

So, quantum mechanics tells us that physical systems are sometimes well described by superposition states in the basis corresponding to some

observable quantities. The completeness of 1.A, together with the linearity of its time evolution in 1.B imply that in such circumstances where the system starts out in a superposition in a measurement basis, the measurement devices will end up in a superposition state too. This is then in conflict with 1.C, as a superposition of determinate outcomes is incompatible with unique determinate outcomes.

We will demonstrate that each of the problems of molecular structure satisfy 1.A-1.C. In effect, all show that one cannot simultaneously hold with the orthodoxy of quantum mechanics, to which 1.A and 1.B refer, while accepting 1.C, that measurements in chemistry reveal determinate properties of one kind or another. This illustrates that the problems of molecular structure just are instances of the measurement problem.

It's important to make a terminological observation at this stage: while the debate in the foundations of chemistry literature has often been phrased in terms of Hamiltonians, the foundations of physics literature discussion of the measurement problem standardly refers to the quantum state (or wavefunction). Nonetheless, there's a straightforward relation between the two: if a system is well described by an asymmetric quantum state, then a Hamiltonian that has the corresponding symmetries cannot be the source of the asymmetry, and, consequently, such asymmetry must come from elsewhere. Hamiltonians and quantum states are used in different ways: for example, Hamiltonians represent the structure of the potential, whereas quantum states, at least in principle, represent all the properties a given system may have.

### 3.1 Enantiomers and Hund's Paradox

Hund's paradox brings out the inconsistency between statements 1.A to 1.C when those statements are applied to the quantum mechanical description of enantiomers. Specifically, in the case of enantiomers, statement 1.A tells us to accept the basic quantum mechanical picture – that the most stable state of chiral molecules generically corresponds to a superposition of right- and left-handed structures, rather than just to one or the other. Statement 1.B is straightforwardly satisfied: a state described by quantum mechanics, unless there is some dynamical modification, will evolve according to the time dependent Schrödinger equation. No-one has suggested a different dynamics for molecules outside discussions of the measurement problem! Statement 1.C is then the fact that only a left-handed or right-

handed structure of the examined molecule is observed.

This case is then just an instance of the measurement problem as there is good reason to accept all three claims and yet they are mutually inconsistent. That inconsistency is the source of Hund's paradox: that a superposition in the chirality basis is incompatible with being observed as left- or right-handed, and yet superpositions in that basis are predicted by quantum mechanics. In fact, MacDermott and Hegstrom ([2004], p. 56) explicitly identify the eigenstates of a chiral molecule with 'genuine Schrödinger's cat-like coherent superpositions', thus further reinforcing our claim.

It's worth noting in addition that some of the proposed solutions to Hund's paradox (as considered in subsection 2.1) are either related to, or refer to interpretations of quantum mechanics – especially appeals to decoherence and to the MHI (see Bahrami et al. [2012] and Fortin et al. [2016]). This also reinforces the claim that Hund's paradox just is the measurement problem applied to the special case of enantiomers.

### **3.2 Isomers and the Inability of Resultant Hamiltonians to Determine Molecular Structure**

Unless additional assumptions are made, one cannot derive observed molecular structure from resultant Hamiltonians. In order to establish that resultant Hamiltonians' failure to determine molecular structure is a special case of the measurement problem, we demonstrate that this case entails the inconsistency of Maudlin's trilemma.

First, eigenfunctions of the resultant Hamiltonian are taken to be a complete description in Maudlin's sense (thus satisfying statement 1.A). This is because, in principle, such wavefunctions specify all the physical properties of the system associated with the nuclear and electronic degrees of freedom. As explained in subsection 2.2, the resultant Hamiltonian takes into account all and only the physical properties and interactions of the particles comprising the molecule by specifying the kinetic and dynamic factors that result from the interactions between the pairs of electrons, the pairs of nuclei, and the pairs of electrons and nuclei.

