Chapter X

Quantum mechanics and molecular structure: the case of optical isomers

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X.1.- Introduction

From its birth, quantum mechanics enjoys great prestige thanks to its success in the explanation and prediction of phenomena at the atomic and molecular scales. Indeed, this theory comes explaining the emission lines observed in the hydrogen atom, and in a few years it can explain the energy spectrum of simple molecules. This type of success, quickly leads scientists to ensure that all chemistry can be explained and reasoned from the physical. An example of this, is the famous Dirac's assertion: "*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). However, over time it has been possible to establish that in the attempt to explain chemistry from physics arise complications that allow to question Dirac's claim. One of these problems is to explain the molecular structure from quantum mechanics. There are many ways to approach this problem but in this work we will do it by introducing a particular case: optical isomers and Hund's paradox.

When young Kant meditated upon the distinction between his right hand and his left hand, he could not foresee that the problem of incongruent counterparts would revive in the twentieth century under a new form. The so-called Hund paradox points to the difficulty of giving a quantum explanation to chirality, that is, to the difference between the members of a pair of optical isomers or enantiomers. The question about whether the quantum formalism can account for chirality concerns philosophy of chemistry for (at least) three reasons. First, it introduces an interesting case for the debate about the relation between physics (quantum mechanics) and chemistry (molecular chemistry), which has been the focus of many philosophical works in recent years. Second, and related to the previous point, the analysis of the paradox can enrich the discussion about whether quantum mechanics can provide an explanation of molecular structure. Third, since some approaches attribute the origins of the paradox to a focus on isolated molecules, the solution is believed to be found in considering molecules in interaction; these views pose a relevant question to the ontology of chemistry: is chirality an intrinsic property of a molecule? These three problematic matters make the resolution of the Hund paradox an issue of the utmost importance for the philosophy of science.

On this basis, in the present article we will analyze the problem of optical isomerism by proceeding in the following steps. In Section 2, the Hund paradox will be presented in formal terms. Section 3 will be devoted to show the relevance of the paradox to the relation between physics and chemistry, to the explanation of molecular structure, and to the ontology of chemistry. In Section 4 the paradox will be conceptualized as a case of quantum measurement, stressing that decoherence does not offer a way out of the problem. Finally, in Section 5 it will be argued for the need to adopt a clear interpretation of quantum mechanics; in particular, we will claim that the modal-Hamiltonian Interpretation (MHI), which conceives measurement as a breaking symmetry process, supplies the tools required to solve the Hund paradox.

X.2.- The Hund Paradox

As it is well known, an empirical formula indicates the elements in a compound and their relative proportions, but it does not offer information about the geometric structure of the molecule. Molecules with the same empirical formula but differing in the spatial disposition of their atoms are called isomers. The class of isomers includes the subclass of optical isomers or enantiomers: the members of a pair of enantiomers are mirrorimages of each other; the property that distinguishes them is called chirality. The peculiarity of enantiomers of a same compound is that they share almost all their chemical and physical properties. They only differ in how they rotate the plane of polarization of plane-polarized light. Depending on the direction of the rotation, dextrorotation or levo-rotation, optical isomers are called *D* or *L*.

The problem of the enantiomers was first formulated by Friedrich Hund (1927), pioneer in the development of quantum chemistry. From a structural point of view, the two members of a pair of enantiomers have the same bonds: the “distance between atoms” is the same. Since the quantum Coulombic Hamiltonian depends only on the inter-nuclear distances, the Hamiltonian is exactly the same for the two members of the pair. Consequently, quantum mechanics provides the same description for two chemical species that can effectively be differentiated in practice by their optical activity (Harris and Stodolsky 1981, Wolley 1982, Berlin et al. 1996, Quack and Stohner 2005, Schlosshauer 2007).

In the quantum domain, the parity operator $\hat{P}$ is associated with spatial reflection: if $|D\rangle$ and $|L\rangle$ are the states of isomers D and L respectively, $\hat{P}$ transforms $|D\rangle$ into $|L\rangle$ and vice versa: $\hat{P}|L\rangle = |D\rangle$, $\hat{P}|D\rangle = |L\rangle$. Let us suppose that the molecule consists of A atomic nuclei and N electrons. Then, the Coulombic Hamiltonian of the complete molecule is

