About the Nature of the Wave Function and its Dimensionality: The case of Quantum Chemistry

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Abstract: The problem of the 3N dimensions of the wave function is of particular interest in the philosophy of physics. In this work, we will recall the main positions about the nature and dimensionality of the wave function and we will introduce a new perspective, coming from quantum chemistry. For this, we will bring to light the formal operations that underlie the Independent Electron Approximation. We show that the concept of the orbital is closely linked to this approximation. Therefore, its characterization as an approximation must be questioned. On this basis, we will point out how quantum chemistry can offer new arguments that contribute to the debate about the ontology of wave function.

1. Introduction

The wave function is a central element in quantum mechanics, since it represents the state of the system and participates in its dynamics through its evolution according to the Schrödinger equation. However, even today, almost a hundred years after the advent of quantum mechanics, the meaning of the wave function remains a matter of debate. In this context, the problem of the $3N$ dimensions of the wave function is of particular interest in the philosophy of physics. In fact, the debates around the issue have an important impact on the way in which we conceive the world around us. This is clearly manifested by the intense discussions that have taken place in recent years (see Monton, 2006; Ney and Albert; 2013).

From his early work, Schrödinger tried to endow the wave function with a physical meaning, first as a kind of vibration in the atom (Schrödinger, 1926a) and later as a tool for obtaining the electron density (Schrödinger, 1926b). With these proposals, Schrödinger intended to develop an ontology of the wave function in a space of three dimensions, in agreement with the world in which we live. However, some years later he was disappointed with those ideas.

In recent years, different views regarding the dimensionality of wave function have been proposed. On the one hand, it is possible to propose an ontology in which the wave function is the most relevant element of quantum theory, so that its mathematical nature is directly related to "reality" (e.g. Albert, 2013). In spite of the fact we only perceive three dimensions, the authors who advocate for this position, commonly called "wave function realism", consider that the real physical space has actually $3N$ dimensions. On the other hand, the wave function can be conceived as a mere mathematical artifact belonging to the formalism of quantum mechanics. The defenders of this view usually postulate a "primitive ontology" that inhabits a real space with only three dimensions (e.g. Monton, 2013; Allori, 2013). Finally, there is a third position that tries to reconcile the two previous ones. It proposes an ontological picture in which both the space of $3N$ dimensions and that of three dimensions coexist (e.g. Monton, 2006). This discussion is still relevant not only in the philosophy of physics, but also in physics.

In this work we will introduce a new perspective, coming from quantum chemistry, an area of study arising from the direct interaction between quantum mechanics and molecular chemistry. In the field of quantum chemistry, the question about the $3N$ dimensions of the wave function has not been discussed as deeply as in the context of quantum mechanics. In fact, even the most theoretical objects of chemists exist in real space; hence, it is natural to try to turn the wave function into a three-dimensional entity. In the context of quantum chemistry, it is common to use the so-called *orbital approximation*, which allows chemists to write the total wave function of a system as a product of mono-electron wave functions (see, e.g, Atkins and de Paula, 2006). Under this approximation, the wave function of an electron depends only on the variables of this electron; therefore, it evolves in the space of three dimensions (Lowe and Peterson, 2006). We will consider how quantum chemists use this approximation, which can be conceived as a particular case of the so-called *independent electron approximation*. On this basis, we will show that it is possible to formalize quantum chemists' strategies as the result of the application of two mathematical operations: first, a projection in Hilbert space and, then, a change of variables. This formalization will allow us to go beyond the approximation itself by propose a new version of the idea of a primitive ontology, now from the perspective of quantum chemistry.

For these purposes, we have structured the work in the following way. In Section 2 we will introduce a brief historical review of Schrödinger's proposals on this subject. Then, in Section 3, we will recall the main positions about the nature and dimensionality of the wave function. We will continue with the detailed description of the orbital approximation, as a particular case of the independent electron approximation in Section 4. In Section 5, we will bring to light the formal operations that underlie the independent electron approximation. Finally, in Section 6, we will point out how quantum chemistry can offer new arguments that contribute to the debate about the ontology of wave function.