Secondly, statement 1.B is satisfied unless a non-linear dynamical modification is introduced to transform the wavefunctions corresponding to a superposition of configurations (the eigenfunctions of the resultant Hamiltonians) into wavefunctions corresponding to a determinate molecular con-

figuration. While such alternate dynamics could be introduced (see section 4.3), to our knowledge this is not a strategy advocated in the literature on this issue.

In the case of isomers (like styrene), what quantum mechanics (via the resultant Hamiltonian) tells us is that the ground state corresponds to a state with no identifiable structure. This is because the corresponding Schrödinger equation is invariant under those transformations which distinguish between different molecular structures (see also Löwdin ([1989])). Specifically:

the symmetry inherent in this complete Hamiltonian as concerns the nuclei (rotational symmetry, reflection symmetry, permutational symmetry for identical nuclei), which is necessarily reflected in the eigenfunctions (notably the ground state one), precludes the existence of a 'molecular structure'. For example, rotational symmetry implies that the system of nuclei should be described as a 'nuclear cloud' (exhibiting spherical symmetry), as well as an electronic cloud, for those molecular eigenstates – the ground state among them – which belong to the identity representation of the rotation group. (Claverie and Diner [1980], p. 58)

Note that the relevant literature is somewhat misleading with respect to the sense in which the resultant Hamiltonian does not describe structure. Even though a resultant Hamiltonian does not determine the molecular structure that is identified empirically (that is, by measurement), it nevertheless, at least in principle, determines all possible structures of the examined molecule. Given this, one can understand the role of the configurational Hamiltonian as picking out that structure which agrees with the result of a particular measurement. This is supported by Claverie and Diner ([1980], p. 60) who directly connect the act of measurement with identifying a particular structure:

if, at any instant of time, we should measure the positions of the nuclei of some molecules, we would find some (relative) configurations of the resulting positions with higher probability, and those (relative) configurations with maximal probability clearly enable us to speak of some underlying structure.

Claverie and Diner's discussion of different probabilities for different molecular configurations may be understood as the claim that the system is in a superposition of such configurations. As a consequence, different resolutions to the measurement problem will lead to the selection of just one of these configurations and thus account for the transition from symmetric to asymmetric descriptions.

Lastly, statement 1.C corresponds to the fact that particular molecules are observed with a specific isomeric structure. For example, styrene is observed with a particular structure which is measurably distinct from the other isomeric structures that the same set of atoms could take.

Note that the superposition of all possible isomeric structures are rarely, if ever, manifest in the sense that, for example, interference experiments could be performed. This is to be expected given that tunnelling from one isomeric structure to another very often involves breaking and reforming different kinds of chemical bonds between the same set of atoms.<sup>23</sup> For example, tunnelling from styrene to cubane would require going from double bonds within styrene to single covalent bonds between all carbon atoms. In quantum mechanical terms, this is explained by the fact that the probability of tunnelling is low enough that, if a system starts off as some particular isomer it will maintain that structure indefinitely.<sup>24</sup> Further interpretation of probabilities and superpositions depends on the resolution of the measurement problem (see section 4).

In many cases, it's very difficult to gain direct evidence of the superpositions discussed in this subsection. Consequently, the measurement problem discussed here may be thought of as more theoretical than in other cases. However, quantum physics does predict that such superpositions are in fact instantiated, even though they are difficult to observe; in addition, superposition states for large molecules can be experimentally observed – see for example (Fein et al. [2019]). As is discussed in the next section, different interpretations of such superpositions have significantly different ontological implications. It's also worth noting how commonly superpositions of measurement devices and cats are discussed in the literature. As such, this is no reason not to count the case of isomers as an

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<sup>23</sup>An exception to this are chiral molecules (enantiomers) which differ only in terms of their inverted structure. For chiral molecules, the probability of tunnelling is higher than for most other types of isomer; see discussion of Hund's paradox above.

<sup>24</sup>Talk of probabilities is licensed by the fact that molecules in an environment have decoherence timescales on the order of femtoseconds; see (Prezhdo and Rossky [1998]).

instance of the measurement problem!

