

# Ontological perspectives in crystal solids

Sebastian Fortin

CONICET – Universidad de Buenos Aires, Buenos Aires, Argentina

Matias Pasqualini

CONICET – Universidad Nacional de Rosario, Rosario, Argentina

email: [sfortin@conicet.gov.ar](mailto:sfortin@conicet.gov.ar)

## Abstract

This paper addresses the issue of the different levels of description of matter and the relationships between them. Specifically, it focuses on the area of crystalline solids, a topic that has been scarcely analyzed in the philosophy of chemistry. Unlike other cases where the relevant levels are clearly defined, the scientific practice related to crystals introduces new entities, such as phonons, which complicate the ontological landscape. In order to organize the discussion, the conceptual implications of describing crystals through three distinct levels are explored: the atomistic, the phononic, and the crystal as a whole. Existing proposals for understanding the phenomenon are analyzed, and based on the introduction of the Tensor Product Structure approach, it is argued that the ontological perspectives of crystals depend on external criteria beyond the formalism that describes them. In the absence of external criteria, a pluralistic ontology is obtained, granting equal status to all entities. On the other hand, privileging the total system or the fundamental components leads to holistic or atomistic ontologies, respectively.

## Keywords

Crystal Solids; Ontological Dependence; Phonons; Emergence; Tensor Product Structures.

## 1.- Introduction

The development of the philosophy of chemistry at the end of the 20th century has been shaped by various debates regarding the relationship between different conceptions of matter arising from distinct levels of description. Addressing these issues has necessitated revisiting and deepening certain discussions within the philosophy of physics, as both disciplines are deeply interconnected when it comes to the ultimate nature of matter. For example, debates have focused on the relationship between the microscopic and macroscopic levels of chemistry, particularly by examining the connections between thermodynamics and statistical mechanics in a gas composed

of molecules (Weisberg et al. 2016). Similarly, the relationship between atoms and molecules has been analyzed in light of discussions about the classical limit, decoherence, and different interpretations of quantum mechanics (Franklin and Seifert 2024, Fortin and Lombardi 2021, Martínez González et al. 2019, Fortin *et al.* 2017).

These and other debates have explored the relationships between entities and theories through concepts such as reduction, emergence, supervenience, and pluralism. Nevertheless, not all of chemistry revolves around molecules, and we argue that examining intertheoretical relationships in the context of other states of matter is equally significant. This paper, therefore, investigates intertheoretical relationships in crystalline solids. The case of crystals, however, presents an additional complexity. While matter is typically described in terms of atoms or molecules interacting with each other, scientific practice suggests that, in the case of crystals, it is more effective to adopt a different framework: that of phonons. Thus, even prior to addressing macroscopic issues, quantum mechanics involves three distinct levels of description: the traditional atomistic level, the phononic level, and the crystalline structure as a whole.

A crystalline solid is usually described as a periodic arrangement of atoms or molecules; let us assume they are simple atoms. In this picture atoms may have relative motion with respect to the rest. Then they are vibrating atoms that may create waves that propagate sound and heat. The significance of these waves propagating within the crystal extends beyond the obvious, as their characteristics have a direct impact on the properties of crystals, such as thermal expansion, heat capacity, thermal conductivity, electrical conductivity, and more. To describe these phenomena, an alternative description can be adopted: the crystalline solid is described as a lattice of fixed atoms and a new particle is introduced. This particle carries the acoustic or thermal energy, and it is known as phonon. The case of phonons is interesting because, this model not only simplifies the calculations that must be performed, but it also provides a picture of the phenomenon that greatly facilitates the explanation of the processes. Nevertheless, they are still considered entities with the diminished ontological status. According to the traditional way of describing the situation, phonons are not "real" particles but merely a mathematical device to simplify calculations. However, in recent years, a proposal has been introduced suggesting that phonons can be understood as an emergent phenomenon. The aim of this paper is to expand this discussion by introducing a perspective that clarifies the formal relationships between the crystal, the vibrating atoms, and the phonons. Based on this, the paper will explore various possibilities for the ontological description by postulating different assumptions. To fulfill this purpose, Section 2 will provide a concise overview of the mathematical formalism commonly employed to describe crystalline solids and deduce phonons. Section 3 will present an example demonstrating