2. Schrödinger's Wave Function

In 1926 Schrödinger published a series of papers in which he introduced his theory of wave mechanics. He postulated the now well-known Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\Psi=\left[-\frac{\hbar^2}{2m}\overline{\nabla}^2+V\right]\Psi\,, \qquad (1)$$

where $\Psi(\overline{r}_1,\overline{r}_2,...,\overline{r}_N)$ represents the wave function, which depends on the spatial coordinates $\overline{r}_i =,(x_i, y_i, z_i)$ of all the particles of the system. Then, the wave function depends on $3N$ dimensions, where N is the number of particles in the system.

The dimensionality of the wave function was a problem that Schrödinger did not ignore, and he addressed it from the very beginning. Very early in his work, he wanted to give a physical meaning to the wave function by associating it with a vibration process in the atom (Schrödinger, 1926a). However, he later pointed out that it is only in the case of a single electron that the interpretation as a vibration in real space of three dimensions can be sustained (Schrödinger, 1926b). When the system has two or more particles, the wave function inhabits a space of six or more dimensions, so it cannot be conceived as a wave in the common three-dimensional space.

In the last of his articles of 1926, Schrödinger emphasizes the idea of dispensing with the wave function in the direct interpretation of physical phenomenon, relegating its use to obtain what he called the *density of electricity* (Schrödinger, 1926c), a quantity that he supposes does have a direct physical meaning and is defined in the space of three dimensions. The process by which he obtains this quantity is described in a letter to Lorentz:

> $\psi * \psi$ (just as ψ itself) is a function of 3*N* variables or, as I want to say, of *N* three dimensional spaces, $\overline{r}_1, \overline{r}_2, ..., \overline{r}_N$. Now first let $\overline{r}_1$ be identified with the real space and integrate $\psi * \psi$ over $\overline{r}_2, ..., \overline{r}_N$; second, identify $\overline{r}_2$ with the real space and integrate over $\overline{r}_1, \overline{r}_3, ..., \overline{r}_N$; and so on. The *N* individual results are to be added after they have been multiplied by certain constants which characterize the particles (their charges, according to the former theory). I consider the result to be the *electric charge density* in real space. (Schrödinger, in Przibram, 1967: 56; emphasis added).

In this way Schrödinger offers a wave-function ontology based on electric charge density. However, later Schrödinger set aside this approach, and by 1935 expressed his regret in the following terms: “I am long past the stage where I thought that one can consider ψ-function as somehow a direct description of reality.” (quoted in Fine, 1996: 82).

The aim of developing an ontology for the wave function in three dimensions, which motivated Schrödinger in the 1920’s, reappeared in the present-day discussions about the nature of the wave function.

3. Positions about the Nature of Wave Function and its Dimensionality

The problem about the nature of the wave function and its dimensionality has been addressed in the light of questions such as: does the wave function have a real physical meaning or is it merely a mathematical artifact? If it has physical meaning, what does it represent? And, in that case, does the real physical space have 3*N* dimensions or only the three that we perceive in our daily life? These and other questions arise naturally from the need to make quantum mechanics more intelligible, one of the most successful and counterintuitive physical theories. Next we will review the different philosophical positions on this issue in the recent bibliography. The intention is not to be exhaustive or go too deep, but to show that this is an important discussion in philosophy of physics that remains current.

In the recent philosophical literature, at least three positions can be identified regarding the dimensionality of the wave function: one that conceives the wave function as the basic ontological item in a 3*N*-dimensional physical space, an opposite view that retains the three-dimensional physical space and deprives the wave function of a basic ontological role, and an intermediate position that admits the coexistence of both spaces.

Some authors, such as David Albert, defend the idea of retaking a realistic project in which scientific exploration informs us about what the world is like. Then, an ontology where the wave function in 3*N* dimensions represents the physical reality is proposed. In short, it is established that the wave function is a real physical entity. So the dimensionality of the wave function shows that the real world has 3N dimensions and the 3 dimensions we see are just an illusion (Albert 2013). The problem of this position, commonly called "wave function realism", is that the real ontology turns out to be radically different from the way in which the world around us is perceived. According to Albert, the appearances in the three-dimensional space are a dynamical result: ultimately, what it means *to be* an object in the real world "is to occupy a certain location in the causal map of the world", and the form in which geometric appearances are constructed is due to a question of *dynamics* (Albert, 2013: 54). So, in accordance with Albert, the Hamiltonian determines the way in which we can perceive the objects of the real world from elementary particles that constitute them.