We have shown that there is good reason to accept all three of Maudlin's lemmas in the context of the resultant Hamiltonian used to describe isomers. Since these lemmas are mutually incompatible, we have demonstrated that the the problem of resultant Hamiltonians' inability to determine structure is an instance of the measurement problem.

In the next subsection we discuss the problem of symmetry breaking; this is the most general example considered here as it applies to all molecules which are observed to have structures with stable asymmetries.

### 3.3 Symmetry breaking

The case of the ammonia molecule, along with that of other molecules exhibiting spatial asymmetries, similarly satisfy Maudlin's trilemma.

Statement 1.A corresponds to the claim that the wavefunction representing a superposition of the pyramid and its inversion is the best way to describe ammonia in the quantum formalism. This is evidenced by discussion of the tunnelling frequency which is derived from the superposed state and the claim that the stationary quantum mechanical state is symmetric. Nonetheless, this first lemma is only satisfied by those molecules which are appropriately described as in superposition states in the position basis. As noted above, some molecules are stably produced in asymmetric states and may not as a consequence illustrate the measurement problem or provide justification for philosophical worries concerning symmetry breaking.<sup>25</sup>

Statement 1.B is a straightforward consequence of the application of quantum mechanics. The Schrödinger dynamics are assumed to be applicable within the physics and chemistry of molecules. While some putative resolutions of the measurement problem posit non-linear dynamics, Anderson's set-up of the problem does not contest this assumption.

The satisfaction of statement 1.C is particularly stark in the case of the ammonia molecule: while the superposed state would not exhibit an electric dipole moment, the observed molecule has such a moment. All observations and measurements of ammonia have this preferred direction, while the initial quantum description is symmetric.

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<sup>25</sup>Though such worries may of course arise further upstream.

Consequently, it should be clear that such cases of symmetry breaking are instances of the measurement problem. Maudlin's trilemma in an abstracted form involves the question: how come a single determinate outcome is observed when, according to quantum mechanics, all outcomes are on a par? Alternatively: why is an asymmetric molecule with a particular orientation observed, when quantum mechanics predicts a symmetric superposition of orientations?

The measurement problem is the observation that no physical mechanism within quantum mechanics allows for that symmetry to be broken and a single outcome to be selected. The putative resolutions of the measurement problem considered in the next section may, thus, all be understood to provide a mechanism either for breaking that symmetry and selecting a single outcome or, in the case of the many worlds interpretation, for hiding the other outcomes of measurement in effectively non-interacting worlds. Any resolution to the measurement problem will, thus, explain how a system may be symmetric before measurement but asymmetric (or effectively asymmetric) after measurement.

The problem of symmetry breaking in molecules is an instance of the measurement problem because all three of Maudlin's lemmas appear to apply to such molecules, and thus the incompatibility of the trilemma is entailed in such cases.

Further evidence that this problem should be thought of as an instance of the measurement problem is found in (Claverie and Diner [1980]; Landsman [2017]; and Wallace [2018]), all of which make the connection between symmetry breaking and putative resolutions of the measurement problem (respectively, Stochastic Electrodynamics, the Flea on Schrödinger's cat, and decoherent histories on the many worlds interpretation).

## **4 Interpretations of Quantum Mechanics: Implications for the Ontology of Chemistry**

One might be persuaded by our argument thus far and nonetheless be worried that the problems of molecular structure would each be resolved by distinct mechanisms. As yet, we haven't provided any way out of the aforementioned problems of molecular structure. In this section we allay this worry by demonstrating that several putative solutions to the measure-

ment problem also resolve the problems of molecular structure. As such, we answer the question: how should we understand molecular structure, given its quantum mechanical description?