how phonons can be understood as an emergent phenomenon. In Section 4, we will closely examine the mathematics that gives rise to phonons, demonstrating that both vibrating atoms and phonons belong to the same theory, making it difficult to consider phonons the result of an inter-theoretical emergence. Then, the Tensor Product Structure (TPS) approach, is introduced to facilitate the study of the relationship between the whole and its parts in a quantum system. This formalism shows that both descriptions of the crystal refer to the same total system but differ in how they divide the whole into parts. Furthermore, it will be demonstrated that without the introduction of an external criterion, it is impossible to select one partition as the ontologically privileged one. Finally, in Section 5, it will be showed that adopting different criteria makes it possible to consider the ontological description of a crystal in different manners. Without introducing any criterion, a pluralistic ontology is obtained, where the crystal, phonons and vibrating atoms are considered on equality. With the introduction of a criterion that privileges the total system, one arrives at a holistic ontology, concluding that phonons and atoms do not correspond to any ontological entity and are merely tools. On the other hand, with the introduction of a criterion that privileges fundamental systems, an atomistic ontology is attained. In this framework, one of the descriptions is taken as fundamental, from which the other can be derived in accordance with inter-theoretical emergence.

## 2.- What is a phonon?

This section summarizes the conventional method of introducing phonons as presented in textbooks. Such an overview is essential, as a thorough examination of the calculations can unveil details that are critical for the accurate interpretation of the phenomenon. A crystalline solid is normally thought of as a group of units in a periodic arrangement and bounded by an interaction. Typically, textbooks use a simplified version of a crystalline solid. While a real crystal has three dimensions and the interactions between its components can be complex, many of its general properties can be studied using a one-dimensional model with a harmonic interaction. Furthermore, the units can be atoms or complex molecules, but initially only atoms are considered. Thus, a first classical model is considered, consisting of a series of particles with mass  $m$ , arranged in a line, interacting with their first neighbors through a force that is proportional to the distance between particles. That is, a one-dimensional infinite chain of atoms interconnected by a harmonic interaction. Advancing with this model leads to a series of differential equations (Ashcroft and Mermin 1976):

$$\frac{m}{C} \frac{\partial^2 u_s}{\partial t^2} = u_{s+1} + u_{s-1} - 2u_s \quad (1)$$

where  $u_s$  is the position of the particle  $s$ ,  $u_{s+1}$  and  $u_{s-1}$  are the positions of its neighbors and  $C$  is a constant that represents the intensity of the force. This classical model is the starting point that establishes the conceptual basis used to understand phenomena within crystals. These bases state that within crystals there are atoms that can move around their equilibrium positions, i.e., vibrating atoms. These vibrations give rise to waves that travel through the crystal lattice, leading to the transmission of both sound and thermal energy. As these waves propagate, they play a crucial role in the transfer of acoustic signals and heat throughout the crystalline structure. However, from an experimental point of view, this model is insufficient because evidence indicates that these vibrations are quantized. For this reason, the model is quantized using standard procedures.

The Hamiltonian  $\hat{H}$  under a quantum description of the model of vibrating atoms reads

$$\hat{H} = \sum_{s=1}^S \frac{1}{2m} \hat{p}_s^2 + \frac{C}{2} (\hat{q}_{s+1} - \hat{q}_s)^2 \quad (2)$$

where  $\hat{p}_s$  and  $\hat{q}_s$  are the momentum and position operators of the atom  $s$  and  $\hat{q}_{s+1}$  the position operator of its neighbor  $s+1$ . To solve a quantum problem, the next step would be to find the eigenvalues and eigenfunctions of this Hamiltonian. However, doing this directly is impossible. The difficulties arise because of the large number of particles and the fact that the interaction causes that the motion of each particle is influenced by the motion of all the others. Mathematically, this can be observed by noting that each term of the summation in (2) involves not only the particle  $s$ , but also the particles  $s+1$  and  $s-1$ . This implies that diagonalizing the Hamiltonian will involve an enormous number of coupled equations. Conceptually, it means that the solutions to the equation will involve collective movements of all the atoms in the system, rather than individual atoms. Fortunately, it is possible to make a change of variables that simplifies the calculations:

$$\hat{Q}_{k_j} = N^{\frac{-1}{2}} \sum_{s=1}^S \hat{q}_s e^{-ik_j sa} \quad (3)$$

$$\hat{P}_{k_j} = N^{\frac{-1}{2}} \sum_{s=1}^S \hat{p}_s e^{ik_j sa} \quad (4)$$

where  $k_j = 2\pi j N^{-1} a^{-1}$ ,  $j = 0, \pm 1, \dots, \frac{S}{2}$  and  $a$  is the equilibrium distance between atoms. These are the phonon variables, using them we obtain an equivalent expression for the Hamiltonian (2), which is

$$\hat{H} = \sum_j \frac{1}{2} (\hat{P}_j^2 + \omega_j^2 \hat{Q}_j^2) \quad (5)$$

where  $\omega_j = (2C/m)^{\frac{1}{2}} (1 - \cos(k_j a))^{\frac{1}{2}}$  is the angular frequency of the oscillator  $j$ . Expression (5) shows the same Hamiltonian as expression (2), but now written in the phononic coordinates. If its origin is forgotten, the structure of  $\hat{H}$  presented in (5) can be reinterpreted. In effect, it can be said that there is another type of particle: particles with momentum  $\hat{P}_j$ , in a potential  $\hat{Q}_j$ , whose Hamiltonian is  $\hat{P}_j^2 + \omega_j^2 \hat{Q}_j^2$ . In summation (5) the neighbors  $i+1$  or  $i-1$  do not appear, so these particles do not interact with each other. At this point, it is possible to consider the crystalline solid as an aggregate of non-interacting harmonic oscillators.

