A new application of the modal-Hamiltonian interpretation of quantum mechanics: The problem of optical isomerism

Sebastian Fortin, Olimpia Lombardi[*], Juan Camilo Martínez González

CONICET — Universidad de Buenos Aires, Instituto de Filosofía, Facultad de Filosofía y Letras, UBA, Puan 480, 1420, Ciudad de Buenos Aires, Argentina

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1. Introduction

The modal interpretations of quantum mechanics found their roots in the works of Van Fraassen (1972, 1974), who claimed that the quantum state always evolves unitarily (with no collapse) and determines what *may* be the case: which physical properties the system may possess, and which properties the system may have at later times. On this basis, since the 1980s several authors presented realist interpretations that can be viewed as belonging to a "modal family" (Bacciagaluppi & Dickson, 1999; Bene & Dieks, 2002; Dieks, 1988, 1989; Kochen, 1985; Vermaas & Dieks, 1995): realist, non-collapse interpretations of the standard formalism of the theory, according to which any quantum system possesses definite properties at all times, and the quantum state assigns probabilities to the possible properties of the system. Given the contextuality of quantum mechanics (Kochen & Specker, 1967), the members of the family differ to each other with respect to their rule of definite-value ascription, which picks out, from the set of all observables of a quantum system, the subset of definite-valued properties, that is, the *preferred context* (see Lombardi & Dieks, 2014 and references therein). In particular, the modal-Hamiltonian interpretation (MHI) (Castagnino & Lombardi, 2008; Lombardi & Castagnino, 2008) endows the Hamiltonian of the system with the role of selecting the subset of the definite-valued observables that constitute the preferred context.

The MHI solves several problems that affected the traditional modal interpretations (Lombardi & Castagnino, 2008; Ardenghi, Lombardi, & Narvaja, 2013; Lombardi, Fortin, & López, 2015). Moreover, it has been reformulated in an explicitly Galilean invariant form (Ardenghi, Castagnino, & Lombardi, 2009; Lombardi, Castagnino, & Ardenghi, 2010), and its compatibility with the theory of decoherence has been proved (Lombardi, 2010; Lombardi, Fortin, Castagnino, & Ardenghi, 2012). In turn, from the ontological viewpoint, the MHI offers a clear picture of an ontology without individuals, where quantum systems are bundles of properties (da Costa, Lombardi, & Lastiri, 2013; da Costa & Lombardi, 2014; Lombardi & Dieks, 2016). Nevertheless, perhaps the main advantage of the MHI in the eyes of scientists is given by its several applications to well-known physical situations, leading to results compatible with experimental evidence: free particle with spin, harmonic oscillator, hydrogen atom, Zeeman effect, fine structure, Born-Oppenheimer approximation (see Lombardi & Castagnino, 2008, Section 5). The purpose of this paper is to add a new application to the list: the case of optical isomerism, which is a central issue for the philosophy of physics and of chemistry. The phenomenon of isomerism points to the core of the problem of the relationship between physics and chemistry, in particular, to the question of whether molecular chemistry can be reduced to quantum mechanics. Here it will be shown that the MHI supplies a direct and physically natural solution to the problem, which does not require putting classical assumptions in "by hand."

With this purpose, the paper is organized as follows. In Section 2, the discussion about the problem of the reduction of chemistry to physics will be introduced in terms of the concept of molecular structure. On this basis, Section 3 will focus on the particular problem of optical isomerism and the so-called Hund's paradox, which points to the difficulty in giving a quantum account to chirality. Section 4 will be devoted to explain the different attempts to solve the paradox and their difficulties. In Section 5, the main features of the MHI will be recalled, emphasizing the aspects that will lead, in Section 6, to offer a solution of Hund's paradox in exclusively quantum terms. Finally, in the Conclusions the general argument will be reviewed, stressing why the MHI supplies a perspective that sounds natural to chemists' ears and provides them with the tools to face some general problems related to the links between chemistry and physics.

* Corresponding author.
  E-mail addresses: sebastian.fortin@gmail.com (S. Fortin), olimpiafilo@gmail.com (O. Lombardi), olimac62@hotmail.com (J.C. Martínez González).

2. Linking physics and chemistry: the problem of molecular structure

Since the advent of quantum mechanics and its application to chemical systems, reduction became a regulative idea in the accounts of the relationship between physics and chemistry. The famous introductory paragraph of Paul Dirac's article of 1929 is usually considered the paradigmatic manifestation of the reductionist attitude in this field: "*The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these equations leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation*" (Dirac, 1929, p. 714). In this quote, the idea is that chemical phenomena can be explained by the laws of physics, in the sense that the descriptions of those phenomena are derivable from the equations of quantum mechanics plus the necessary specific conditions. Of course, Dirac explicitly acknowledges that the explanation does not require effective derivation: in practice, due to the complexity of the target, the application of quantum mechanics to molecular systems requires the introduction of different approximation strategies. Nevertheless, since at that time it was commonly assumed that chemical systems are nothing else than complex quantum systems (see discussion in Lombardi & Labarca, 2005, 2006), approximations were seen as conceptually innocuous techniques that could be in principle removed to obtain a more precise description. The approximate methods referred to by Dirac are the core of what later would be known as quantum chemistry (see Hendry, 1998).

The problem of the relationship between physics and chemistry, in particular between molecular chemistry and quantum mechanics, finds one of its main manifestations in the debate about the nature of molecular structure, which, according to molecular chemistry, is given by the spatial arrangement of the atoms in a molecule. The debate focuses not on an auxiliary or secondary notion, but on a central concept of molecular chemistry: molecular structure is the main factor in the explanation of reactivity, it is "*the central dogma of molecular science*" (Woolley, 1978, p. 1074). As Robin Hendry claims, "*molecular structure is so central to chemical explanation that to explain molecular structure is pretty much to explain the whole of chemistry*" (Hendry, 2010, p. 183). Or, in Hans Primas terms: "[t]*he alpha and omega of molecular chemistry is the doctrine that molecules exist as individual objects and that every molecule has a shape, characterized by its molecular frame*" (Primas, 1994, p. 216).

At present, the discussion about the boundaries between physics and chemistry distinguishes between epistemic reduction and ontological reduction (Lombardi & Labarca, 2005, 2006) or, in Hendry's terms (2010; see also 2004, 2008), between the intertheoretic and the metaphysical aspects of the reduction debate. In the epistemic field, Hinne Hettema (2012) is extremely optimistic: he adopts an explicitly reductionist stance by considering that the intertheoretic relationship between molecular chemistry and quantum mechanics fulfills the conditions required by the traditional Nagelian model of reduction (see debate between Lombardi, 2014; Hettema, 2014). Another epistemic reductionist strategy is that based on the concept of quantum decoherence: conceived as the process that accounts for the classical limit of quantum mechanics (Zurek, 1991, 2003), environment induced decoherence would supply the necessary link between the classical concepts of molecular chemistry and the concepts of the quantum domain (Trost & Hornberger, 2009; Scerri, 2011, 2013).

Nevertheless, at present epistemic reductionism is not the usual stance in the philosophy of chemistry community: nowadays almost everybody agrees that classical intertheoretic reductions of chemistry to physics are not currently available (see several examples in Lombardi & Labarca, 2005). In spite of the role played by approximations, the obstacles are particularly serious in the case of the explanation of molecular structure. Already in his works of the 70's and the 80's, Guy Woolley points out that, by means of the description of a molecule from "first principles", "*one cannot even calculate the most important parameters in chemistry, namely, those that describe the molecular structure*" (Woolley, 1978, p. 1074); he considers that the impossibility of determining the geometry of a molecule by means of quantum mechanics is a proof of the fact that molecular structure is only a "*powerful and illuminating metaphor*" (Woolley, 1982, p. 4). Other authors stress that conceiving the molecule as an individual object with its own spatial structure requires to ignore quantum correlations: "*The shape of a molecular state should of course not show holistic correlations to other molecular quantities and hence be unambiguously defined.*" (Amann, 1992, p. 32).

Notwithstanding the agreement about epistemic matters, ontological reductionists and non-reductionists differ in their interpretation of the practical impossibility of explaining molecular structure in quantum terms: "*the issue is essentially future directed −both sides must wait and see, even if they would bet different ways. But why do the two sides make different bets? Perhaps the answer concerns their different underlying metaphysical views.*" (Hendry, 2010, p. 184).