Peter Lewis (2004), in turn, although conceiving the wave function as the central element of quantum mechanics, considers that its dependence on 3*N* variables is only the most convenient way to represent the correlations between quantum particles. The wave is a function of spatial parameters (positions of particles), but these do not necessarily have to be related to the spatial dimensionality of the system. Under this view, the wave function is a real entity but not a 3D spatial entity. Then, the 3N dimensions of quantum mechanics can be taken as three-dimensional in a relevant sense (Lewis 2004). This is a position similar to the one that we adopt with the spin. The spin part of the wave function has dimensions that are not spatial. Lewis says the same with the surplus dimensions of the wave function. Indeed, Lewis admits that the common use of the notion of *spatial* corresponds to a three-dimensional space. Nevertheless, he does not rule out the possibility that, in a future paradigm, the use of '*spatial*' will change in favor of a notion corresponding to a 3*N*-dimensional world (For a review of Lewis's ideas 10 years later see Lewis 2013).

The other option is to discard the central role of the wave function from the construction of the ontology, that is to relegate the wave function to a secondary role. This is the case of Bradley Monton (2013), who claims that the wave function can be defined by the properties of the system. From this perspective, within quantum mechanics the wave function represents an state of the system and the observables, i. e., the system properties, are given by lineal operators that act on the wave function. When the system has a well defined property, we have that the wave function corresponds to an eigenstate of that property and the eigenvalues corresponds to the results obtained in a measurement of that property. Then, the information about the system contained in the wave function is "carried" by the properties in the real space of three dimensions; hence, the wave function itself is not indispensable. Then, the real world has 3 dimensions but the wave function has a physical meaning only when it is an eigenstate of some observables. In this way, it is not necessary to take into account all the degrees of freedom of the wave function because it has a weak ontology (Monton 2013), and we can save the traditional 3-dimensional physical space.

In the same end of the spectrum stand those positions that look for a *primitive ontology* as the reference of quantum mechanics. According to this view, any physical theory must try to account for the world in which we live, a world that is constituted by entities in a three-dimensional space. These entities are the foundation of the real world, and the theory must describe them and account for their time evolution. Then, the theory must include primitive variables associated with this ontology, and non-primitive variables that describe the way in which the former change over time (Allori, 2013). In the context of this position, the wave function turns out to be a *non-primitive variable*, which describes the dynamics of particles, whose representative magnitudes are the *primitive variables*.

The third intermediate position is briefly outlined by Morton (2006), who introduces two versions. In the first one, two independent spaces coexist, one of 3*N* dimensions where the wave function evolves, and the three-dimensional space where the *N* particles evolve. What remains to be explained is the type of connection that links these two spaces: the problem is that, although there is a lawful relationship, in principle there is no causal link between them. In the second version, the two spaces are hypersurfaces of a space of ($3N$+3) dimensions, which might be the stage for a kind of causal connection, however it is still unclear what kind of connection could link the two spaces.

A common feature of all the arguments in the debate is that they rely on very abstract elements: the discussions are confined to the quantum mechanics as a formal theory. But if science is a practice, the way in which quantum mechanics is used should also be taken into account. But quantum mechanics is not used in the same way in different disciplines. In particular, it is interesting to consider how quantum chemists integrate quantum mechanics in the core of their theoretical practice in order to open new ontological questions.

4. A Different Approach from Quantum Chemistry

Schrödinger original view about the *electric charge density* was rapidly dismissed in the physicists' community and, for this reason, it was never taken seriously into account in the philosophy of physics. But this is not the case in quantum chemistry, where it reappears under the name of '*electronic density*' as the central element of the discipline.

The issue of the dimensionality of the wave function is not an object of debate in the field of quantum chemistry. Although both physicists and chemists deal with phenomena that occur in a three-dimensional space, physicists are used to appeal to very abstract entities that go beyond the features of our perceived physical world. By contrast, even the most abstract entities studied by chemistry inhabit the three-dimensional space. This particularity is inherited by quantum chemistry: molecules, its main object of study, are three-dimensional objects, and the links between their components are relationships in three-dimensional space. Therefore, it is no surprising to find that a basic theoretical move in quantum chemistry is to turn the wave equation into a three-dimensional entity.