We argue that identifying the problems of molecular structure as special cases of the measurement problem significantly informs both our understanding of the nature of molecular structure and our philosophical understanding of chemistry's relation to quantum physics. Recall that the problems of molecular structure have been invoked in favour of specific forms of anti-reductionist emergence. Therefore, insofar as the different solutions to the measurement problem resolve the problem of molecular structure, such solutions will also affect how one should think of the relations between chemistry and quantum physics. Note that our goal is not to advocate for any particular theory or interpretation of quantum mechanics. Rather, we argue that many of the currently available solutions also have the potential to resolve the problems of molecular structure.

This section is organised into three subsections, each of which focuses on one specific solution to the measurement problem; namely, the Everett (or Many Worlds) interpretation, the de Broglie-Bohm theory, and spontaneous Collapse Theories.<sup>26</sup>

Each subsection explains how the examined interpretation solves the problems of molecular structure. In the course of such explanations it will be made clear how the given interpretation informs our understanding of molecular structure with reference to isolated and non-isolated molecules, and how the interpretation affects the tenability of strong emergence and reduction with respect to chemistry's relation to quantum physics. In fact, we argue that, to the extent that strong emergence and anti-reductionism about chemistry are supported by the problems of molecular structure, then under all three interpretations of quantum mechanics these positions are undermined.<sup>27</sup>

The distinction between isolated and non-isolated molecules plays an

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<sup>26</sup>While we acknowledge that this is far from an exhaustive list of realist interpretations of quantum mechanics, these three hold most currency in the philosophy literature – see for example (Maudlin [2019]; Bacciagaluppi [2016]). It's also important to note that some of the problems of molecular structure have already been considered with reference to the Modal Hamiltonian interpretation in (Fortin et al. [2018]).

<sup>27</sup>We primarily have in mind Hendry's strong emergentism, but we take it that any form of emergence and anti-reduction that invokes the problems of molecular structure to support its claims is likewise undermined by our analysis.



important role in our analysis in this section. Chemists often talk as if there is structure in isolation and quantum mechanics is often taken to describe molecular systems in isolation (Woolley [1988], p. 58; Seifert [2019]). Moreover, anti-reductionist and emergentist views about molecular structure argue that quantum mechanics is inadequate since it cannot identify an isolated molecule's structure in a way consonant with chemistry's description; this implies that they assume there is structure in isolation which should be identified by the more fundamental theory. However, this assumption is challenged to the extent that interpretations of quantum mechanics imply that isolated molecules do not generically have determinate molecular structure.

If, on the one hand, molecular structure is not to be found in isolated systems, then the purported failure of quantum mechanics to identify structure is no longer an indication of anti-reduction. This is because there is no structure to be captured in isolation. Instead, it is only in the context of interactions with the environment that there is any requirement to account for molecular structure. On the other hand, insofar as an interpretation of quantum mechanics predicts that there is molecular structure in isolation, whichever particular molecular structure is instantiated is explained by the initial conditions and the dynamics of the isolated system.

While this paper has important implications for how to understand structure for isolated and non-isolated molecules and we discuss these implications, 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. For example, when a molecule is part of a chemical substance, then its structure is partially determined by factors that relate to the conditions and environment in which that substance is found. Such considerations go beyond the scope of this paper

This section's analysis illustrates that any metaphysical claims about molecular structure have to assume some or other solution to the measurement problem. Questions of reduction and emergence are contentious on any resolution of the measurement problem and while we do not purport to demonstrate the reducibility of chemistry *in toto*, nonetheless, the identification of the problems of molecular structure as special cases of the measurement problem removes significant hurdles facing the reductionist.

## 4.1 The Everett Interpretation

The Everett (or Many Worlds) interpretation of quantum mechanics is given its best modern presentation in (Wallace [2012]). On this interpretation, when environmental or measurement device degrees of freedom become entangled with a quantum system, the wavefunction does not collapse. Rather, if the quantum system is in a superposition in the measurement basis, then the measurement device will enter into a superposition. If decoherence is as the Everettians suppose, then within a very short time period (on the order of femtoseconds) after interaction with the measurement device or environment, interference between branches of the superposition will be suppressed and each branch may be considered to instantiate approximately independent worlds.<sup>28</sup> The Everettian avoids the inconsistency of Maudlin's trilemma by rejecting statement 1.C and claiming that measurements only have determinate outcomes relative to an emergent world.