$$\hat{H} = \sum_{g}^{A} \frac{P_g^{\,2}}{2m_g} + e^2 \sum_{g<h}^{A} \frac{Z_g Z_h}{2m_g} + \sum_{N}^{i} \left(\frac{P_i^2}{2m_e} - e^2 \sum_{g}^{A} \frac{Z_g}{\hat{r}_{ig}} \right) + e^2 \sum_{i<j}^{N} \frac{1}{\hat{r}_{ij}} \tag{X.1}$$

where $\hat{P}_g$, Z_g and m_g are the momentum operator, the atomic number and the mass of the nucleus g, respectively, with $g = 1, 2, ..., A$; e and m_e are the charge and the mass of the electrons respectively; $\hat{P}_i$ is the momentum operator of the electron i, with $i = 1, 2, ..., N$; $\hat{r}_{ij}$ is the operator "distance" between the electron i and the electron j, and $\hat{r}_{ig}$ is the operator "*distance*" between the electron i and the nucleus g. Since the Coulombic interaction only depends on the distance between the interacting particles, it is symmetric under spatial reflection; therefore, the Hamiltonian commutes with the parity operator $\hat{P}$:

$$\left[\hat{P}, \hat{H}\right] = 0 \tag{X.2}$$

This means that the eigenstates $|\omega_n\rangle$ of the Hamiltonian have definite parity. In particular, the ground state $|\omega_0\rangle$ is invariant under space reflection: $\hat{P}|\omega_0\rangle = |\omega_0\rangle$. As a consequence, $|\omega_0\rangle$ cannot be a chiral state $|D\rangle$ or $|L\rangle$, but it is a superposition of them:

$$|\omega_0\rangle = \frac{1}{\sqrt{2}}\left(|D\rangle + |L\rangle\right) \tag{X.3}$$

The question is, then, why chiral molecules are never found in this superposition state. The states obtained in the laboratory are $|D\rangle$ and $|L\rangle$, which are not eigenstates of the Hamiltonian and do not correspond to the ground state. So, why do certain chiral molecules display an optical activity that is stable over time, associated to a well-defined chiral state? Why do chiral molecules have a definite chirality? (Berlin et al.1996). The Hund paradox points to the core of certain traditional problems of the philosophy of chemistry. Let us consider them briefly.

X.3.- Interteoric relationships and molecular structure

The relationship between chemistry and physics is one of the hottest topics in the philosophy of chemistry. In this context, the links between theories coming from the two disciplines have been explored with great detail from different perspectives. However, despite this effort, there is still no agreement with respect to the best intertheoretic relationship model to describe those links. Although the idea of reducing different disciplines to physics is much older, the success of the applications of quantum mechanics to chemical systems turned reduction into a regulative idea in the accounts of the relationship between chemistry and physics. Following Dirac's famous dictum (1929), the idea that chemistry can be reduced to quantum mechanics pervaded both the communities of physics and of chemistry. The approximations necessary for such a reduction led to the constitution of quantum chemistry as a new area of scientific research (Gavroglu and Simões 2012). However, frequently the approximate methods distort the principles of quantum mechanics in such a way that the interpretation of the intertheoretical links as reductive is seriously disputed (Woolley 1978, 1982; Primas 1983). In fact, the strategies that make possible the description of chemical phenomena in quantum terms, such as the Born Oppenheimer approximation or the models of Valence Bond and Molecular Orbital, do not strictly satisfy the conditions of Nagelian reduction: not only they establish loose and non-continuous connections between chemistry and physics (Lombardi 2014), but they also introduce assumptions that stand in conflict with quantum mechanics itself (Lombardi and Castagnino 2010).

The case of enantiomers would provide a new insight in the discussion about the reduction of chemistry, because it involves a difficulty that does not depend on approximations. In this case the challenge is more fundamental since it stands beyond the Born-Oppenheimer approximation. In fact, even if we cannot write down the exact Hamiltonian due to its complexity, we know that it only depends on the distance of the component particles and, therefore, it cannot account for the difference between the members of a pair of enantiomers.

X.3.1. The concept of molecular structure

Molecular structure, given by the spatial arrangement of the nuclei in a molecule, is a main character of molecular chemistry: it is "the central dogma of molecular science" (Woolley 1978, 1074), since it plays a key role in the explanation of reactivity. However, the concept of molecular structure finds no comfortable place in the theoretical framework of quantum mechanics, inasmuch as it appeals to the classical notion of individual nuclei in fixed positions. This problem can be viewed as a particular manifestation of the general problem of the intertheoretical links between molecular chemistry and quantum mechanics. Following the traditional reductionist perspective, some authors consider that the difficulties are only due to our partial knowledge of the molecular systems in the theoretical framework of quantum mechanics (Sutcliffe and Woolley 2011, 2012).