On the one hand, authors with ontologically reductionist disposition consider that the impossibility of deriving molecular structure from quantum mechanics is the consequence of our partial knowledge of the molecular systems. For instance, Guy Woolley and Brian Sutcliffe claim that: "*We have never claimed that molecular structure cannot be reconciled with or reduced to quantum mechanics, or that there is something 'alien' about it; our claim is much more modest. We do not know how to make the connection.*" (Sutcliffe & Woolley, 2011, p. 94; see also 2012). On the contrary, other authors stress that the problem is not merely practical and contingent, but derives from the fact that the very concept of molecular structure finds no place in the theoretical framework of quantum mechanics. For instance, according to Hans Primas, the classical idea of definite spatial position for the atomic nuclei, conceived as individual objects, is, at least, strongly controversial in the quantum context. The author highlights non-locality as a specific feature of quantum mechanics that excludes the spatial concept of molecular structure: "*the holistic correlations between the nuclei and electrons are suppressed, so the description of a molecule reduces to the description of the motion in the electrical field of a classical nuclear framework*" (Primas 1983, p. 91; see also 1998). Following Primas' ideas, Robert Bishop (2005) also recognizes the conceptual limitations of quantum mechanics to account for molecular structure, and points out that proper attention to the context relevant to a particular situation can resolve otherwise intractable problems (see also Bishop & Atmanspacher, 2006). In turn, Hendry (2004, 2008, 2010), who has largely addressed the issue of molecular structure in the context of the debate about reduction, claims that the debate must turn to consider the ontological relationships between the entities, processes, and laws studied by different sciences. From this perspective, he argues that the relationship between quantum mechanics and molecular chemistry, embodied in concept of molecular structure, must be conceived in terms of emergence.

A central element in the discussion about molecular structure is the role played by the Born-Oppenheimer approximation, whose fundamental premise is the possibility of decomposing the

Hamiltonian of the molecule into its electronic and its nuclear components. This move relies on assuming the nuclei as classical-like particles at rest in a definite position: on this basis, the terms of kinetic energy associated to the nuclear motion are removed (*clamped-nuclei assumption*). In the Hamiltonian resulting from that assumption, the molecular structure is described by the positions of the nuclei. In turn, the so-called 'potential energy surface' that affects the electrons of the molecule can be calculated by means of this Hamiltonian. Nevertheless, from the viewpoint of reduction, the Born-Oppenheimer approximation faces at least two difficulties. First, it introduces the molecular structure into the quantum description from the very beginning, since the positions of the nuclei are established with the appeal to classical geometric considerations. Second, the assumption of the nuclei at rest in fixed spatial positions contradicts the Heisenberg principle, which prevents quantum systems from having definite values of position and velocity simultaneously (see Chang, 2015; Lombardi & Castagnino, 2010). As Hendry (1998, 2010) points out, the "proxy" defense of Born-Oppenheimer models is based on the assumption that using them instead of the exact solution makes only a small difference to the energy; but, from a theoretical viewpoint, those models "*simply assume the facts about molecular structure that ought to be explained*" (Hendry, 2010, p. 186). Hasok Chang clearly makes the point: "*The difficulty here is not only about the practicalities of the calculation, and the clamping-down of nuclei is not merely an approximation. Aside from assuming that the nuclei are fixed, it is necessary to know exactly where exactly the nuclei in question should be placed. Otherwise it is not possible to specify the potential function, which needs to be inserted into the Schrödinger equation, whose solution determines the wavefuncion of the electrons in the molecule. In other words, without knowing the locations of the nuclei in the molecule it is impossible even to set up (not to mention solve) the Schrödinger equation.*" (Chang, 2015, p. 198).

The discussion around the nature of molecular structure is often related to the interpretation of the Born-Oppenheimer approximation. However, there is a specific problem regarding molecular structure that plays a central role in the debate about the relationship between molecular chemistry and quantum mechanics. This is the problem of isomerism. The particular relevance of this case is that, as it will be explained in the next section, the difficulties derived from it are independent from the assumptions involved in the Born-Oppenheimer approximation.

3. Isomerism and optical activity: Hund's paradox

The composition of a molecule is given by its chemical formula, which specifies in what stoichiometric proportion the component elements are present in the chemical compound. But the formula supplies no information about the geometrical arrangement of the component atoms. For instance, $C_2H_4O_2$ corresponds to different chemical compounds: methyl formate, acetic acid and glycolaldehyde. Compounds that contain the same number of atoms of each element (and, therefore, have the same chemical formula) but have different spatial arrangements of their atoms are called

isomers (see Fig. 1). Isomerism is a phenomenon highly relevant in chemistry, since it explains the difference in the physical and chemical behaviors of substances with the same composition.

There are two main forms of isomerism: structural isomerism and stereoisomerism. In *structural isomers*, sometimes referred to as *constitutional isomers*, the component atoms and the functional groups are connected together in different ways. On the other hand, in *stereoisomers*, the component atoms are linked together in the same way, but the geometrical positioning of atoms and functional groups in space differs. The class of stereoisomers includes the subclass of *enantiomers*: the structures of the members of a pair of enantiomers are non-superimposable mirror-images of each other, that is, the molecules are *chiral* (see Fig. 2 below).

When present in a symmetric environment, enantiomers have identical chemical and physical properties. Nevertheless, they differ in the kind of interaction with polarized light. In particular, the members of a pair of enantiomers can be distinguished by their ability to rotate plane-polarized light by equal amounts but in opposite directions. It is for this reason that they are called *optical isomers* and it is usually said that they are *optically active*. When the plane of polarization is rotated clockwise (as seen by a viewer towards whom the light is traveling), the optical isomer is called *dextro-rotatory* (D); in the case of counterclockwise rotation, the optical isomer is called *levo-rotatory* (L).

Chiral molecules have an important function in the enzymatic reactions of biological systems: many pharmacological drugs are chiral, and generally only one of the members of the pair exhibits biological activity. The action of drugs is usually explained by means of the idea of "receptor". Receptors are protein molecules in human body, which are exclusively built from L-aminoacids. This means that protein molecules are chiral and, as a consequence, they have different reactions with the two enantiomers of a chiral drug. For instance, aspartame is a sweetening agent that has two enantiomers: one of them is more than a hundred times sweeter than sucrose; the other, is tasteless or slightly bitter. A dramatic example of the different biological activity of enantiomers is that of thalidomide, a drug of molecular formula $C_{13}H_{10}N_2O_4$ introduced to the market in 1957 by a pharmaceutical company in West Germany. It was prescribed to pregnant women as a sedative and to prevent nausea; its use spread rapidly to 46 countries. But the drug was made and marketed as a mixture of D-thalidomide and L-thalidomide: the D-thalidomide is an effective sedative, whereas the L-thalidomide is a teratogen, that is, an agent affecting the
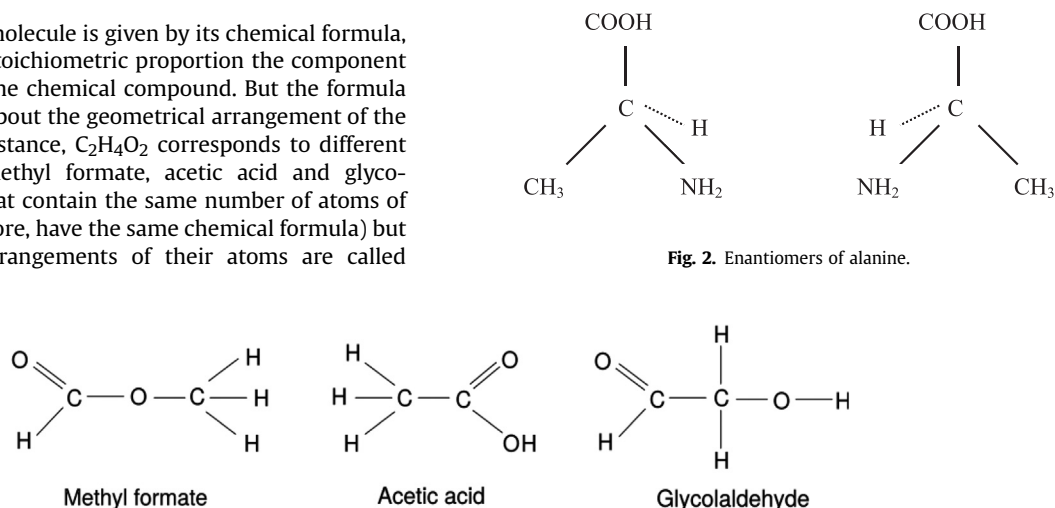
Fig. 2. Enantiomers of alanine.