In this theoretical background, the usual story proceeds as follows. Given the impossibility to apply quantum mechanics in an exact way to the study of chemical systems, alternative approximate methods have been developed. The most popular of them is the so-called *orbital approximation*. This is not a very precise approximation since it ignores electronic interactions. Nevertheless, it is a powerful tool for the study of molecular structure. As Peter Atkins and Julio de Paula point out in their famous textbook:

> The wave function of a many-electron atom is a very complicated function of the coordinates of all the electrons, and we should write it $\psi(\overline{r}_1,\overline{r}_2,...)$ where $\overline{r}_i$ is the vector from the nucleus to electron *i*. However, in the *orbital approximation* we suppose that a reasonable first approximation to this exact wavefunction is obtained by thinking of each electron as occupying its "own" orbital, and write
>
> $$\psi(\overline{r}_1,\overline{r}_2,...)=\psi(\overline{r}_1)\,\psi(\overline{r}_2)...$$
>
> We can think of the individual orbitals as resembling the hydrogenic orbitals, but corresponding to nuclear charges modified by the presence of all the others electrons in the atom. This description is only approximate, but it is a useful model for discussing the chemical properties of atoms, and is the starting point for more sophisticated descriptions of atomic structure. (Atkins and de Paula, 2006: 336).

This approach is what justifies the fact that phrases like "the 2p orbital of a fluorine atom is compact" are common in the chemists' discourse. According to quantum mechanics, the 2p orbital is an eigenfunction of the Hamiltonian of an atom with only one electron. Since a fluorine atom has 9 electrons, the 2p orbital is not an eigenfunction of its Hamiltonian. However, under the orbital approximation chemists can talk about the 2p orbital of a fluor atom and to make inferences with it.

The orbital approximation is very imprecise because it does not take into account the interaction between the electrons in the atoms. However, the procedure can be refined in the so-called *independent electron approximation*, by taking into account the interactions but at the same time retaining an orbital for each electron. Consider a chemical system of N electrons that interact with each other, and that are influenced by the Coulomb potential of the positive charges of nuclei. The Hamiltonian of that system is given by the following equation (in atomic units),

$$\hat{H}=-\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2-\sum_{i=1}^{N}V(\overline{r}_i)+\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{1}{r_{ij}}\,, \qquad (2)$$

where the $\overline{r}_i$ are the coordinates of each electron of the system, the first term corresponds to the kinetic energy, the second term includes the traditional coulombic potentials $V(\overline{r}_i)$ due to the nucleus-electron attraction, and the third term represents the electric repulsion between each pair of different electrons, where the distance between them is $r_{ij} = \left|\overline{r}_i - \overline{r}_j\right|$.

The difficulty to solve this equation lies in the third term, since it couples the electron motions. A way to solve this problem is to consider that each electron moves in an average potential due to the rest of electrons, in such a way that its motion is decoupled from the others; in this way, the Hamiltonian turns out to be a function of a single electron and the Schrödinger equation can be solved using independent wave functions $\psi_i(\overline{r}_i)$ for each electron. Precisely, the Hamiltonian takes the form

$$\hat{H}' = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - \sum_{i=1}^{N} V(\overline{r}_i) + \sum_{i=1}^{N} v(\overline{r}_i), \tag{3}$$

Now, the new problem is to determine the form of the potential $v(\overline{r}_i)$ for each electron, a problem not trivial at all, since it involves fundamental information about the interaction between all the remaining electrons inside a chemical system. The solution to this difficulty has been the subject of intense research in the field of quantum chemistry. Just to mention two of the most important approaches: the Hartree-Fock method and the density functional theory (see Gill, 1998). In the former, the wave functions ψ_i are used to obtain the potential $v(\overline{r}_i)$, while in the latter the electron densities $\rho(\overline{r})$ is appealed to.