From the opposite perspective, Robin Hendry (2004, 2008, 2010), who rejects the epistemological reduction of chemistry to physics, claims that the problem of molecular structures must be addressed within the ontological domain: the interesting philosophical question is how the entities and processes studied by different disciplines are related to each other. In particular, the author considers that the links between quantum mechanics and molecular chemistry, embodied in the problem of molecular structure, must be conceived non-reductively, in terms of emergence. Optical isomerism introduces a new perspective to the discussion. In fact, the difference between two enantiomers lies in their structure. But, again, in this case no arguments concerning how to interpret approximations in quantum mechanics are involved: the Hund paradox arises in terms of the exact Hamiltonian of the molecules. Due to this particularity, a clarification of the paradox would certainly enrich the debate about whether quantum mechanics can provide an explanation of molecular structure.

X.3.2. The ontology of chemistry

Although not as extensively treated as the relationship between chemistry and physics, a central topic in the philosophy of chemistry is that related with the ontology of chemistry, that is, with the object of study of the discipline (see Hendry 2016). The central question in this field of inquiry is about what items inhabit the realm of chemistry and what ontological categories they belong to. For instance, certain works analyze the nature of the chemical bond (Vemulapalli 2008, Hendry 2012), the reference of the concept of chemical orbital (Labarca and Lombardi 2010, Llored 2010), or even the ontological status of electronegativity (Leach 2013). The common ground in those discussions is the effort to identify and to categorize chemical properties. Does the term ‘chemical bond’ have an ontic reference? Is the shape of the orbitals a real property or a mere theoretical tool? Is electronegativity an intrinsic property of atoms or a loosely defined property of elements?

From a traditional perspective, chirality was usually conceived as an intrinsic property of molecules, defined by the molecular structure. But, more recently, some approaches consider that the Hund paradox is the consequence of focusing on isolated molecules. From this viewpoint, then, the solution must be based on studying the interactions in which the molecule is involved. Therefore, chirality would no longer be a property of a particular molecule, but rather it would turn out to express the result of a relation linking the molecules with its environment. This view, that modifies the traditional ontological picture regarding chirality, began to prevail with the development of the theory of decoherence.

X.3.3. The reductionist program: Quantum mechanics plus

Hinne Hettema (2009, 2012) claims that molecular structure can be understood in term of reduction in the light of certain recent developments in quantum chemistry, such as the Quantum Theory of Atoms in Molecules, from now QTAiM (Bader 1994).

The QTAiM was introduced by Richard Bader in the nineties and is based on the fact that the distribution of electron density associated to the atoms and molecules represents the physical manifestation of matter in space (Bader 2010b). Therefore, the topology of electron density encodes and reflects the concepts of atom, bond, structure and structural stability (Bader 2011). In this way, Bader argues that a theory based on electron density allows to link the language of chemistry with that of physics. According to Bader, the atoms are bounded by a zero-flux surface in the gradient vector field, which is a result of the dominant morphology of the electron density distribution, which leads to the natural partition of the molecular space into mononuclear regions associated to the atoms. The zero-flux surface is not crossed by any trajectory of the gradient vector field. This fact can be interpreted in principle as no electron crosses said surface, in such a way that the electron density of each atom in the molecule remains unchanged over time.

Likewise, it is possible to define the molecular structure by mean of critical points at which the gradient vector is canceled. A local maximum is associated to nuclear positions and a saddle point is linked to a chemical bond (according to the theory is particularly called bond path). Moreover, with the help of these critical points the classical view of molecular structure with “balls and sticks” is recovered through the molecular graphs, which are constructed by employing “balls” to represent nuclear positions and “sticks” to represent bond paths (Bader 2010a). Under this context, QTAIM claims to offer a reductionist scheme for molecular structure. In the author words: *The reductionist approach afforded by QTAIM offers a clear solution to the myriad of personal views and models of bonding. As has been amply demonstrated by appeal to physics, the presence of a bond path linking a pair of atoms fulfills the sufficient and necessary conditions that the atoms are bonded to one another. This definition, which necessarily applies to quantum mechanical densities, transcends all bonding schemes and categories and provides a unified physical understanding of atomic interactions.*

One assumes such unification to be a primary goal of any physical theory (Bader 2011, page 20).