In general, on this interpretation, isolated molecules are in superpositions of different atomic configurations. Since superpositions are interpreted physically and the quantum state is complete, when the system is in a superposition of different atomic arrangements there may be no determinate molecular structure.<sup>29</sup> Thus, for example, if the system is in a superposition of right- and left-handed enantiomers, that is all there is to say about the molecule and it has no determinate handedness. Likewise, if the system is in a superposition of the different molecular structures which correspond to the same resultant Hamiltonian or if the system is in a superposition of different dipole moments as discussed, respectively, in sections 2.2 and 2.3, then the system may have no determinate molecular structure.<sup>30</sup> That is, in each case, the system may not have a unique determinate atomic spatial configuration.

Determinate molecular structure emerges once the interference between the branches of the superposition have been sufficiently suppressed

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<sup>28</sup>See (Prezhdo and Rossky [1998]) for a discussion of decoherence timescales for molecules and (Dawid and Thébault [2015]) for an argument that not all the Everettian claims about decoherence go through.

<sup>29</sup>This needn't imply ontic vagueness: a set of atoms may be determinately in a superposition of molecular structures even while they have no unique determinate structure.

<sup>30</sup>Note that molecules which have a symmetric molecular structure (such as the hydrogen molecule H<sub>2</sub>) will not be predicted to be in a superposition of different structures, though their atoms will still be in a superposition of different positions.

due to decoherence (of both environmental and non-environmental kinds). When that has occurred we can ascribe molecular structure to each branch of the superposition, and consequently, relative to each emergent world there is determinate molecular structure.

The problems of molecular structure are resolved on the Everett interpretation by acknowledging that our fundamental symmetric quantum mechanical description determines a superposition of molecular structures for isolated molecules, but that macroscopic observers will only ever come into contact with particular branches of those superpositions. This is because macroscopic observers inhabit effectively non-overlapping emergent worlds. In other words, on the Everett interpretation, the full quantum description is symmetric and this symmetry is hidden by the different emergent worlds which each corresponds to some part of the complete quantum state. The fact that observed molecular structure appears to be underdetermined by quantum mechanics is consequently explained.

It remains to define more precisely the circumstances in which molecules can be correctly said to have molecular structure in isolation. As noted above, when in a non-decohered superposition of configurations, it is incorrect to say that there is determinate molecular structure. However, if, due to some external asymmetry a molecule is in an eigenstate of just one configuration, then it can be said to have structure in isolation. As such, the biologically produced sugar molecule discussed at the end of section 2.3 may well have molecular structure in isolation.

It's also worth noting that decoherence is not only the result of environmental interactions. As Wallace ([2018]) discusses, a molecule with a sufficiently low amplitude for tunnelling may undergo a different kind of decoherence such that, even in isolation, it may be considered to have molecular structure.

This kind of decoherence builds on Halliwell's analysis ([1998, 2010]): once you have an approximately conserved quantity, there is strong suppression of interference terms between various values of such quantities. This gives rise to approximate decoherence, and, on the Everettian view, emergent worlds. In the case of superpositions considered in section 2, this might allow one to think of, say, the right- and left-handedness of the enantiomers as conserved relative to some faster changing variables such as the rotation of these molecules. The approximate decoherence would thus enable us to conceive of such molecules as having determinate structure in

isolation in the sense that the worlds with each molecular configuration would effectively not interact.

For these reasons, while the Everettian approach implies that, generically, molecules do not have structure in isolation, there are circumstances in which they will have such structure. And whether or not they have such structure in isolation, their exhibiting molecular structure on measurement is explained insofar as the Everettian approach provides a satisfactory resolution of the measurement problem.

This brings us to the question: according to the Everett interpretation, is molecular structure reducible? Since in isolation, in general, we've argued that there is no molecular structure, then the anti-reductionist claim that quantum mechanics cannot recover structure becomes moot. When in contact with an environment, according to the Everettian account, such structure is also reducible. This is because the Everettian claims that decoherence effects follow from an application of the Schrödinger equation.