Fig. 1. Isomers corresponding to the chemical formula $C_2H_4O_2$.

development of the fetus and causing structural or functional abnormality. It is not known exactly how many worldwide victims of the drug there have been, although estimates range from 10.000 to 100.000. These are only some examples of the fact that, at present, the control and production of enantiomers is a key activity in the pharmaceutical industry.

Chemists not only successfully explain the behavior of enantiomers in terms of the geometrical shape of the molecules, but they have also developed many techniques for the preparation of compounds where the proportions of the enantiomers can be controlled. The problem with chirality arises not at the chemical level, but with the attempts to explain the phenomenon in quantum terms.

When a molecule is described by quantum mechanics, the Coulombic Hamiltonian only depends on the distances between the particles composing the molecule; in particular, if only the atomic nuclei are considered, the Hamiltonian depends exclusively on the inter-nuclear distances. In the case of structural isomers, the difference between them is manifest in the Hamiltonian. But in the case of optical isomerism, all the inter-atomic distances are the same for the two members of the pair and, as a consequence, the Hamiltonian is exactly the same for both. This means that quantum mechanics supplies the same description for two structures that can effectively be distinguished in practice through their optical and biological activity.

It is very important to stress that the problem of optical isomerism is completely independent of the Born-Oppenheimer approximation. Let us suppose, for instance, that we write down the exact Hamiltonian H (with no approximation) of a molecule of alanine $C_3H_7NO_2$, which includes three nuclei of carbon, one of nitrogen, and two of oxygen, plus all its electrons (Fig. 2).

Even if we cannot solve this Hamiltonian due to its complexity, we know that it only depends on the distance of the component particles and, therefore, not even the exact Hamiltonian can account for the difference between D-alanine and L-alanine. As Sutcliffe and Woolley claim: "*Clearly then, an eigenstate of H does not correspond to a classical molecule with structure! That observation begs the question: what are the equations that determine the quantum state of molecules? Beyond the BO* [Born-Oppenheimer] *approximation we have no idea.*" (Sutcliffe & Woolley, 2012, p. 416; emphasis in the original). In short, the problem of the quantum mechanical distinction of optical isomers of the same substance is beyond the Born-Oppenheimer approximation and its underlying assumptions.

The problem embodied in optical isomerism points to a deep difficulty in the attempts to account for molecular structure in quantum terms. This was already noticed by Friedrich Hund, pioneer in the development of quantum chemistry, in the 1920s. Hund's paradox can be formulated in two versions. The first one, due to Hund himself (1927), reads as follows: since chiral states (states $|L\rangle$ and $|D\rangle$ corresponding to levo-rotation and dextrorotation, respectively) are not eigenstates of the Hamiltonian (since it is invariant under spatial reflection, further discussion below), and none of them corresponds to the basal state, why do certain chiral molecules display an optical activity that is stable in time, associated to a well-defined chiral state?, why are they not in a superposition of the two possible chiral states? More recently, Hund's paradox was formulated in a slightly stronger version (Berlin, Burin, & Goldanskii, 1996): why do certain molecules have the property of chirality?

Let us consider the total Hamiltonian H of any molecule, which takes into account all the interactions among nuclei, among electrons and among electrons and nuclei. Since the Coulombic interaction only depends on the distance between the interacting

particles, the Hamiltonian is symmetric under spatial reflection; therefore, it commutes with the parity operator P:

$$[P, H] = 0 \tag{1}$$

This means that the eigenstates of the Hamiltonian have definite parity. Moreover, this feature is preserved during the time evolution of the system, because the parity operator commutes with the Hamiltonian and, as a consequence, is a constant of motion.

With these elements, Hund's paradox can be expressed in formal terms. Let us consider a chiral molecule from the perspective of quantum mechanics. The eigenstates $|\omega_n\rangle$ of the Hamiltonian of the molecule have parity symmetry:

$$P|\omega_n\rangle = \pm|\omega_n\rangle \tag{2}$$

In particular, the even levels have even parity, and the odd levels have odd parity. For instance, the ground state $|\omega_0\rangle$ is symmetric and the first excited state $|\omega_1\rangle$ is anti-symmetric:

$$P|\omega_0\rangle = +|\omega_0\rangle \cdot P|\omega_1\rangle = -|\omega_1\rangle \tag{3}$$

However, on the basis of experimental data it is possible to know that the states of optical isomers do not have this symmetry. In fact, if the isomers correspond to the chiral states $|L\rangle$ and $|D\rangle$, each isomer is the mirror image of the other, since:

$$\begin{aligned} P|L\rangle &= |D\rangle \\ P|D\rangle &= |L\rangle \end{aligned} \tag{4}$$

Therefore, the states $|L\rangle$ and $|D\rangle$ cannot be eigenstates of the Hamiltonian, which, as explained above, are symmetric or anti-symmetric (see eq. (3)). On the contrary, $|L\rangle$ and $|D\rangle$ can be expressed as superpositions of $|\omega_0\rangle$ and $|\omega_1\rangle$:

$$\begin{aligned} |L\rangle &= \frac{1}{\sqrt{2}}(|\omega_0\rangle + |\omega_1\rangle) \\ |D\rangle &= \frac{1}{\sqrt{2}}(|\omega_0\rangle - |\omega_1\rangle) \end{aligned} \tag{5}$$

On the other hand, the ground state is a superposition of the chiral states:

$$|\omega_0\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |D\rangle) \tag{6}$$

Why, then, do we always observe chiral states and never superpositions of them? The paradox might be expressed in the following terms: since the ground state of optical isomers is a superposition of chiral states, in that state isomers should not manifest the optical activity corresponding to states $|D\rangle$ states $|L\rangle$; but we have empirical access to the optical activity associated to those states; how to avoid this seeming contradiction? In other words: "*What is the shape of the hypothetical superposition of these two species? Is there a proper reason to exclude such superpositions? What reason can be given —from a quantum-mechanical point of view— for chemical systematics?*" (Amann, 1992, p. 32).

4. Some attempts to solve the paradox

Once it is concluded that chiral states are not eigenstates of the Hamiltonian, it is necessary to explain why those states are observed in the laboratory. One strategy consists in maintaining the Coulombic Hamiltonian, identifying the states $|L\rangle$ and $|D\rangle$ as superpositions of the eigenstates of the Hamiltonian, and then supplying a reason why the molecule does not decay to the ground
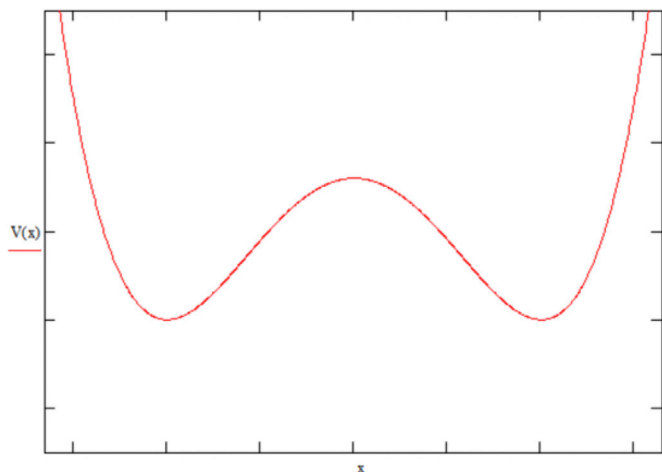
Fig. 3. Potential $V(x)$ with mirror symmetry.

state, eigenstate of the Hamiltonian: this is Hund's strategy, based on graphical visualization.

Let us consider a quantum system with a potential $V(x)$ with mirror reflection symmetry, such as that of Fig. 3. The states "at rest on the left" and "at rest on the right" break the symmetry of the situation and, for this reason, they cannot be eigenstates of the Hamiltonian. In fact, if the wavefunctions of the ground state $|\omega_0\rangle$ and of the first excited state $|\omega_1\rangle$ are graphed, the results of Fig. 4 are obtained. Fig. 4 clearly shows that the eigenfunctions of the Hamiltonian preserve parity: they do not correspond to states localized on the left or on the right, since both occupy both "wells." However, experimentally it is possible to place a quantum particle in one of the two minima of the potential, for instance, on the left. It is clear that this particle is not in an eigenstate of the Hamiltonian, but is in a superposition. The chiral states $|L\rangle$ and $|D\rangle$ correspond to wavefunctions as those shown in Fig. 5.