The simplest form to solve the problem is to consider that electrons do not interact with each other, so the term corresponding to the interelectronic interaction is neglected and the equation (3) becomes,

$$\hat{H}_{OA} = -\frac{1}{2}\sum_{i=1}^{N}\nabla_i^2 - \sum_{i=1}^{N} V(\overline{r}_i) = \sum_{i=1}^{N} h(\overline{r}_i), \tag{4}$$

where $h(\overline{r}_i)$ represents a hydrogen-like Hamiltonian. In this way, the orbital approximation is recovered. Since each mono-electron Hamiltonian $h(\overline{r}_i)$ corresponds to an hydrogenic ion, its eigenfunctions are the same as those of the Hamiltonian of the hydrogen atom, i.e., 1s, 2s, 2p, … etc., and are called *atomic orbitals*. It is interesting to stress that these atomic orbitals are one of the foundations for the construction of the electronic configurations of the atoms according to the periodic table.

As it is quite clear, either when interelectronic interactions are considered or when they are neglected, the wave function of the total system, which depends on the coordinates of all the electrons, is approximated by combinations of monoelectron wave functions, each one of them is a functioof the coordinates of a single electron. This shows that, long before arriving at the problem of interpretation the 3*N* dimensions of the wave function, quantum chemists face a calculation problem. Then the theory is intervened, modified: the wave function of 3*N* dimensions is transformed into *N* wave functions of three dimensions in real space, one for each electron. As we will see, this strategy, which originally arises as a computational need, becomes the conceptual basis to conceive the nature of quantum-chemical systems.

5. Dimensional Marginalization

In order to understand how the wave function is conceived by quantum chemistry, but now from the viewpoint of physics, the strategy described in the previous section will be mathematically formalized.

The wave function $\psi(\overline{r}_1, \overline{r}_2, ..., \overline{r}_N)$ of a molecule is defined in a space of 3N dimensions, since it is a function of the variables $\overline{r}_1, \overline{r}_2, ..., \overline{r}_N$. As usual in these cases, we assume that the wave function is separable (the results can be generalized to the more general case):

$$\psi(\overline{r}_1, \overline{r}_2, ..., \overline{r}_N) = \psi(\overline{r}_1)\,\psi(\overline{r}_2) ... \psi(\overline{r}_N)\,, \tag{5}$$

However, in the independent electron approximation, this function is somehow projected onto a three dimensional space. Indeed, according to the standard procedure, it is said that the function $\psi(\overline{r}_i)$ corresponds to the orbital occupied by electron *i*, and this orbital is represented in the physical space of three dimensions. This means that the label that identifies the electron *i* is transferred from the variable to the function

$$\psi(\overline{r}_i) \;\rightarrow\; \psi_i(\overline{r})\,, \tag{6}$$

Therefore, a change of variables is introduced, which makes possible to represent the different orbitals in the same physical space.

From a mathematical viewpoint, this procedure can be formalized as the result of the successive application of a projector $\hat{P}_i$, followed by the application of an operator $\hat{C}$ that changes the variables to mono-electron wave functions:

a) In the first step, a projector $\hat{P}_i$ is defined as an operator that selects the mono-electron wave function that corresponds to electron *i* and eliminates the rest. This can be done by means of the following mathematical operation:

$$\hat{P}_i\,\boldsymbol{\psi}(...) = \int ... \int \boldsymbol{\psi}(...)\,\psi^*(\bar{r}_1)d\bar{r}_1 ... \psi^*(\bar{r}_{i-1})d\bar{r}_{i-1}\psi^*(\bar{r}_{i+1})d\bar{r}_{i+1} ... \psi^*(\bar{r}_N)d\bar{r}_N\,, \qquad (7)$$

Where $\boldsymbol{\psi}(...) : \psi(\bar{r}_1, ..., \bar{r}_{i-1}, \bar{r}_{i+1}, ..., \bar{r}_N)$. Then, the application of $\hat{P}_i$ to $\psi(\bar{r}_1, \bar{r}_2, ..., \bar{r}_N)$ gives the desired result:

$$\hat{P}_i\,\psi(\bar{r}_1, \bar{r}_2, ..., \bar{r}_N) = \psi(\bar{r}_i)\,, \qquad (8)$$

b) In the second step, the operator $\hat{C}$ can be defined as:

$$\hat{C}\,\psi(\bar{r}_i) = \psi_i(\bar{r}) \quad \text{for } i = 1, ..., N \qquad (9)$$

Thus, the successive application of $\hat{P}_i$ and $\hat{C}$ describe the implicit operation in the independent electron approximation:

$$\hat{C}\,\hat{P}_i\,\psi(\bar{r}_1, \bar{r}_2, ..., \bar{r}_N) = \psi_i(\bar{r}) \qquad (10)$$

Since this operation extracts a mono-electron wave function from the total wave function of $3N$ dimensions and projects it onto a three dimensional space, it can be called *dimensional marginalization*.