This serves to undermine the claims due to Hendry ([2010a]) that the problem of molecular structure is in-principle evidence for strong emergence. Contra such views, molecular structure does not need to be imposed from the top down; it's derivable, for each emergent world, that the observed molecular structure of that world will correspond to some branch of the superposition of molecular configurations described by the resultant Hamiltonian. While strong emergence is thus undermined, the Everettian worlds might be said to emerge weakly from the underlying quantum state.<sup>31</sup>

The discussion of molecular structure on the Everettian interpretation demonstrates that the principal moral of this paper – that the problem of molecular structure just is the measurement problem – allows for progress to be made in the question of the reducibility of molecular structure. It is clear that, in principle, observed molecular structure may be derived from the underlying quantum theory, and whether or not such derivation is successful depends on an ongoing physics research programme. We are therefore rescued from the logjam engendered by pointing out the different symmetries of molecular structure and more fundamental physics, and claiming that these are irreconcilable. The resolution of this problem is not

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<sup>31</sup>See (Knox [2016]; Franklin and Knox [2018]) for an account of weak emergence, though development of an account of weak emergence adequate to the full Everettian picture is an ongoing research project.

straightforward, but through recognising the commonality with the measurement problem, positive steps may be made.

## 4.2 De Broglie-Bohm Theory

The de Broglie-Bohm theory (also known as ‘Bohmian mechanics’) has a dualist ontology where a configuration of particles with determinate positions is guided by the wavefunction, known as the ‘pilot wave’.<sup>32</sup> The application of Bohmian mechanics to some of the problems of molecular structure is also discussed in (Fortin et al. [2017]), however, this paper does not offer a detailed analysis of the existence of molecular structure in isolation.

To understand how de Broglie-Bohm theory solves the measurement problem, it’s important to distinguish between how the wavefunction evolves and the consequences for the particle configuration. Note that particle positions have no effect on the wavefunction – the latter evolves deterministically according to the Schrödinger equation. As such, on this interpretation, quantum systems’ wavefunctions are in real, physical superpositions.<sup>33</sup> On the other hand, particles always have determinate positions (they may also be assigned charge and mass).

Where the wavefunction governing the particles is in a superposition of positions, then one may think of the parts of the wavefunction which overlap the particle positions as ‘filled’, and the remainder of the wavefunction as ‘empty’. Where there is non-trivial interference between the filled and empty parts of the wavefunction, the particles will exhibit interference phenomena in their locations. Decoherence, and the consequent suppression of interference between empty and filled branches of the wavefunction, will result in only the filled branches’ being dynamically relevant to the particle trajectories. In such circumstances particles will follow approximately classical trajectories; see (Rosaler [2015]).

The de Broglie-Bohm theory renders Maudlin’s trilemma consistent by denying statement 1.A: the wavefunction does not offer a complete description because the particles also determine some of the physical properties of quantum systems. Whenever quantum mechanics describes a molecule or

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<sup>32</sup>See the discussion in (Maudlin [2019]) for more details.

<sup>33</sup>Some advocates of Bohmian mechanics are eliminativist about the wavefunction, see (Miller [2014]), and (Dewar [2016]) for a critique of that position.

set of molecules as in a superposition, the particles will still have determinate positions, but, prior to decoherence, their trajectories will exhibit the effects of interference. After decoherence, if the wavefunction is in a superposition in the measurement basis, the particles will only fill one branch of that superposition.

The resultant Hamiltonian describes a quantum wavefunction that is in a superposition of enantiomers, isomers, and inversions of some collection of atoms. The de Broglie-Bohm theory specifies preferred branches of this superposition through its initial conditions – one assumption required in the set-up of the theory is that the configuration of particles at the beginning of time has its probability given by the modulus squared of the initial wavefunction. As such, unlike on the Everett interpretation, the full quantum description does not treat all branches of the superposition on a par. There are always facts about the positions of the Bohmian particles which are sufficient to break any symmetry of the wavefunction.