In their article "On the time dependence of optical activity", Robert Harris and Leo Stodolsky (1981) face the problem of optical isomers and emphasize the limitations of Hund's proposal. In particular, since chiral states are not eigenstates of the Hamiltonian, it is necessary to admit the existence of an exceptional kind of molecules that do not remain in their ground states. For these

authors, the key to solve this difficulty is the interaction between molecules; they modify the Hamiltonian of the system with the purpose of describing such interaction. The central idea is that the paradox arises when the molecule is considered in isolation, whereas a real system actually consists of many molecules in interaction. For this reason, they propose to study the molecules in collision with each other: intermolecular collisions would modify the dynamics of the whole composite system.

The solution to Hund's paradox offered by Harris and Stodolsky is based on considering the interaction of the molecule with its environment, in this case composed of other similar molecules. But in this case it is not clear how the interaction breaks the symmetry of the problem. As Hendry claims: "*The particular form of the symmetry-breaking addition must be justified however, and it is quite mysterious how that could work if all one has in the environment are more molecules described by Coulombic Hamiltonians. The Coulomb Schrödinger equation for an n-molecule ensemble of hydrogen chloride molecules has precisely the same symmetry properties as a Coulomb Schrödinger equation for a 1-molecule system. If the particular form of the symmetry-breaking addition is not justified, then it is just ad hoc: a deus ex machina.*" (Hendry, 2010, p. 186).

Once the possibility of solving the problem of optical isomerism in terms of the interaction with an environment was considered, it did not take long for the idea of decoherence to enter the stage (see, e.g., Joos, 1996). In fact, although the ground state of the molecule is a superposition of the chiral states $|L\rangle$ and $|D\rangle$, through the rotation of polarized light we always measure a definite rotational property. Analogously to the traditional quantum measurement problem, here the problem is to account for the transition from the superposition to one of the chiral states, say, $|L\rangle$:

$$|\omega_0\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |D\rangle) \to |L\rangle \qquad (7)$$

During the last decades, the quantum measurement problem is being faced in the light of the theory of *environment induced decoherence* (Zurek, 1981, 1991, 2003), which relies on the study of the effects of the interaction between a quantum system, considered as an open system, and its environment. On the basis of the analysis of the evolution of the reduced state of the open system, it is proved that, under certain conditions, that state becomes diagonal, that is, loses the interference terms that preclude classicality. The reduced state is conceived as a mixed state containing only the representation of classical correlations and, as a consequence, it can
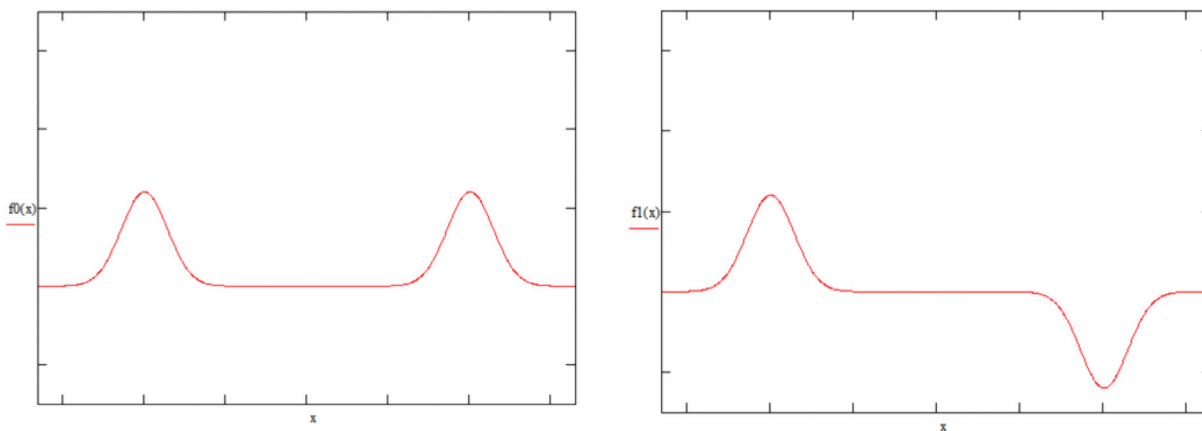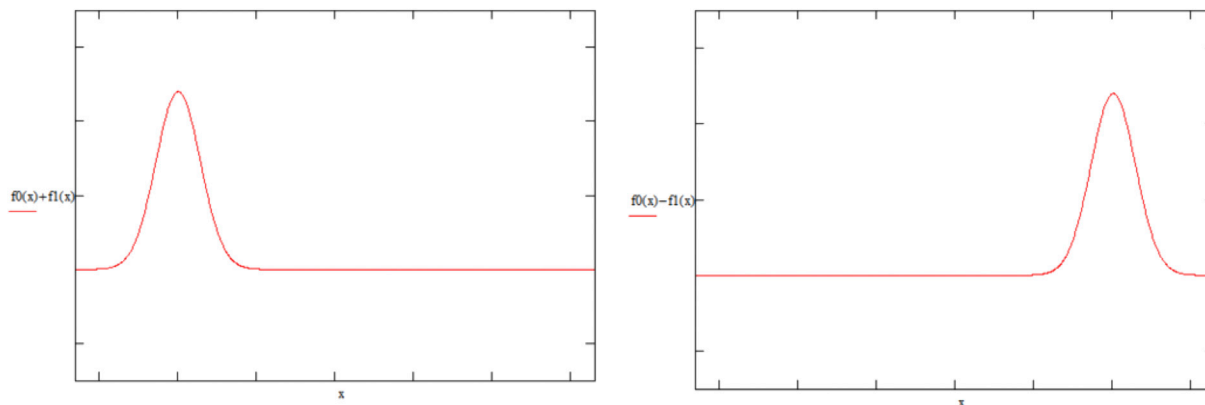

Fig. 4. Shape of the eigenfunctions of a particle subject to the potential $V(x)$. On the left, the ground state, symmetric under space reflections. On the right, the first excited state, anti-symmetric under space reflections.

Fig. 5. Shape of the eigenfuncions of a particle in the states $|L\rangle$ and $|D\rangle$. On the left, the state $|L\rangle$ corresponds to a particle located on the left side. On the right, the state $|D\rangle$ corresponds to a particle located in the right side.

be interpreted in terms of ignorance. When this idea is applied to the problem of isomerism, the conclusion is that the molecule is in one of the states $|L\rangle$ or $|D\rangle$, and the probabilities measure our ignorance about its definite state. In this way, the theory of deco-herence would have solved the problem underlying Hund's paradox.

This idea was widely accepted in the philosophy of chemistry community. For instance, in the Editorial 37 of the journal *Foundations of Chemistry*, its editor Eric Scerri (2011) explicitly considers optical isomerism in the context of the debate about the possibility of accounting for molecular structure in quantum-mechanical terms. He relates the problem of isomerism to the measurement problem in quantum mechanics, and states that the question about molecular structure "*is part of a bigger problem that has long plagued the foundations of quantum mechanics, namely the problem of the collapse of the wavefunction.* […] *this problem has gradually begun to dissolve with the growing realization of the role of quantum deco-herence in physics and other disciplines.*" (Scerri, 2011, p. 4). On the basis of the extensive literature on decoherence (e.g. Zurek, 1981, 1991, 1994, 1998, 2003; Joos, 1996; Joos & Zeh, 1985; Schlosshauer, 2007), Scerri claims that the problem of optical isomerism is dissolved by taking into account the interaction of the molecule with its environment: "*The study of decoherence has shown that it is not just observations that serve to collapse the su-perpositions in the quantum mechanics. The collapse can also be brought about by molecules interacting with their environment.*" (Scerri, 2011, p. 4; for a similar claim, see Scerri, 2013).