6. Toward an Ontology of Quantum Chemistry

Various compatibility problems between quantum mechanics and chemistry are shown in several of the Chapters of this book. Faced with the fait accompli that there are compatibility problems, it is possible to adopt three positions. The conservative position will try to smooth the rough edges between disciplines. Either from a reductionist or emergentist position, it is possible to work from a technical and conceptual point of view to reconcile chemical and physical concepts. The introduction of decoherence and other modern quantum techniques invoked by authors such as Scerri 2011 or Franklin and Seifert 2020 have this objective (see also Trost and Hornberger 2009 and Scerri 2013). As an alternative, it is possible to adopt a more radical position according to which the incompatibilities between physics and chemistry show that there are insurmountable differences that make a joint description of the phenomena impossible. This position has two versions, the first invites us to abandon the concepts coming from chemistry, considering them outdated and incompatible with those of modern physics. This position should not be confused with reductionism, it is not about reducing chemistry to physics, but about abandoning certain concepts as obsolete in a similar way to which the epicycles were abandoned in cosmology. This is the direction that Sutcliffe and Woolley take when they point to the incompatibility between quantum mechanics and molecular structure (see Sutcliffe and Woolley 2012 and their chapter in this book). Finally, within the group of those who consider the differences between chemistry and physics irreconcilable are those who claim for the ontological independence of chemistry. According to this position, if concrete scientific practice is considered then there are enough arguments to consider that chemistry develops and evolves in contact with physics but conceptually independent of it. Chemistry takes from physics what is useful to it, and combines this with elements of chemistry to give rise to different theories and procedures. As in practice, these theories or procedures are developed without any concern about whether or not they will be compatible with the ontology of quantum mechanics, there is a conceptual and ontological independence of chemistry. The works of Lombardi and Labarca (2005 and 2010) are framed in this trend (see also Fortin *et al*. 2021, and Fortin and Lombardi 2021), same as Klaus Ruthenberg chapter in this book. The present work is framed precisely in this last tendency. The argument that follows attempts that the 3N-dimensional problem can contribute to the development of an ontology of its own for quantum chemistry.

As explained in the previous sections, although according to quantum mechanics the wave function of a molecule cannot be expressed in terms of just three variables, in the field of quantum chemistry endowing each electron with its own wave function is a standard procedure that lies at the very core of the discipline and, as a consequence, has more implications than a mere approximation.

When trying to solve the Schrödinger equation applied to chemical systems, quantum chemists use the orbital approximation for simple cases, and the independent electron approximation for more complex situations. By means of these strategies, the energy levels in chemical systems can be computed; besides this, it make possible to describe the electronic structure in systems of relative complexity.

In Chapter 5 of this book there is an in-depth analysis of the meaning and characteristics of approximations and idealizations. There, it is shown that the well-known Born-Oppenheimer approximation is not a true approximation. This is very important because confusing an approximation with an idealization, or simply with the act of exchanging one system for another, can have profound consequences in the ontology (for a full discussion on this topic see the Chapter 5 of this book). The names given to the procedures known as "independent electron approximation" and "orbital approximation" imply that, these strategies used by quantum chemists are mere approximations. As such, they should be only formal tools designed to obtain approximate solutions of an equation that cannot be solved with complete precision. As Norton (2012: 207) says, "approximations merely describe a target system inexactly"; they do not even carry the novel semantic import carried by idealizations. In Frigg and Hartmann's words, "approximation is a purely formal matter" that is introduced in a mathematical context (2017: 8). As a mere tool, the effectiveness of an approximation lies in the adequacy of the results that it allows to obtain. If the practical or formal obstacles to obtain the exact solution were overcome, the approximation could be removed. To the extent that approximations are in principle eliminable, they carry no conceptual import: they do not discover new properties of the target nor supply new elements for explanations.