The advantage of using a sum of harmonic oscillators is that the solutions are known. Indeed, eigenvalues and eigenstates for this Hamiltonian  $j$  are:

$$\varepsilon_j = \hbar \omega_j (n_j + 1/2) \text{ and } |n_j\rangle \quad (6)$$

where  $n_j = 0, 1, 2, \dots$ . In this case, the energy is quantized, and each quantum has a value  $\hbar \omega_j$ , so referring to the energy  $\varepsilon_j$  or to the number  $n_j$  of quanta of energy is the same. Then we can represent the energy states as  $|n_j\rangle$ . At this point, it is possible to make a conceptual shift and move to the description of phonons by means of the introduction of a different mathematical formalism. This change involves thinking that the state  $|n_j\rangle$  represents a system with  $n_j$  particles called phonons, each with energy  $\hbar \omega_j$ . Thus, the energy is a direct measure of the number of phonons: an increase in the system's energy means that there are more phonons in it, and a decrease in energy is represented as the transition to states with fewer phonons. In analogy with photons, which represent quanta of electromagnetic energy, phonons represent quanta of vibrations. In this way, the total energy  $E$  of the system is the sum of the energy of the phonons plus the vacuum energy  $\varepsilon_{vacuum}$ , which is the energy of the crystalline solid when there are no vibrations.

$$E = \sum_j \varepsilon_j = \sum_j \hbar \omega_j \left( n_j + \frac{1}{2} \right) = \sum_j \hbar \omega_j n_j + \varepsilon_{vacuum} \quad (7)$$

where  $\hbar \omega_j$  is the energy of a phonon with frequency  $\omega_j$  and  $n_j$  is the number of phonons with frequency  $\omega_j$ . This mathematical approach facilitates the determination of the system's solutions and offers an alternative characterization of the vibrations within a crystalline solid. Viewed through this lens, the oscillations are represented as discrete particles, where a higher magnitude of oscillation corresponds to an increased number of these particles. This is the central idea of the

phonon model and the approach that allows us to refer to phonons. For greater elegance, it is possible to move to second quantization and use the formalism based on creation and annihilation operators (Sakurai 1994).

Currently, the use of phonons is widespread in the field of condensed matter. This is because it allows for the simplification and solution of the equations posed in each case, but also because the picture provided by phonons facilitates the formulation of the problems and improves the explanation of phenomena. For example, to study thermal conductivity in metals, the phonon model provides a very intuitive picture (see Ashcroft and Mermin 1976 for details). When a point in a crystal is heated, the vibrations of the lattice at that point increase, creating phonons that will move through the material. Thus, phonons transport heat from one point to another, and thermal conductivity is related to how easily phonons can move within the material. Depending on the type of material, phonons can interact with each other, with other particles such as electrons, material impurities, other excitations in the material, etc. Therefore, in materials with many impurities or defects, phonons scatter more, and thermal conductivity decreases. In contrast, in materials with fewer impurities or defects, phonons scatter less, and thermal conductivity is usually higher. In this way, the model offers two advantages: on one hand, instead of framing the calculation as a complex interaction among elements of an infinite lattice, it is treated as a simple collision of particles. On the other hand, the phenomenon of thermal conductivity can be explained in a very intuitive manner. The phonon model has an explanatory power that the model of vibrating atoms lacks.

### **3.- Emergentist description of phonons**

In considering the relationship between phonons and the original lattice of atoms, several theoretical approaches can be explored. Two significant perspectives are emergence and reduction. These frameworks assume the existence of a basal level, where fundamental entities reside, and an upper level, where emergent entities exist. Typically, the connection between these two levels is established through a mathematical deduction, allowing for an understanding of the relationship in either a reductive or non-reductive manner. Emergence posits an ontological dependence between the upper and lower domains, wherein emergent entities or properties are seen as arising from, yet distinct from, the foundational entities at the basal level. In contrast, intertheoretic reduction implies an epistemic dependence between a less fundamental and a more fundamental theory, where reducible phenomena are fully explained by more basic principles. Applying these basic notions to the study of phonons, the basal level comprises vibrating atoms, while the upper level consists of phonons. Additionally, a mathematical derivation of phonons is

available, making possible to defend the case of phonons as one of emergence that may be compatible with intertheoretic reduction. This scenario gives rise to an attempt to describe an emergence compatible with intertheoretic reduction, wherein both ontological and epistemic dependencies are integrated.