QTAiM was very successful to describe many chemical molecules. However, it is doubtful that it is a reduction of chemistry by quantum mechanics:

- Bader discards the wave function and adopts the density of electrons as a fundamental entity.
- QTAim considers that the maximum of electron density are the positions of the atoms ¿why? Is this a new postulate of quantum mechanics?
- The theory find zero flux surfaces and it say that this surfaces encloses atoms. However, it doesn't consider the holism of quantum systems and its peculiar individuality problems.

Bader itself present his theory as an extension of quantum mechanics for chemical systems. Then, he has to modify quantum mechanics to obtain his results. The idea of modifying quantum mechanics to achieve the results of chemistry is not acceptable in a reductionist program with ontological pretensions. In fact, the most accepted proposal to describe molecular structure (in general and isomers in particular) from quantum mechanics is based on quantum decoherence (Eric Scerri 2011).

X.4.- Decoherence, enantiomers and quantum measurement

As explained in Section 2, the ground state of the molecule is not one of the chiral states $|D\rangle$ or $|L\rangle$, but a superposition of them (see eq. (3)). Then, why do we always find the molecule either in the state $|D\rangle$ or in $|L\rangle$? It is not hard to see that the question is the same as that of the quantum measurement problem: following Schrödinger's famous example, if the cat is in a superposition of "alive" and "dead", we have to explain why we always see the cat dead or alive. In technical terms, the problem is to explain why we measure definite values of an observable when the system is in state of superposition of the eigenstates of that observable. In the particular case of chirality, the problem is to account for the fact that, although the molecule is in a superposition of the chiral states, it always manifests a definite chirality.

The orthodox answer to the measurement problem is the collapse hypothesis (or von Neumann's projection postulate), according to which, when we measure the system, the state collapses to one of the states of the superposition. Then, if the result of a single measurement is, say, dextro-rotation, then the system is actually in the state $|D\rangle$:

$$|\omega_0\rangle = \frac{1}{\sqrt{2}}\left(|D\rangle + |L\rangle\right) \rightarrow |D\rangle \tag{X.4}$$

If many measurements are performed on identical systems with the same initial conditions, it is possible to define an ensemble, whose state is represented by a density operator:

$$\hat{\rho}_{collapsed} = \frac{1}{2}\left(|D\rangle\langle D| + |L\rangle\langle L|\right) \tag{X.5}$$

This state is interpreted as stating that there is a probability 0.5 of finding the system in the state $|D\rangle$ and a probability 0.5 of finding the system in the state $|L\rangle$: the state is a mixture of equal number of definite chiral states. The collapse hypothesis is very successful in reproducing the experimental results, but has no explanatory power to the extent that it is an *ad hoc* hypothesis specifically designed to account for the quantum measurement problem. Moreover, collapse is a non-unitary process that breaks the Schrödinger evolution; however, the hypothesis does not explain why or when the process happens. For this reason, during the last decades quantum measurements have been approached from different perspectives; one of them is that given by the theory of decoherence.

According to the orthodox approach −the so-called environment induced decoherence (Zurek 1981, 1993, 2003), decoherence is a phenomenon resulting from the interaction between an open quantum system with its environment. Let us consider a closed system U with two subsystems: the open system S in the initial state $\hat{\rho}_S$, and the environment E in the initial state $\hat{\rho}_E$. Then, the initial state of the total system is $\hat{\rho}_U = \hat{\rho}_S \otimes \hat{\rho}_E$. This state evolves in a unitary way according to the Schrödinger equation. But the theory of decoherence studies the behavior of the reduced state of the open system, $\hat{\rho}_{redu} = Tr_E\left(\hat{\rho}_U\right)$, obtained by applying the partial trace on the state of the whole closed system; the partial trace in an operation that removes the degrees of freedom of the environment from $\hat{\rho}_U$. As a consequence, the reduced state of the open system is no longer governed by the Schrödinger equation, but is ruled by a master equation: $\hat{\rho}_{redu}$ may evolve in a non-unitary way. Moreover, when the number of degrees of freedom of the environment is very high, the reduced state may become diagonal and mimic the $\hat{\rho}_{collapsed}$ obtained by means of the collapse hypothesis (see eq. (5)).