This position, however, does not take into account that, in spite of the wide application of the decoherence program, its ability to solve the traditional measurement problem has been largely dis-cussed, and doubts about such ability have been raised on the basis of different arguments. In fact, no matter how the open molecule evolves, the state of the whole system molecule + environment is a superposition at any time: the superposition never disappears through its unitary evolution. For this reason, although the reduced state operator of the molecule lacks interference terms, this does not allow us to suppose that what is observed at the end of the process is one of two definite events: either the event associated with $|L\rangle$, or the event associated with $|D\rangle$. In this sense, Stephen Adler concludes: "*I do not believe that either detailed theoretical calculations or recent experimental results show that decoherence has resolved the difficulties associated with quantum measurement the-ory*" (Adler, 2003, p. 136). The criticism of Jeffrey Bub (1997) is even stronger: stating that what is observed at the end of the mea-surement process is a definite event not only is unjustified, but also

contradicts the eigenstate-eigenvalue link, a standard assumption in quantum mechanics.

Another way to criticize the solution to the measurement problem via decoherence relies on stressing the difference between a proper mixture –the mixed state of a closed system– and an improper mixture –the state of an open system, obtained by tracing off the degrees of freedom of its environment– (d'Espagnat, 1966, 1976): improper mixtures cannot be interpreted in terms of ignorance. As Maximilian Schlosshauer emphasizes in his well-known book about decoherence: "*Since the two systems A and B are entangled and the total composite system is still described by the superposition, it follows from the standard rules of quantum me-chanics that no individual definite state can be attributed to either one of the subsystems. Reduced density matrices of entangled subsystems therefore represent improper mixtures*" (Schlosshauer, 2007, p. 48). The difference between proper and improper mixtures turns out to be even clearer when it is proved that the reduced state of the open system, obtained by partial trace, is a kind of coarse-grained state of the composite system to which the open system belongs (Fortin & Lombardi, 2014). Perhaps confusions are due to the fact that proper and improper mixtures cannot be distinguished from a mathe-matical viewpoint. However, that mathematical indistinguish-ability essentially depends on the formalism used to express the theory, in particular, the Hilbert space formalism. But the situation might be different in other cases. For instance, it has been proved (Masillo, Scolarici, & Sozzo, 2009) that proper and improper mix-tures are represented by different density operators in the so-called quaternionic formulation of quantum mechanics (Adler, 1995); hence, in this formalism they can be distinguished also from a mathematical viewpoint. In a recent article, Scerri (2012) recog-nizes that the question of whether decoherence explains quantum measurement is a subtle matter, and refers to the review paper of Guido Bacciagaluppi (2012). In this paper Bacciagaluppi points out that, although naive claims of the kind that decoherence gives a complete solution to the measurement problem are still somewhat part of the "folklore" of the matter, decoherence as such does not provide that solution, at least not unless it is combined with an appropriate interpretation of quantum mechanics (for a detailed argument, see Fortin, Lombardi, & Martínez González, 2016).

In summary, the different answers to the problem of optical isomerism offered in the literature are far from conclusive. Perhaps it is time to follow an interpretive strategy: tackling the problem by means of an interpretation of quantum mechanics that can be applied not only to the abstract model of quantum measurement,

but also to situations commonly treated in the practice of physics and chemistry.

5. The modal-Hamiltonian interpretation

5.1. Modal interpretations

As advanced in the Introduction, modal interpretations are realist views, according to which the quantum state evolves unitarily and encodes possibility (Dieks & Vermaas, 1998). In spite of the differences among them, all the modal interpretations agree on the following points (Lombardi & Dieks, 2014):

- The interpretation is based on the standard formalism of quantum mechanics, without the projection postulate.
- The interpretation is realist: quantum systems possess definite properties at all instants of time and they do not depend on the observer.
- Quantum mechanics is conceived as a fundamental theory: it applies both to microscopic and macroscopic systems.
- The state of the system (pure or mixed) tells us what the possible properties of the system and their corresponding probabilities are.
- A quantum measurement is an ordinary physical interaction. There is no collapse: the state always evolves unitarily according to the Schrödinger equation.

Due to the constraints imposed by the Kochen-Specker theorem (Kochen & Specker, 1967), all the modal interpretations are committed to selecting the subset of definite-valued properties, that is, the preferred context. Therefore, despite the agreements, each modal interpretation supplies its own "rule of definite-value ascription" or "actualization rule." In the so-called Kochen-Dieks modal interpretation (Dieks, 1988; Kochen, 1985), the biorthogonal (Schmidt) decomposition of the pure quantum state of the system picks out the definite-valued observables. The Vermaas-Dieks version (Vermaas & Dieks, 1995), a generalization of the Kochen-Dieks interpretation to mixed states, is based on the spectral resolution of the reduced density operator: the range of the possible properties of a system and their corresponding probabilities are given by the non-zero diagonal elements of the spectral resolution of the system's reduced state, obtained by partial tracing.

These traditional modal interpretations, however, faced some difficulties. On the one hand, given the multiple factorizability of a given Hilbert space, their rules of definite-value ascription may lead to contradictions of the Kochen-Specker variety (Bacciagaluppi, 1995; Vermaas, 1997). This difficulty motivated the development of an atomic modal version (Bacciagaluppi & Dickson, 1999), based on the assumption that there exists a special set of disjoint systems, which are the building blocks of all other systems. That set fixes a preferred factorization of the Hilbert space; the properties of a system supervene on the properties ascribed to its "atomic" subsystems. In turn, Gyula Bene and Dennis Dieks (2002) developed a perspectival modal interpretation, according to which properties are not monadic but always have a relational character.

On the other hand, those traditional modal interpretations do not pick out the right properties for the apparatus in non-ideal measurements, that is, in measurements that do not introduce a perfect correlation between the possible states of the measured system and the possible states of the measuring apparatus (Albert & Loewer, 1990, 1991, 1993; Elby, 1993; Ruetsche, 1995). Since ideal measurement is a situation that can never be achieved in practice, this shortcoming was considered a "silver bullet" for killing modal interpretations (Harvey Brown, cited in Bacciagaluppi & Hemmo, 1996). Perhaps these problems explain the decline of the interest in modal interpretations since the end of the 90's. Jeffrey Bub's preference for Bohmian mechanics in those days can be understood in this context: given the difficulties of the modal interpretations whose preferred context depends on the state of the system, the natural alternative for a realist is Bohmian mechanics, which can be conceived as a member of the modal family whose preferred context is a priori defined by the position observable (Bub, 1997).

But position is not the only observable that can be appealed to in order to define the state-independent preferred context of a modal interpretation. The modal-Hamiltonian interpretation (MHI) (Castagnino & Lombardi, 2008; Lombardi & Castagnino, 2008) endows the Hamiltonian of a system with the role of selecting the subset of the definite-valued observables of the system. This makes the MHI immune to the non-ideal measurement's "silver bullet", since it accounts for ideal and non-ideal measurements (Lombardi & Castagnino, 2008): no matter whether the correlations between measured system and measuring apparatus are perfect or not, the apparatus' pointer observable always acquires a definite value. Furthermore, the MHI also supplies a criterion to distinguish between reliable and non-reliable measurements in the non-ideal case: despite the fact that correlations are not perfect, repeated measurements allow the experimenter to reliably reconstruct the state of the system under definite conditions (Lombardi & Castagnino, 2008; Ardenghi et al., 2013; Lombardi et al., 2015). This explains a common experimental fact: perfect correlation is not a necessary condition for "good" measurements. If the reliability condition is satisfied, then the coefficients of the system's state can be approximately obtained even when the correlation is not perfect. Nevertheless, both in the reliable and in the non reliable case, a definite reading of the apparatus' pointer is obtained in each single measurement.

As pointed out by Harvey Brown, Mauricio Suárez, and Guido Bacciagaluppi (1998), any interpretation that selects the set of the definite-valued observables of a quantum system in a given state is committed to considering how that set is transformed under the Galilean group. The study of this question is particularly urging in the case of realist interpretations, which conceive a definite-valued observable as a physical magnitude that objectively acquires an actual value among all its possible values: the actualization of one of the possible values must be an objective fact. Therefore, the set of the definite-valued observables of a quantum system should be left invariant by the Galilean transformations: from a realist viewpoint, it would be unacceptable that such a set changed as the mere result of a change in the perspective from which the system is described. This Galilean invariant feature cannot be guaranteed in the modal interpretations whose preferred context does not depend on invariant observables. On the contrary, in spite of the fact that the Hamiltonian is not Galilean invariant, the MHI can be reformulated under an explicitly Galilean-invariant form in terms of the Casimir operators of the Galilean group (Ardenghi et al., 2009; Lombardi et al., 2010). Such a reformulation not only leads to results that agree with usual assumptions in the practice of physics, but also suggests the extrapolation of the interpretation to quantum field theory by changing accordingly the symmetry group: the definite-valued observables of a system in to quantum field theory would be those represented by the Casimir operators of the Poincaré group, and the observables commuting with them and having, at least, the same symmetries. Since M and S^2 are the only Casimir operators of the Poincaré group, they would always be definite-valued observables (Ardenghi, Castagnino, & Lombardi, 2011). This conclusion stands in agreement with a usual physical assumption in quantum field theory: elemental particles always have definite values of mass and spin, and those values are precisely what define the different kinds of elemental particles of the theory.