The notion of emergence has been developed over many years and remains as a topic of discussion. For this reason, depending on the author, there are many ways to understand it. This section does not aim to exhaustively cover all existing ways of understanding emergence, but rather shows that, in general terms, the case of phonons can be framed within an emergentist scheme. For this, we rely on a proposal made by Franklin and Knox (2018), in which they describe phonons as an emergent phenomenon by adopting a notion of emergence compatible with reduction.

### 3.1 A notion of emergence compatible with reduction

Traditionally, emergence and reduction have been conceived as opposing notions, such that they offer mutually incompatible claims. However, it is possible to argue that this is not the case, as these notions refer to different domains. On one hand, emergence is an ontological notion that establishes a degree of ontological dependence of emergent entities on those at the fundamental level. On the other hand, reduction is an epistemic notion, it is a type of relationship between different theories. Indeed, Butterfield (2011) has proposed a version of emergence compatible with inter-theoretical reduction that has gained popularity among philosophers of physics. In this work, Butterfield conceives emergence as a behavior that is novel and robust concerning a fundamental domain. Reduction is conceived as a deduction, with the caveat that it is typically aided by appropriate definitions or bridge principles that link the vocabularies of the two theories, as is the case of Nagel (1961) and Schaffner (2013). That is, Butterfield adheres to the notion of reduction according to which, by adding appropriate definitions of terms, a less detailed theory can be deduced within a more detailed theory. Regarding mathematical deduction, the examples used in that article employ singular limits at some point. Indeed, according to Batterman's (2011) book on emergence and reduction, in most cases of emergence, novelty arises after the use of singular limits. In these cases, singular limits introduce a mathematical irreversibility that is crucial in determining the novel character of the emergent description (Knox, 2016). However, in their article, Franklin and Knox (2018) argue that singular limits can opaque the novelty that emergent behavior is supposed to exhibit. For this reason, they present the case of phonons as an example of emergence that does not rely on the use of singular limits.

### 3.2 Phonons as an emergent phenomenon

A simplified version of the deduction of phonons according to Franklin and Knox (2018) is reconstructed. As a preliminary step, they propose a simple example of two masses connected to each other and to fixed points by three springs. The equations of motion for the masses are:

$$m\ddot{x}_1 = -kx_1 - k'(x_1 - x_2) \quad (8)$$

$$m\ddot{x}_2 = -kx_2 - k'(x_2 - x_1) \quad (9)$$

Where  $k'$  is the constant associated with the spring that connects the two masses, and  $k$  is the constant associated with the springs that connect the masses to fixed points. To solve the equations, they propose the change of variables:

$$\begin{aligned} \eta_1 &= x_1 + x_2 \\ \eta_2 &= x_1 - x_2 \end{aligned} \quad (10)$$

By means of the change of variables, equations (8) and (9) are transformed into two decoupled differential equations for two simple harmonic oscillators:

$$m\ddot{\eta}_1 = -k\eta_1 \quad (11)$$

$$m\ddot{\eta}_2 = -(k + 2k')\eta_2 \quad (12)$$

Substituting  $\omega_1 = \sqrt{k/m}$  and  $\omega_2 = \sqrt{(k + 2k')/m}$ , the following solutions representing normal modes of the system are obtained:

$$\eta_1 = \alpha_1 e^{i\omega_1 t} + \alpha_1^* e^{-i\omega_1 t} \quad (13)$$

$$\eta_2 = \alpha_2 e^{i\omega_2 t} + \alpha_2^* e^{-i\omega_2 t} \quad (14)$$

Where  $\alpha_1, \alpha_1^*, \alpha_2, \alpha_2^*$  are fixed by the initial conditions. In this way they show that a change of variables can simplify the equations of the system. Expressions (8) and (9) correspond to the equations of two masses  $m$  connected by a spring with constant  $k'$ , with each mass also attached to fixed points by two additional springs, each with constant  $k$ . In other words, this is a system of two interconnected masses and three springs, which we will refer to as *System 1*. On the other hand, expressions (11) and (12) correspond to the equations of two masses  $m$  that are not