In the Editorial 37 of the journal *Foundations of Chemistry*, Eric Scerri (2011) explicitly relates the problem of optical isomerism to the quantum measurement problem. According to the author, the Hund paradox would dissolve if the interaction of the molecule with its environment were taken into account: “The study of decoherence has shown that it is not just observations that serve to collapse the superpositions 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). The idea is that the enantiomer molecule is in interaction with the environment (air, particles, other molecules, etc.). If the initial states of the molecule and the environment are $|\omega_0\rangle$ and $|\varepsilon_0\rangle$ respectively, the initial state of the whole system is $\left(1/\sqrt{2}\right)\left(|D\rangle+|L\rangle\right)\otimes|\varepsilon_0\rangle$.The interaction between the molecule and its environment define the evolution of the total system, which, in some cases, produces a correlation between the possible states of the system and the environment:

$$\frac{1}{\sqrt{2}}\left(|D\rangle+|L\rangle\right)\otimes|\varepsilon_0\rangle \rightarrow \frac{1}{\sqrt{2}}|D\rangle\otimes|\varepsilon_D\rangle+\frac{1}{\sqrt{2}}|L\rangle\otimes|\varepsilon_L\rangle \qquad \text{(X.6)}$$

Decoherence occurs when, as the result of the evolution, the states of the environment become rapidly orthogonal: $\langle\varepsilon_L|\varepsilon_L\rangle\rightarrow 0$. As a consequence, after an extremely short decoherence time, the reduced state of the molecule acquires the same structure as that of the mixed state after collapse (see eq. (5)):

$$\hat{\rho}_{decoh}=\frac{1}{2}\left(|D\rangle\langle D|+|L\rangle\langle L|\right) \qquad \text{(X.7)}$$

As in the case of the quantum measurement, this state is interpreted as stating that the molecule is in one of the states $|L\rangle$ or $|D\rangle$, and probabilities measure our ignorance about which that state is. In this way, the theory of decoherence would solve the problem underlying Hund paradox.

Although there was a time when decoherence was considered the “new orthodoxy” in the physical community to explain quantum measurements (Leggett 1987, Bub 1997), at present it is quite clear that decoherence does not solve the measurement problem. In fact, collapse is the change of the state of the system, from a superposition to a definite state; on this basis, $\hat{\rho}_{decoh}$ can be interpreted as a legitimate mixture. On the contrary, in the case of decoherence, the state of the whole system never collapses, but evolves always according to the Schrödinger equation: the superposition never vanishes through the unitary evolution. Therefore, it cannot be supposed that what is observed at the end of the decoherence process is one of two definite events: either that associated with $|L\rangle$ or that associated with $|D\rangle$ (see Adler 2003). Jeffrey Bub (1997) even claims that the assumption of a definite event at the end of the process not only is unjustified, but also contradicts the eigenstate-eigenvalue link. These conclusions about decoherence can also be drawn from the traditional distinction between a proper mixture −the mixed state of a closed system− and an improper mixture −the reduced state of an open system: as Bernard d'Espagnat (1966, 1976) repeatedly stressed, improper mixtures cannot be interpreted in terms of ignorance (for additional arguments, see Fortin and Lombardi 2014).

Summing up, at present some authors still consider that decoherence, by itself, solves many conceptual problems in quantum physics (e.g. Crull 2015). Nevertheless, in the community of the philosophy of physics it is well known that, although decoherence is a powerful tool to deal with conceptual problems, it does not dispense us from interpreting the formalism (Vassallo and Esfeld 2015). In the next section we will follow precisely an interpretive path to deal with the Hund paradox.

X.5.- Symmetry breaking, enantiomers and MH interpretation

As it is well-known, the contextuality of quantum mechanics, derived from the KochenSpecker theorem, implies that all the observables of a quantum system cannot acquire definite actual values simultaneously. Therefore, any realist interpretation of quantum mechanics is forced to select a preferred context, that is, the set of the definite-valued observables of the system. The modal-Hamiltonian interpretation (MHI, Lombardi and Castagnino 2008, Lombardi, Castagnino and Ardenghi 2010) is a realist, non-collapse interpretation that places the Hamiltonian of the system in the center of the stage: according to the modal-Hamiltonian actualization rule, the observables that acquire actual definite values are the Hamiltonian $\hat{H}$ and all the observables that commute with $\hat{H}$ and have, at least, its same symmetries (that is, that do not break the symmetries of $\hat{H}$).

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. In fact, the MHI actualization rule has been applied to several well-known physical situations, leading to results consistent with empirical evidence (Lombardi and Castagnino 2008, Section 5), and accounts for quantum measurements both in the ideal an in the non-ideal cases (Lombardi and Castagnino 2008, Section 6, Lombardi, Fortin and López 2015). In the present discussion about the Hund paradox, the relevant point is that the MHI describes measurement as a symmetry-breaking process: measurement breaks the symmetry of the Hamiltonian and, then, turns an otherwise non-actualized observable into an actually definite-valued observable, which becomes thus empirically accessible.