Does the de Broglie-Bohm theory thus predict determinate molecular structure in isolation? As soon as decoherence occurs in the way described above in section 4.1, then molecules will have determinate configurations which conform to the standard description in chemistry. One might think that, given that the particles in this theory always have determinate positions, then there is always molecular structure in isolation. However, while particles always have determinate positions on this theory, it's misleading to describe such structure as that given by chemistry. This is because when there is interference between branches, the particle trajectories can be utterly non-classical. For example,

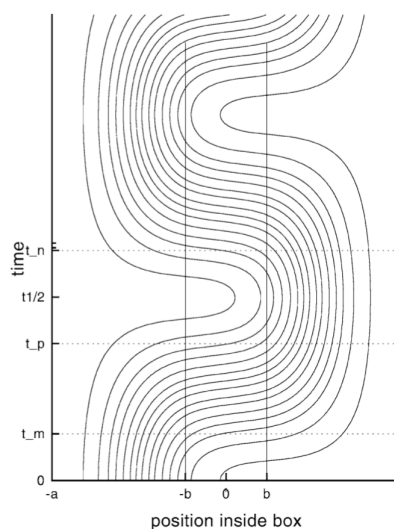


Figure 2: From (Stomphorst [2002], p. 216). This figure depicts the possible trajectories of a particle in a double well potential as predicted by de Broglie-Bohm theory. The barrier of height  $V > E$  is between  $b$  and  $-b$ , the initial wavefunction has energy  $E$ .

see figure 2 for a depiction of particle trajectories over time when in a double well potential, as described by Stomphorst ([2002]). Needless to say, the potentials experienced by the atoms in a molecule are far more complicated than a double well, and before interference is suppressed, particles governed by a wavefunction described as a superposition of positions will not be located in the relative positions predicted by chemists.

This brings us once again to the question of the reducibility of molecular structure. In isolation, particles have determinate positions, but are not organised in structures that chemists would recognise. Insofar as the de Broglie-Bohm theory resolves the measurement problem in a reductionist-friendly manner then it allows for the reduction of molecular structure. Upon interaction with the environment, the theory has, as part of its fundamental structure, particles arranged in exactly the molecular structures which chemistry describes. While one might question the reductionist credentials of the other aspects of the theory, including the status of the wavefunction and the role of decoherence, the particle configurations reduce molecular structure.

This also serves to undermine the claims to strong emergence due to Hendry ([2010a]). Not only is the imposition of molecular structure by chemistry unnecessary, but for molecules in isolation, the molecular structure described by chemistry does not conform to the true positions of the Bohmian particles.

In conclusion, while the de Broglie-Bohm theory has the in-principle resources to resolve the problems of molecular structure, this theory does not, in general, give rise to the molecular structure in isolation which corresponds to chemists' description and representation of structure. Like the Everett interpretation, the extent to which it can be said that this theory resolves the problems of molecular structure is hostage to technical developments in decoherence theory.

### 4.3 Spontaneous Collapse Theories

Spontaneous collapse theories resolve the measurement problem by positing a spontaneous stochastic physical process which collapses wavefunctions in superpositions of position onto approximate eigenstates of position; see (Ghirardi [2018]). While there are a number of ways of constructing such theories, all those which are consistent with current empir-

ical data have tuneable parameters which guarantee that superpositions involving collections of a few hundred to a few thousand particles have very low probabilities of collapsing, while collections of  $10^{23}$  particles have extremely high probabilities of collapsing.

As such, Maudlin's trilemma is rendered consistent by the denial of statement 1.B: the Schrödinger dynamics are occasionally interrupted by spontaneous collapses which break the symmetry between the branches of the superposition. There is no problem of symmetry breaking because the process is spontaneous and stochastic, which means that the choice between the different branches of the superposition is explicitly made by a real physical process according to the probabilities assigned by the Born rule.