connected to each other by any spring, with each mass attached to fixed points by two springs with constants  $k$  and  $k + 2k'$ , respectively. This constitutes a system of two unconnected masses and two springs, which we will refer to as *System 2*. The change of variables can be understood as the replacement of System 1 by another system, System 2. As noted by Sebastian de Haro (2019) in his analysis of the paper by Franklin and Knox, the role of the change of variables is to simplify calculations, while the change of system introduces explanatory novelty. To illustrate the idea, suppose the spring with constant  $k'$  emits light when compressed, and the goal is to study the frequency at which the light is emitted (Franklin and Knox 2018). If one attempts to solve this problem using System 1, it is necessary to use expressions (8) and (9) to find solutions for  $x_1$  and  $x_2$ , and then compute  $x_1 - x_2$ , which is the variable relevant to light emission. This means solving a system of two equations with two unknowns. In contrast, if System 2 is used, it suffices to solve equation (12) for a single unknown  $\eta_1$ , since in this coordinate system, the equations for  $\eta_1$  and  $\eta_2$  can be solved independently. According to de Haro's interpretation, for the authors, this transformation allows the essential physics to be abstracted from the irrelevant details present in the original description, thereby introducing a form of explanatory novelty. The second description is more explanatory because it focuses on the relevant physics.

Then, they propose a model that better approximates a real crystalline solid: a classical arrangement of  $N$  basic units, each with  $m$  atoms. In this instance, the adiabatic and harmonic approximations are used. The first involves assuming that the degrees of freedom of the nuclei are independent of the degrees of freedom of the electrons, so the electronic degrees of freedom are not considered. The second involves assuming that atomic displacements are negligible compared to interatomic distances. Thus, displacement variables are obtained along with their coupled differential equations, since the arrangement is three-dimensional. Next, a change of variables is made, analogous to the one done for the masses connected by springs (see eq. 10). A series of phonon variables  $q_{kj}$ , which represent harmonic oscillators, is obtained. From the Lagrangian of the system, a series of decoupled equations of motion is derived. Namely

$$\ddot{q}_{kj} = -\omega_{kj}^2 q_{kj} \quad (15)$$

It is worth noting that, in equations (15), the authors obtained the normal mode variables commonly called phonons, but according to them, these do not yet resemble particles. To obtain particle-like phonons, they reformulate the description within quantum mechanics. Specifically, they perform second quantization using creation and annihilation operators to make the phonons appear as particles. This formalism represents vibrations as particles that are created or destroyed as the magnitude of the vibration increases or decreases. If the state of the system is  $|n\rangle$  where  $n$

is an integer that represents the number of particles, and  $\{\hat{a}^\dagger, \hat{a}\}$  are respectively the creation and annihilation operators, then

$$\hat{a}^\dagger |n\rangle = |n+1\rangle \quad \hat{a} |n\rangle = |n-1\rangle \quad (16)$$

On this basis, the Hamiltonian is expressed as (see Kittel 2005 for details):

$$\hat{H} = \sum_k \hbar \omega_k \left( \hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right) \quad (18)$$

Then, the phonon mode variables  $q_{kj}$  and their associated momenta  $p_{kj}$  reads

$$q_{kj} = \sqrt{\frac{\hbar}{2\omega_{kj}}} (\hat{a}_{-kj}^\dagger + \hat{a}_{kj}) \quad p_{kj} = i\sqrt{\frac{\hbar\omega_{kj}}{2}} (\hat{a}_{-kj}^\dagger - \hat{a}_{kj}) \quad (19)$$

At this point, they allow for the possibility of thinking of quanta of vibration as particles, i.e., phonons. Additionally, they propose a parallel with the equations that give rise to photons, which are exactly the same. In this way, they establish that the relationship that phonons have with the underlying description of the crystal is almost identical to the relationship that quantum particles have with the underlying quantum field. And since, for them, the inter-theoretical relationship between quantum particles and the field indicates emergence, it does so in the case of phonons as well.

Also, in their defense of the emergent status of phonons, adopt Butterfield's notion of emergence compatible with inter-theoretic reduction. As stated above, there are three conditions for this type of emergence: novelty, robustness, and reduction. The authors present a comprehensive argument supporting that novelty is indeed satisfied in the context of phononic descriptions. Their reasoning is that phononic descriptions allow for the introduction of abstractions that are not immediately possible in the previous atomic-level description, as in the classical model. This abstraction allows for a more sophisticated understanding of material behavior, which is not possible when using the basic atomic framework alone.

Furthermore, the authors address the criterion of robustness, demonstrating that it is equally well met. They provide examples where phononic behavior withstands significant disturbances, indicating that the phononic framework remains stable even under challenging conditions. The primary focus of their paper lies in establishing the novelty and robustness of the phononic description. However, while the authors emphasize these aspects, they do not delve deeply into the topic of reducibility. Instead, they operate on the assumption that there exists a theoretical leap between the phononic and atomic descriptions. In this context, by theoretical leap we refer to

a situation in which transitioning from one description to the other necessarily requires a change of theory. This assumption is predicated on the idea that the theory of phonons is less fundamental than the underlying atomic theory of the crystal.