As a simple example, let us consider the case of a free particle. In this case the Hamiltonian is symmetric under space-displacements in all space directions: all the directions are equivalent with respect to the linear motion of the particle. The three components of the momentum, P_x , P_y , P_z , are the generators of this symmetry, but they cannot acquire definite values simultaneously because they do not commute with each other. According to the MHI, none of these three observables belong to the preferred context: they are not definite-valued observables because they have less symmetries than $\hat{H}$, and this means that the actualization of any of them would distinguish a direction of space in a completely arbitrary way. Let us now suppose that we want to measure one of those observables, say, the component P_y in direction *y*. For this purpose, we have to place a wall normal to the direction *y*, in such a way that the new Hamiltonian is the original one plus a term that represents the asymmetric potential barrier. It is precisely this term that breaks the symmetry of the original Hamiltonian and renders the observable P_y actually definite-valued and, as a consequence, accessible to measurement. But the point to stress here is that now the system is no longer the free particle: it is a new system, whose Hamiltonian is not symmetric with respect to displacements in direction *y*.

In the light of these interpretive ideas, now the Hund paradox can be rephrased in MHI's language. As stressed in Section 2, the exact Hamiltonian $\hat{H}$ of the enantiomeric molecule (see eq.(1)) is symmetric under spatial reflection: it commutes with the parity operator $\hat{P}$ (see eq. (2)). Now, let us consider the observable chirality $\hat{C}$, whose eigenstates are $|D\rangle$ and $|L\rangle$: the eigenvalues *d* and *l* of $\hat{C}$ represent the properties dextro-rotation or levo-rotation, respectively. It is easy to see that $\hat{C}$ does not commute with $\hat{P}$: $\left[\hat{P},\hat{C}\right] \neq 0$. As in the above example of the free particle, in this case the actualization of the observable $\hat{C}$ would determine the chirality 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, $\hat{C}$ has no actual value: chirality is indefinite in the isolated molecule.

If the observable $\hat{C}$ is to be measured, the parity symmetry of the molecule has to be broken. For this purpose, the molecule must interact with another system *M*, which plays the role of the apparatus, in such a way that the Hamiltonian $\hat{H}_T$ of the new composite system is no longer parity invariant. For instance, this is obtained when

$$\hat{H}_T = \hat{H} + \hat{H}_M$$

where the Hamiltonian $\hat{H}_M$ of the new system breaks the original parity invariance: $\left[\hat{H}_M,\hat{P}\right] \neq 0 \Rightarrow \left[\hat{H}_T,\hat{P}\right] \neq 0$. A good candidate for $\hat{H}_M$ is the Hamiltonian usually introduced in quantum chemistry to describe the interaction between molecules and polarized light (see Shao and Hänggi 1997), which is a function of the electric field $\hat{H}_T$ and the magnetic field $\overline{B}$ of the light. Additionally, $\hat{C}$ must commute with the total Hamiltonian $\hat{H}_T$ in order to obtain a stable reading of chirality. Under these conditions, according to the MHI the observable $\hat{C}$ acquires a definite actual value: we measure dextro-rotation or levo-rotation, but now the system is no longer the isolated molecule, but the molecule in interaction with the polarized light. In a certain sense, this answer to the Hund paradox agrees with the view according to which the solution must be looked for in the in interaction of the molecule with its surroundings: chirality is not an intrinsic property of the molecule, but of the composite system molecule plus polarized light. However, our view does not appeal to decoherence, but rather to an interpretation of quantum mechanics that explicitly accounts for measurement from the perspective of the symmetries of the system.

X.6.- Final remarks

In this paper we have argued that the problem of enantiomers cannot be solved by appealing to decoherence, but it requires a precise interpretation of quantum mechanics capable to deal with quantum measurement. In particular, we have shown that the MHI provides us with the adequate tools, since it conceptualizes measurement as a symmetry breaking process. It is important to stress that, nevertheless, this result does not supply an indisputable answer to the problem of molecular structure. In fact, the proposed interpretive approach only accounts for the different behavior of the members of a pair of enantiomers in their interaction with polarized light, but it does not take a stand about molecular structure understood as a spatial geometric property. This is an issue that deserves a further discussion, even in the context of the present solution of the Hund paradox.

X.7.- References

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