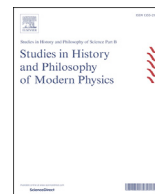




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A new application of the modal-Hamiltonian interpretation of quantum mechanics: The problem of optical isomerism

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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.

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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 inter-theoretic 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

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