#### 4.- A pluralistic description of phonons

This section presents an alternative approach to study the ontological status of phonons, according to which phonons do not arise from the mathematical manipulation of vibrating atoms. On the contrary, both vibrating atoms and phonons, are different ways to decompose the Hilbert space of the whole system.

##### 4.1 The theoretical affiliation of phonons and vibrating atoms

In the previous sections, two ways of deriving phonons have been presented, one in Section 2 and another in Section 3. Although the two presentations are similar, they have a significant difference: in one case, the change of coordinates is made before quantization, and in the other case, after. This is a detail that may go unnoticed but is crucial in determining which theory describes vibrating atoms and which describes phonons. Without delving into the details of the calculations and without claiming exhaustiveness, it is possible to assert that there are two pathways to derive phonons. In both cases, one begins with Equation (1), which represents classical vibrating atoms. This equation originates from a model of the crystal as a chain of atoms interacting with nearest neighbors through a harmonic potential. In one pathway:

$$\frac{m}{C} \frac{\partial^2 u_s}{\partial t^2} = \dots \xrightarrow{\text{phonons coordinates}} \frac{d^2 Q_k}{dt^2} = \omega_k^2 Q_k \xrightarrow{\text{quantization}} \hat{H} = \sum_k \frac{1}{2} \left( \hat{P}_k^2 + \omega_k^2 \hat{Q}_k^2 \right)$$

the system's variables are converted to phonon coordinates. This leads to the derivation of new classical equations. This equation characterizes what are referred to as classical phonons (Dagotto 2013). Despite its nomenclature, this framework essentially consists of a collection of equations describing multiple independent classical harmonic oscillators. It is important to note, however, that this representation does not inherently account for the creation and annihilation of particles. Subsequently, by applying the quantization process, the desired equation is derived, leading to the concept of quantum phonons. This last equation allows for the discussion and analysis of phonons within the quantum mechanical framework, as has been outlined in Section 2. This approach might give the impression that transitioning from vibrating atoms to phonons necessitates a shift in theoretical frameworks. However, the other pathway reveals that this transition can occur within the same theoretical framework, moving from one description to another without requiring a change in theory. Indeed, in the other pathway:

$$\frac{m}{C} \frac{\partial^2 u_s}{\partial t^2} = \dots \xrightarrow{\text{quantization}} \hat{H} = \sum_{s=1}^S \frac{1}{2m} \hat{p}_s^2 + \frac{C}{2} (\hat{q}_{s+1} - \hat{q}_s)^2 \xrightarrow{\text{phonons coordinates}} \hat{H} = \sum_k \frac{1}{2} (\hat{P}_k^2 + \omega_k^2 \hat{Q}_k^2)$$

the process begins with the quantization to derive a Hamiltonian for quantum vibrating atoms. Then, a coordinate transformation is performed to shift from atomic coordinates to phonon coordinates, thereby obtaining the equations for quantum phonons. By adopting this last approach, it becomes evident that the transition from atoms to phonons occurs within the quantum domain. Before the change of coordinates, one has a quantum model for vibrating atoms, which belongs to the quantum framework and is governed by quantum theory. Upon applying the phonon coordinates, a quantum model for phonons is obtained, which also belongs to the quantum domain, and it is governed by the same quantum theory. Consequently, both vibrating atoms and phonons belong to the same theoretical level. This indicates that although there are two different descriptions, in principle it is incorrect to think that there are necessarily a higher-level and a lower-level theoretical domain. This result has been taken as a basis to question the proposal of emergence with inter-theoretic reduction as presented in Section 3 (Fortin and Pasqualini 2025). However, it is not, by itself, an argument to dismiss an emergentist description of phonons. Nonetheless, we take this result as motivation to seek an alternative description to emergence.

#### 4.2 The whole and the parts in a quantum system

A composite quantum system is typically defined by specifying its constituent entities and the interactions between them. This approach represents a bottom-up perspective, as it starts with the analysis of the subsystems and their interactions within them. Conversely, a top-down approach can also be highly fruitful (Fortin & Lombardi 2016). This perspective begins with an examination of the entire closed system and its evolution, subsequently informing the analysis of its individual components and their interactions. One of the advantages of adopting a top-down approach is that it immediately becomes apparent that there are many ways to divide the entire system into parts.