However, the above characterizations do not apply to the independent electron approximation used in quantum chemistry. The idea that each electron can be described by its three-dimensional wave function is at the core of the discipline and shapes the quantum-chemical picture of the molecule: a structure given by the geometrical disposition of the nuclei, and electrons that can be conceived as particles that "occupy" the orbitals, identified by the wave functions of the hydrogen atom (1s, 2s, etc.). The orbital approximation is an approximation since it ignores the interaction between the electrons of this quantum-chemical target. But even when the interactions are reintroduced, the global wave function of 3N-dimensions is not recovered: the target is still described in terms of monoelectronic wave functions. In this case, quantum chemists often describe the situation as follows: the 1s orbital was modified with the new correction, but the idea of each electron with its orbital is not set aside. In the context of this picture, the Hartree-Fock method and the density functional theory are only approximations to compute the potential that each electron “sees” in the presence of the rest of the electrons of the molecule. But even if the computational obstacles could be removed and the exact inter-electronic interactions could be computed, this would not remove the assumption that the behavior of each electron is described by its own wave function, now modified accordingly.

This quantum chemical picture also plays an essential role in the explanations of the processes that occur in atoms and molecules. For example, in order to explain that the SF_6 compound exists while the OF_6 does not, although both oxygen and sulfur have the same external electronic structure (two s-electrons and four p-electrons), it is usually argued that the difference is that the sulfur is in the third period while the oxygen is in the second period of the periodic table. Let us see the argument. Sulfur has two electrons in a 3s orbital and four in two 3p orbitals; therefore, it has a free 3p orbital, but also has five free 3d orbitals, and they allow it to extend its valence shell to be bonded with many fluorine atoms. In the case of oxygen, the external electronic structure consists in two electrons in a 2s orbital and four in two 2p orbitals. But the difference is that there are no 2d orbitals, so oxygen only has one free orbital (one 2p-orbital). Then it can only be linked to 2 fluorine atoms and the OF_6 does not exist while the OF_2 does. Explanations of this kind do not make any sense from the physical point of view, because according to quantum mechanics there are not mono-electronic wave functions, but only multi-electronic wave functions in a space of $3N$ dimensions. However, even if considered approximate, they offer a clear understanding of many molecular phenomena: the chemistry of molecules could not exist without them. And the scientific status of these studies cannot be denied, in the light of their empirical success not only in describing and predicting phenomena, but mainly in creating new substances.

The above considerations point to the fact that, actually, the so-called ‘independent electron approximation’ is not a mere approximation, but it is at the basis of a conceptual framework specific of quantum chemistry. In this framework, the notion of orbital as monoelectronic wave function plays a central role, since it is indispensable in the descriptions of the electronic structure in atoms and molecules and the explanation and production of molecular phenomena. This points to the fact that, when the empirical success of quantum chemistry is take into account, it is not easy to conceive the description in terms of monoelectronic wave functions as a mere fiction that could be left aside in favor of a more precise description of the molecular realm. On the contrary, it should be accepted that there is a quantum-chemical ontology, that is, the particular reference of quantum chemistry, that is essentially different than the ontology of quantum mechanics (whatever it be) (see Lombardi and Labarca, 2005; Labarca and Lombardi, 2010).

Now, the question is: what is the relationship between the quantum-chemical ontology and that based on pure quantum mechanics? According to a traditional reductionist view, in spite of its scientific efficiency, the quantum-chemical ontology is an appearance arising from a coarse description of the quantum world. However, the reductionist position faces several difficulties, in general derived from the fact that incompatible assumptions, coming from structural chemistry and quantum mechanics, coexist in quantum chemistry and constitute the theoretical body of the new discipline (Lombardi, 2014; Fortin, Lombardi, and Martínez González, 2017, 2018). If the antireductionist stance is adopted, then the quantum-chemical ontology can be conceived as the primitive ontology of quantum chemistry, different from the primitive ontology corresponding to the quantum realm (see Allori, 2013; Esfeld, Lazarovici, Hubert, and Dürr, 2013; Egg and Esfeld, 2015). But the full discussion of the issue of the intertheory relation in this case is beyond the limits of the present article, and will be addressed in a future work.

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