This, then, resolves the problems of molecular structure: whenever there is a superposition involving different enantiomers, isomers, or inversions, that superposition is, with high probability, maintained until it becomes entangled with a large enough system that spontaneous collapse is overwhelmingly likely to occur.

On these theories there is, in general, no determinate molecular structure in isolation. There will be, in relative isolation, superpositions of a variety of different molecular structures. The eventual determination of molecular structure is the consequence of an irreducibly stochastic process.

Note that, unlike in the previous two subsections, decoherence does not play a central role in these theories' resolution of the problems of molecular structure. That's because, if these are to be single world theories, they had better deny the Everettian's claim that approximately decoherent branches should be interpreted as distinct emergent worlds. Rather, the spontaneous collapse theorist must maintain that, even where the branches of a superposition are effectively non-interacting, a physical collapse is required for us to obtain the values we measure. As such, determinate molecular structure is much less common for these theories than for those discussed above.

On this approach, is molecular structure reducible? Since, in general, there is no molecular structure in isolation, this question is moot before collapse onto a particular molecular structure has occurred. Insofar as sufficient collapses take place there is a well-defined molecular structure which is consequent on the dynamical localisations of the wavefunction. As such, strong emergence is not required to resolve the problems of molecular structure.



## 5 Conclusion

This discussion does not mean that the central idea of classical chemistry – namely molecular structure – is somehow ‘wrong’. Nor does it mean that quantum mechanics is ‘wrong’. Both assertions are plainly ludicrous. What it does mean is that the eigenvalues and eigenfunctions of the Coulomb Hamiltonian for a collection of electrons and nuclei — the notional starting point of quantum chemistry — without the Born-Oppenheimer approximation, (or equivalently, a conscious decision to disregard the indistinguishability of identical nuclei) do not provide a basis for a quantum theory of chemistry. [...] We agree with Löwdin’s view in his late papers, see for example (Löwdin [1989]), that some new idea is required. (Sutcliffe and Woolley [2012], pp. 422-423)

This statement emphasises just how close the problems of molecular structure are to the measurement problem. Indeed, the fact that the eigenvalues and eigenfunctions of Hamiltonians are not sufficient to explain all the properties we observe could be understood as a formulation of the measurement problem! We agree that the problems of molecular structure are real problems, however, it may not be necessary to come up with a new idea to solve any of them – the various putative resolutions of the measurement problem have been around for a while!

Nevertheless, it would be unfair not to acknowledge that those who have talked (in some form) about the problems of molecular structure have correctly identified central features of these problems. For example, Fortin et al. ([2016, 2018]) argue that Hund’s paradox is analogous to the measurement problem and have proposed an interpretation of quantum mechanics to solve both issues. Scerri ([2011]) has pointed out that the shift from resultant to configurational Hamiltonians is an instance of the collapse of the wavefunction, while Sutcliffe and Woolley ([2012]) and Primas ([2013]) discuss the role of classical concepts and complementarity in the context of this problem. So the current literature admits that the problems of molecular structure are very closely connected to problems in quantum mechanics.

Our novel contribution has been to explain exactly how the problems of molecular structure relate to each other and to the measurement problem. Overall, we demonstrate that three problems generally distinguished in the

philosophy of chemistry literature ought to be regarded as instances of the same problem — one that is central to debates in the philosophy of physics. This paper may be understood as unificatory in the following sense: central problems of the philosophy of chemistry and the philosophy of physics are one and the same!

Lastly, it is a consequence of our argument that the different interpretations of quantum mechanics have implications throughout the philosophy of chemistry. Our work should, thus, open the way for a mutually informative interchange between the foundations of quantum mechanics and the foundations of chemistry communities. While work in the former has clear implications for the latter discipline, it is also our belief that insights from chemistry and its foundations could lead to a deeper understanding of the nature of quantum mechanics. While we are advocating the conflation of the central problems of two disciplines, this ought not to undermine the value of any of the research programs discussed.

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