Consider a composite quantum system  $U$  with the associated Hilbert space  $\mathcal{H}_U$ . The mathematical framework of Hilbert spaces permits various decompositions of this space. Depending on the dimensionality of  $\mathcal{H}_U$ , it will be possible to decompose it into more or fewer subspaces. Each decomposition is called Tensor Product Structure (TPS), because the total Hilbert space must be equal to the tensor product of the Hilbert spaces of the parts, in the case of  $N$  parts

$$\mathcal{H}_U = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_N = \bigotimes_{j=1}^N \mathcal{H}_j \quad (20)$$

In this case,  $\mathcal{H}_U$  may be represented as a tensor product of  $N$  Hilbert spaces corresponding to  $N$  particles. These particles might have certain properties such as mass, charge, and spin. We will refer to this way of splitting the system as  $\text{TPS}_N$ . Alternatively, if the system is decomposed differently, it could involve a different number of particles with distinct properties, resulting in a different tensor product of Hilbert spaces. For example, taking the  $\text{TPS}_N$  subsystems in pairs, the total system would have  $N/2$  parts

$$\mathcal{H}_U = \mathcal{H}_{1-2} \otimes \mathcal{H}_{3-4} \otimes \dots \otimes \mathcal{H}_{N/2} = \bigotimes_{i=1}^{N/2} \mathcal{H}_i \quad (21)$$

Now,  $\mathcal{H}_U$  is represented as a tensor product of  $N/2$  Hilbert spaces corresponding to  $N/2$  particles. These particles must have other mass, other charge, and other spin. We will refer to this way of splitting the system as  $\text{TPS}_{N/2}$ . From a detailed examination of the subsystems, the two different decompositions may imply that the systems are fundamentally different: one with  $N$  particles with certain mass, charge, and spin and the other with  $N/2$  with other properties. However, despite these seemingly divergent characterizations of the subsystems, the total quantum system remains invariant.

This very simple example shows that the different ways of dividing a total system into parts give rise to different descriptions in terms of different entities. From a formal mathematical point of view, there is no criterion that allows one to choose a partition as the privileged one. Thus, without introducing an external criterion, it is not possible to determine the correct composition of a total system. By “TPS approach” we understand a line of research carried out by several authors, considering the relativity of certain notions closely linked to quantum formalism with respect to the previous specification of a TPS for a system. This approach has been widely used in the study of quantum systems. In some cases, an external criterion has been introduced to choose a privileged TPS. For example, in the context of measurement theory, Zanardi et al. (2004) introduced a criterion according to which the set of operationally accessible interactions and measurements chooses the privileged partition. For their part, Harshman and Wickramasekara (2007) use the invariance under global symmetry transformations and dynamical transformations, to privilege some partition of the system. The Modal Hamiltonian Interpretation (Lombardi et al. 2008, 2010) uses a criterion of non-interaction to establish which is the partition with the elementary subsystems with ontological relevance. In the context of quantum information theory, Andreadakis et al. (2024) use a minimally scramble information criterion to determine what are the natural system partitions. In other cases, no external criterion is introduced to select a partition, or the criteria that are introduced do not work as expected, and the fact that certain phenomena are relative to the TPS used is accepted. For example, Dugić and

Jeknić (2008) strive to find criteria that allow distinguishing “real” and “virtual” subsystems from the approach of quantum decoherence and quantum information. Given the current lack of a precise formulation for these criteria, the authors acknowledge that the concept of separability between subsystems, as well as the definition of a “system” itself, must be viewed as relative. It has also been noted that depending on the chosen TPS, the description of the classical limit emerging from a study of decoherence may vary (Castagnino et al. 2010 and Lombardi et al. 2012). On the other hand, according to Earman (2015), a quantum system can be entangled with respect to one partition but not entangled with respect to another, thereby conceiving the entanglement of the state as a notion relative to the TPS. Moreover, Fortin and Lombardi (2022) applied the TPS approach to study the relativity of the notion of entanglement in the case of indistinguishable particles. According to them, indistinguishability should be considered no longer as a relation between particles but between properties. In addition, Pasqualini and Fortin (2022) use different partitions of a quantum system to establish the relativity of the notion of statistical identity. They show that, given a TPS, the state of a system can be symmetric under the permutation of particles, but also be antisymmetric in another TPS.

#### 4.3 Phonons and vibrating particles as different partitions of the whole system

The fact that crystalline solids can be described with components as vibrating atoms in one description and as phonons in another, is another example where the total system can be divided in different ways to yield different partitions. The crucial point is that the transformation to phonon coordinates involves a straightforward Discrete Fourier Transform, which leads to normal coordinates. This means that the coordinate transformation, that connects the Hamiltonian of vibrating atoms  $\hat{H}_{V.Atoms}$  with the phonon’s Hamiltonian  $\hat{H}_{phonons}$ , can be done in both directions without losing information

$$\hat{H}_{V.Atoms} = \sum_{s=1}^S \frac{1}{2m} \hat{p}_s^2 + \frac{C}{2} (\hat{q}_{s+1} - \hat{q}_s)^2 \xrightarrow{\text{phonons coordinates}} \hat{H}_{phonons} = \sum_k \frac{1}{2} (\hat{P}_k^2 + \omega_k^2 \hat{Q}_k^2)$$

With a change of coordinates, it is possible to start from the description of vibrating atoms, transition to the description of phonons, and then return to the initial description, with the result being exactly the same as at the beginning. This is important because, unlike the examples provided by Butterfield (2011) and Batterman’s (2011), where the application of a singular limit makes the connection between two descriptions asymmetric, in this case, there is complete symmetry.