In the MHI, decoherence is not explicitly appealed to in order to account for the definite value of the observables of the preferred context. The MHI perspective seems to be at odds with the decoherence program, according to which the decoherence of a system in interaction with its environment is what causes the apparent "collapse" that suppresses superpositions. However, this apparent conflict vanishes when the measurement situation is considered in detail. In fact, the measuring apparatus is always a macroscopic system with a huge number of degrees of freedom, and the pointer must be a "collective" and empirically accessible observable; as a consequence, the many degrees of freedom corresponding to the degeneracies of the pointer play the role of a decohering "internal environment". It can be proved that the states einselected by decoherence (but whose definite-valuedness the phenomenon of decoherence cannot explain) are precisely eigenstates of the observables selected by the MHI's rule of definite-value ascription (for a detailed explanation, see Lombardi, 2010; Lombardi, Ardenghi, Fortin, & Castagnino, 2011a, 2011b; Lombardi et al., 2012). The compatibility between the MHI and decoherence becomes clearer when the phenomenon of decoherence is understood from a closed-system perspective (Castagnino & Lombardi, 2004, 2005a, 2005b; Castagnino, Laura, & Lombardi, 2007; Castagnino, Fortin, & Lombardi, 2010, 2014; Lombardi & Fortin, 2016).

5.2. The postulates of the modal-Hamiltonian interpretation

By adopting an algebraic perspective, the MHI defines a quantum system S as a pair $(\mathscr{O}, H)$ such that (i) $\mathscr{O}$ is a space of self-adjoint operators acting on a Hilbert space $\mathscr{H}$, representing the observables of the system, (ii) $H \in \mathscr{O}$ is the time-independent Hamiltonian of the system S, and (iii) if $\rho_0 \in \mathscr{O}'$ (where $\mathscr{O}'$ is the dual space of $\mathscr{O}$) is the initial state of S, it evolves according to the Schrödinger equation.

A quantum system so defined can be decomposed in parts in many ways; however, not any decomposition will lead to parts which are, in turn, quantum systems. The expression 'tensor product structure' (TPS) is used to call any partition of a closed system S, represented in the Hilbert space $\mathscr{H} = \mathscr{H}_A \otimes \mathscr{H}_B$, into parts S_A and S_B represented in $\mathscr{H}_A$ and $\mathscr{H}_B$ respectively. Nathan Harshman and Sujeev Wickramasekara (2007a, 2007b) point out that quantum systems admit a variety of TPSs, each one leading to a different entanglement between their parts. However, there is a particular TPS that is invariant under time evolution: the TPS is *dynamically invariant* when there is no interaction between the parts. In other words, in the dynamically invariant case the components' behaviors are dynamically independent from each other; each one evolves unitarily according to the Schrödinger equation. On this basis, according to the MHI, a quantum system can be split into subsystems when there is no interaction among the subsystems.

Composite systems postulate: A quantum system S: $(\mathscr{O}, H)$, with initial state $\rho_0 \in \mathscr{O}'$, is *composite* when it can be partitioned into two quantum systems S^1: $(\mathscr{O}^1, H^1)$ and S^2: $(\mathscr{O}^2, H^2)$ such that (i) $\mathscr{O} = \mathscr{O}^1 \otimes \mathscr{O}^2$, and (ii) $H = H^1 \otimes I^2 + I^1 \otimes H^2$, (where I^1 and I^2 are the identity operators in the corresponding tensor product spaces). In this case, we say that S^1 and S^2 are *subsystems* of the composite system $S = S^1 + S^2$. If the system is not composite, it is *elemental*.

With respect to the preferred context, the basic idea of the modal-Hamiltonian interpretation is that the Hamiltonian of the system, with its own symmetries, defines the subset of observables that acquire definite actual values. The group of transformations that leave the Hamiltonian invariant is usually called "Schrödinger group" (Tinkham, 1964). Since each symmetry of the Hamiltonian leads to an energy degeneracy, much valuable information on the energy spectrum of the system can be obtained by applying the machinery of the group theory to the study of the symmetries of the Hamiltonian. The degeneracies with origin in symmetries are called "normal" or "systematic" (Cohen-Tannoudji, Diu, & Laloë, 1977). On the contrary, degeneracies that have no obvious origin in symmetries are called "accidental". However, deeper study usually shows either that the accidental degeneracy is not exact, or else that a hidden symmetry in the Hamiltonian can be found which explains the degeneracy. A classical example is the degeneracy, in the hydrogen atom, of states of different angular momentum l but the same principal quantum number n (for instance, 2s and 2p functions). In this case, Vladimir Fock (1935) showed that the degeneracy arises from a four-dimensional rotational symmetry of the Hamiltonian in momentum space. For this reason it is assumed that, once all the symmetries of the Hamiltonian have been considered, a basis for the Hilbert space of the system is obtained and the "good quantum numbers" are well defined. This strategy is what underlies the group approach to quantum mechanics, where the physical features of the quantum system are studied by analyzing the symmetry properties of its Hamiltonian (Tung, 1985; Weyl, 1950).

Now we have all the conceptual elements necessary to present the MHI rule of definite-value ascription, here called 'actualization rule'. The basic idea can be expressed by the classical Latin maxim "*Ubi lex non distinguit, nec nos distinguere debemus*": where the law does not distinguish, neither ought we to distinguish. The Hamiltonian of the system, with its symmetries, is what rules actualization; then, no observable whose eigenvalues would distinguish among eigenvectors corresponding to a single degenerate eigenvalue of the Hamiltonian has to acquire definite value, since its actualization would introduce in the system an asymmetry not contained in the Hamiltonian. Once this idea is understood, the actualization rule can be formulated in a very simple way.

Actualization rule: Given an elemental quantum system S: $(\mathscr{O}, H)$, the actual-valued observables of S are H and all the observables commuting with H and having, at least, the same symmetries as H.

Given an elemental quantum system S: $(\mathscr{O}, H)$, the actual-valued observables of S are H and all the observables commuting with H and having, at least, the same symmetries as H.

The justification for selecting the Hamiltonian as the preferred observable ultimately lies in the physical relevance of the MHI and in its ability to solve interpretive difficulties. Here we will focus on the first point, in order to show that the case of Hund's paradox can be counted as a further successful application of the interpretation.

5.3. Measuring as breaking symmetries

As already mentioned, the MHI scheme has been applied to several well-known physical situations, leading to results consistent with empirical evidence (see Lombardi & Castagnino, 2008, Section 5). Let us recall some of them, in order to stress the role played by symmetries in those situations.

The Hamiltonian of the free particle reads

$$H_{free} = \frac{P^2}{2m} = \frac{P_x^2 + P_y^2 + P_z^2}{2m} \qquad (8)$$

where P is the momentum observable, with components P_x, P_y, P_z, and m is the mass of the particle. H_{free} is invariant under space-displacements in any direction, and the components P_x, P_y, P_z are

the generators of the symmetry. Since the Hamiltonian is degenerate, the components of P need to be used for the theoretical description of the system: usually any two of them are added to H_{free} to constitute a complete set of commuting observables (CSCO), $\{H_{free}, P_x, P_y\}$, $\{H_{free}, P_y, P_z\}$ or $\{H_{free}, P_x, P_z\}$, that defines a basis of the Hilbert space. But this fact does not mean that those observables have to be considered definite-valued; in fact, this would be not possible since P_x, P_y, P_z do not commute with each other. The MHI is completely consistent with this fact: according to its actualization rule, H_{free} acquires a definite value, and also P^2 since it is proportional to H_{free}; nevertheless, P_x, P_y, P_z are not definite-valued because the actualization of any of them would introduce an asymmetry not contained in the Hamiltonian: it would *arbitrarily* break the symmetry of the free particle. This result of the application of the MHI agrees with the empirical non-accessibility to the values of P_x, P_y, P_z in the free particle. If we want to know those values, we must perform a measurement on the particle, in particular, a measurement that involves an interaction that breaks the symmetry of the original system by modifying its Hamiltonian. For instance, we can introduce a screen acting as a potential barrier that breaks the homogeneity of space. This means that, under measurement, the particle is no longer free: the symmetry breaking introduced by the interaction with the measuring system is what allows us to have empirical access to an observable that was a symmetry generator of the original free system.

In the case of the free particle with spin, the Hamiltonian is

$$H = H_{free} + H_{spin} = \frac{P^2}{2m} + k\,S^2 \tag{9}$$

According to the MHI, in this case the system is composite because it can be decomposed into two non-interacting subsystems: a free particle without spin, represented in $\mathcal{H}_{free}$ and with Hamiltonian $H_{free} = P^2/2m$, on which the rule applies as explained above, and a spin system, represented in $\mathcal{H}_{spin}$ and with Hamiltonian $H_{spin} = k\,S^2$, with $k = const$. The spin subsystem is invariant under space-rotation: the generators of this symmetry are the three components J_x, J_y, J_z of the total angular momentum J. But since in this case the orbital angular momentum L is zero, the total angular momentum $J = L + S$ turns out to be simply $J = S$, and the three components S_x, S_y, S_z of the spin S are the generators of the space-rotation symmetry. As in the previous case, the three observables S_x, S_y, S_z cannot simultaneously be definite-valued since they do not commute with each other. The MHI agrees with this fact: according to the actualization rule, in this case H_{spin} acquires a definite value, and also S^2 since it is proportional to H_{spin} (S^2 is the Casimir operator of the group generated by S_x, S_y, S_z); nevertheless, S_x, S_y, S_z are not definite-valued since they are the generators of the space-rotation symmetry, and the actualization of any of them would break the symmetry of H_{spin} in an arbitrary way. Again, this conclusion agrees with the fact that we have no empirical access to the spin components of the free particle with spin. If we want to know the value of those components, we have to perform a measurement on the system: we have to introduce a magnetic field B of modulus $|B|$ in some direction, say z, which breaks the isotropy of space and, as a consequence, the original space-rotation symmetry. Under the action of B, the Hamiltonian H_{spin} is not invariant under space-rotation anymore, because now it includes an interaction proportional to $|B|S_z$ that privileges a particular direction of space. In other words, we can have experimental access to the spin component S_z only by means of a measurement that breaks the space-rotation symmetry of the original Hamiltonian and, therefore, makes the system no longer free. This is the usual way in which a spin component is measured in a Stern-Gerlach experiment.

The Hamiltonian of the hydrogen atom reads

$$H_{free} = \frac{P_e^2}{2m_e} + \frac{P_p^2}{2m_p} + \frac{e^2}{|Q_e - Q_p|} \tag{10}$$

where the subindexes e and p refer to the electron and to the proton respectively, and e is the electric charge of the electron. When the spin of the electron is not considered, the atom is invariant under space-rotation, and the total angular momentum $J = L + S$ is simply $J = L$. Then, the three components L_x, L_y, L_z of L are the generators of the symmetry group. The possible states of the atom are labeled by the quantum numbers: the principal quantum number n, the orbital angular momentum quantum number l and the magnetic quantum number m_l, which correspond to the eigenvalues of the observables H, L^2 and L_z respectively. Since the Hamiltonian is degenerate due to its space-rotation invariance, the hydrogen atom is described in terms of the basis $\{|n, l, m_l\rangle\}$ defined by the CSCO $\{H, L^2, L_z\}$. Nevertheless, its space-rotation invariance makes the selection of L_z a completely arbitrary decision: given that space is isotropic, we can choose L_x or L_y to obtain an equally legitimate description of the free atom. The arbitrariness in the selection of the z-direction is manifested in spectroscopy by the fact that the spectral lines of the free hydrogen atom give no experimental evidence about the values of L_z: we have no empirical access to the number m_l of the free atom. The MHI agrees with those experimental results since it does not assign a definite value to L_z: the actualization of the value of L_z would arbitrarily break the symmetry of the Hamiltonian of the free hydrogen atom.

Analogously to the measurement on a free particle with spin, in the case of the hydrogen atom a magnetic field B along the z-axis breaks the isotropy of space and, as a consequence, the space-rotation symmetry of the atom's Hamiltonian. In this case, the symmetry breaking removes the energy degeneracy in m_l: now L_z is not arbitrarily chosen but selected by the direction of the magnetic field. But, in turn, this implies that the atom is no longer free: the Hamiltonian of the new system is approximately

$$H = H_{free} + \frac{e}{2m_e e} B\,L \tag{11}$$

where H_{free} is the Hamiltonian of the free atom. As a consequence, the original degeneracy of the $(2l + 1)$-fold multiplet of fixed n and l is now removed: the energy levels turn out to be displaced by an amount $\Delta\omega_{nlm_l}$, which is also function of m_l: this is the manifestation of the so-called *Zeeman effect*. This means that the Hamiltonian, with eigenvalues ω_{nlm_l}, is now non-degenerate: it constitutes by itself the CSCO $\{H\}$ that defines the preferred basis $\{|n, l, m_l\rangle\}$. According to the MHI actualization rule, in this case H and all the observables commuting with H are definite-valued: since this is the case for L^2 and L_z, in the physical conditions leading to the Zeeman effect both observables acquire definite values.

When the spectral lines of the hydrogen atom corresponding to $n > 1$ are examined at a very high resolution, they are found to be closely spaced doublets: the energy levels of the atom are affected by the "coupling" between the electron spin S and the orbital angular momentum L. Now the Hamiltonian of the system reads

$$H = H_{free} + H_{spin} + H_{s-o} \tag{12}$$

where H_{free} is again the Hamiltonian of the free atom, $H_{spin} = k\,S^2$ is the Hamiltonian of the spin, and H_{s-o} is the Hamiltonian representing the spin-orbit interaction. When the spin-orbit interaction is neglected ($H_{s-o} = 0$), the system is composite and can be described in terms of the basis $\{|n, l, m_l, s, m_s\rangle = |n, l, m_l\rangle \otimes |s, m_s\rangle\}$, where the $s(s + 1)\hbar^2$ are the eigenvalues of S^2, and the $m_s\hbar$ are the

eigenvalues of S_z. But when the spin-orbit interaction is taken into account, the observables L_z and S_z no longer commute with H and, therefore, they are not constants of motion of the system: it is usually said that m_l and m_s are not good quantum numbers anymore. Nevertheless, the Hamiltonian is still invariant under space-rotation: the components J_x, J_y, J_z of the total angular momentum J are the generators of the symmetry group. In turn, $J = L + S$ is the sum of the orbital angular momentum L and the spin angular momentum S, and $m_j = m_l + m_s$, where m_j corresponds to the eigenvalue of J_z. So, now m_j is a good quantum number. Then, the basis $\{|n, l, j, s, m_j\rangle\}$ of the Hilbert space of the system is defined by the CSCO $\{H, L^2, J^2, S^2, J_z\}$. In this case, the spin-orbit coupling removes the original degeneracy of the eigenvalues ω_{nl} of the atom with no coupling; therefore, the MHI actualization rule selects L^2, J^2 and S^2 as definite-valued observables, because all of them commute with H and have the same degeneracy in m_j as H. But the space-rotation symmetry still present in the system leads to a degeneracy of H, manifested by the fact that the energy eigenvalues ω_{nljs} do not depend on m_j. Then, according to the MHI, although in this case m_j is a good quantum number, J_z does not acquire a definite value, and this result agrees with the arbitrariness of the selection of the z-direction for J_z.

When a magnetic field is applied to the atom, the spectral lines split in different ways. The "normal" Zeeman effect, explained above, is observed in spin 0 states where, obviously, the spin-orbit coupling has no effect. In the states where the spin-orbit coupling is effective, the action of the magnetic field produces a further splitting of the energy levels known as *"anomalous" Zeeman effect*. Nevertheless, the explanation of the anomalous effect is the same as that of the normal effect: the action of the magnetic field along the z-axis breaks the space-rotation symmetry of the Hamiltonian by privileging the z-direction, and this leads to the removal of the original degeneracy of the Hamiltonian in the quantum number m_j (instead of in the quantum number m_l as in the normal effect). In this case, the MHI actualization rule prescribes that J_z will be also definite-valued, in agreement with the experimental accessibility of m_j.

All the cases described above point to a feature of the quantum measurement that is not noticed in the usual, merely formal treatments of the process. In fact, in the von Neumann model, the observable A to be measured on the system S of interest is considered in formal terms and deprived of its physical content. Then, the interaction between S and the measuring apparatus M is endowed with the only role of introducing the correlation between A and a pointer P. However, the physical situations just considered show that we have no empirical access to the observables that are generators of the symmetries of the system's Hamiltonian; and, in the context of measurement, A may be one of those observables. This is precisely the case in the Stern-Gerlach experiment, where S_z is a generator of the space-rotation symmetry of $H_{spin} = k\,S^2$; it is the interaction with the magnetic field $B = B_z$ that breaks the isotropy of space by privileging the z-direction and, as a consequence, breaks the space-rotation symmetry of H_{spin}.

This physical account of quantum measurement shows that, when the observable A to be measured on the system S is a generator of a symmetry of the Hamiltonian H_S of S, the interaction with the apparatus M not only must establish a correlation between A and the pointer P, but also must break that symmetry. Therefore, from a physical viewpoint, measurement can be conceived as a process that breaks the symmetries of the system to be measured and, in this way, allows us to have access to an otherwise empirically inaccessible symmetry-generator observable. This suggests that the formal von Neumann model of quantum measurement should be complemented by a physical model in terms of which measurement is a symmetry breaking process that renders a symmetry generator of the system's Hamiltonian empirically accessible.

6. The modal-Hamiltonian account of optical isomerism

In the light of the above account of quantum measurement, now Hund's paradox can be rephrased in MHI's language.

As explained in Section 3, the exact Hamiltonian H of an enantiomer molecule is symmetric under spatial reflection: it commutes with the parity observable P (see eq. (1)). Now, let us consider the observable C, whose eigenstates are $|D\rangle$ and $|L\rangle$, and call it *chiral-rotation*: the eigenvalues d and l of C represent the properties dextro-rotation and levo-rotation, respectively. The observable C should be definite-valued for the molecule to be dextro-rotatory (D) or levo-rotatory (L).

It is easy to see that C does not commute with H: $[C, H] \neq 0$. As in the examples of the previous section, in this case the actualization of the observable C would determine the rotation property of the molecule in a completely arbitrary way: it would introduce in the molecule an asymmetry not contained in its Hamiltonian. As a consequence, from the MHI viewpoint, the observable C of the enantiomer molecule is not definite-valued, that is, it does not belong to the preferred context. In other words, strictly speaking the isolated molecule is not dextro-rotatory (D) or levo-rotatory (L): chiral-rotation is a property that has no definite value in it.

The fact that chiral-rotation does not have a definite value in the isolated molecule is compatible with experience: we have no experimental evidence of the handedness of an *isolated* molecule. In order to make chiral-rotation manifest as a definite-valued property, it is necessary to interact with the molecule. But the necessary interaction must be such that it breaks the parity symmetry of the original Hamiltonian H. More precisely, the molecule must interact with another system M, which plays the role of the apparatus, in such a way that the Hamiltonian H_T of the new composite system is no longer parity invariant. For instance, this happens when

$$H_T = H + H_M \tag{13}$$

where the Hamiltonian H_M of the new system breaks the original parity invariance of H: $[H_M, P] \neq 0 \rightarrow [H_T, P] \neq 0$. Additionally, the observable C must commute with the total Hamiltonian H_T in order to obtain a stable reading of chiral-rotation. Under these conditions, according to the MHI C acquires a definite actual value: we measure dextro-rotation or levo-rotation. However, now the system is no longer the isolated molecule, but the molecule in interaction with the measuring system M.

This is precisely what happens when the molecule rotates the plane of polarization of plane-polarized light. In this case, a good candidate for H_M is the Hamiltonian usually introduced in quantum chemistry to describe the interaction between molecules and polarized light (see Shao & Hänggi, 1997), which is a function of the electric field $\bar{E}$ and the magnetic field $\bar{B}$ of the light. Therefore, the observable C turns out to be a definite-valued observable of the new composite system. In other words, optical activity is not an intrinsic property of the molecule, but of the system 'molecule plus light'. In a certain sense, this answer to Hund's paradox agrees with the view according to which the solution must be sought in the interaction of the molecule with its environment. However, our approach does not appeal to decoherence, but relies on an interpretation of quantum mechanics that explicitly accounts for measurement from the perspective of the symmetries of the system.

It is important to stress that, from the MHI viewpoint, symmetries are not conceived as generated by the spatial shapes of molecules: symmetries are internal features of the Hamiltonian of the

whole closed system; they do not have to be conceived in terms of spatial configurations. According to the MHI, it is not correct to suppose that an enantiomer molecule has, before being observed, a definite handedness depending on its shape, and that such a property is discovered when the molecule interacts with a system with the opposed handedness. From the MHI perspective, isolated molecules have no definite handedness; this property becomes definite when the molecule turns into a part of a composite system that is no longer parity symmetric.

As well known by chemists, optical activity is stably correlated with other properties, usually conceived as structure-based as the property of optical activity itself: if, say, dextro-rotation is observed, the corresponding values of the correlated properties must also be observed. In theoretical terms, the definite value of chiral-rotation must lead to the definite-valuedness of those properties, and the actual value acquired by chiral-rotation must be correlated with the actual values acquired by the correlated properties. This can easily be explained in the context of the MHI. In fact, if the properties are stably correlated with chiral-rotation C, they must be represented by observables that commute with and are functionally related to the observable C. Therefore, according to the MHI, if the molecule interacts with another system in such a way that C acquires a definite value in the new composite system, then the observables commuting with C will also acquire a definite-value. In turn, the functional relation between C and those commuting observables guarantees the proper correlations between their actual values. Summing up, from the viewpoint of the MHI, the same symmetry breaking that explains why a definite value of chiral-rotation is observed also explains why the definite values of the properties correlated with chiral-rotation are also observed.

The problem of isomerism is a particular case of what can be called, following Woolley and Sutcliffe (1977), the *symmetry problem* in chemistry: if the interactions embodied in the Hamiltonian of the molecule are Coulombic, the solutions of the Schrödinger equation have certain symmetries that cannot account for the asymmetries of the molecular structure. For instance, Coulombic molecules are spherically symmetrical; however, the asymmetry of polyatomic molecules is essential in the explanation of their chemical behavior. As Hendry stresses, according to quantum mechanics an isolated molecule in a general energy eigenstate may possess no directional property (Hendry, 1998, p. 131). The author considers the example of the hydrogen chloride molecule, which has an asymmetrical charge distribution that explains its acidic behavior and its boiling point; however, according to quantum mechanics, the expectation value of the dipole moment of a molecule in an arbitrary eigenstate of the full molecular Hamiltonian is always zero. On this basis, he concludes that "*if the acidic behaviour of the hydrogen chloride molecule is conferred by its asymmetry, and the asymmetry is not conferred by the molecule's physical basis according to physical laws, then surely there is a prima facie argument that ontological reduction fails.*" (Hendry, 2010, p. 186). The MHI casts new light on this problem, since it suggests that, although the isolated molecule lacks the necessary asymmetry, an adequate interaction may break the symmetry of the original Hamiltonian in the way needed to explain the asymmetric features that become manifest when the system is experimentally measured.

7. Conclusions

In the context of the debates about the nature of molecular structure, in this paper we have focused on Hund's paradox, derived from the difficulty in giving a quantum explanation for optical isomerism. We have revised different attempts to solve the paradox, in particular, the widespread appeal to decoherence in recent literature; we have argued that none of these attempts is completely successful. On this basis, we have recalled the main features of the MHI in order to show how this interpretation offers a solution of Hund's paradox in exclusively quantum terms.

Since its first formulation in 2008, the MHI was developed in several articles, and was presented many times to varied audiences. It is interesting to notice the different reactions to the same proposal. Philosophers of physics usually insist on requiring the justification for the selection of the Hamiltonian as the key to determine the preferred context, by claiming that no basis of the Hilbert space has a privileged status. By contrast, philosophers of chemistry (and chemists) are always surprised by our insistence in justifying that selection, since in chemistry it is usual to work in the basis of the energy. In fact, the MHI is in resonance with molecular chemistry, in the context of which molecules are almost always described in their stationary states, that is, in eigenstates of the Hamiltonian, and a great deal of relevant knowledge is obtained from studying the symmetries of the Hamiltonian. The MHI account to optical isomerism fits in the framework of this resonance.

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