Regarding the Hilbert space, the group of atomic nuclei is represented in the total space  $\mathcal{H}_r$ , which is a tensor product of the spaces  $\mathcal{H}_j$  of each vibrating atom

$$\mathcal{H}_T = \bigotimes_{j=1} \mathcal{H}_j \quad (22)$$

In this case the eigenstates  $|\varepsilon_j\rangle$  of  $\hat{H}_{V.Atoms}$  span the Hilbert space  $\mathcal{H}_T$ . Nevertheless, both Hamiltonians are the same but expressed in different normal coordinates  $\hat{H}_{V.Atoms} = \hat{H}_{phonons}$ . Then the space spanned by the eigenvectors of  $\hat{H}_{phonons}$  is the same, but we can decompose it in another way

$$\mathcal{H}_T = \bigotimes_k \tilde{\mathcal{H}}_k \quad (23)$$

where  $\{\tilde{\mathcal{H}}_k\}$  are the Hilbert spaces for different number of phonons. Then, the shifting to phonon variables involves adopting an alternative Tensor Product Structure (TPS). Consequently, the models representing vibrating atoms and phonons are distinct methodologies for partitioning the same total system. On the other hand, there is a third TPS that could be considered: treating the total Hilbert space  $\mathcal{H}_T$  as a whole without dividing it into parts. Thus, there is a third description that regards the crystal as a unified whole. Of course, there are infinitely many possible TPSs, but we will not analyze all of them. The fact that an infinite number of descriptions are mathematically possible does not imply that all of them are scientifically relevant. The TPS based on vibrating atoms is significant because it serves as the starting point for microscopic models of crystalline solids. Moreover, the atom-based description is compatible with those used in other areas of quantum chemistry, such as structural chemistry. As noted in previous sections, we agree with the arguments put forward by emergentist authors in support of the claim that phonons meet the criteria of novelty and robustness. These two features suggest a certain degree of independence for phonons, and may serve as a basis for take this TPS into account in an ontological analysis. Finally, the TPS corresponding to the whole is relevant because it refers to the crystal itself. If the TPS approach is accepted without introducing additional considerations, it follows that there is no justification for preferring one TPS over another. This perspective suggests a form of ontological pluralism, wherein vibrating atoms, quantum phonons and the total system are regarded as having equal ontological priority.

Of course, this is not the only option, it is always possible to try to introduce an external element that allows giving a privileged category to one of the partitions. This is what will be shown in the next section.

## 5.- Possible ontological relations

In the previous section, it was demonstrated that the descriptions of phonons, vibrating atoms, and the crystal as a whole arise from the application of different partitions to the total system. According to the TPS approach, there is no way to designate a privileged TPS without introducing an external criterion. Zanardi (2001, 4) emphasizes this point in his paper about virtual quantum subsystems: “without further physical assumption, no partition has an ontologically superior status with respect to any other”. This paves the way for various approaches to establishing the nature of phonons and their relationship with vibrating atoms. In what follows, different general options will be briefly explored. The objective of this section is not to argue in favor of any particular option but to show how the TPS approach allows for a neat expansion of the range of possibilities and can be used to organize the discussion.

### 5.1 A pluralist view

In the field of crystal solids, the use of phonons is widespread and essential for formulating scenarios, solving problems, and describing processes. The conceptualization of a crystal provided by phonons differs significantly from that offered by vibrating atoms, and both differ from the conception of the crystal as a whole. However, in practice, these perspectives complement each other, and it would be impractical to discard one. If this pragmatism is applied to ontology, a pluralistic view about the ontology associated with crystals can be developed. If this ontological pluralism is taken to its ultimate consequences, it can be asserted that the term 'crystal' does not refer to the same ontological entity in one TPS as it does in another. In the TPS of vibrating atoms, a crystal is a quantum system composed of atoms that can move around their equilibrium positions. On the contrary, in the TPS of phonons, a crystal is an entity composed of phonons that can move and a fixed background. Regarding energy, in the atomic crystal, the energy of the system is associated with the collective vibrational modes of the lattice. In contrast, in the phononic crystal, each individual phonon contributes a quantum of energy. In other words, from this position, the term 'crystal' has different meanings in the two TPSs, and asking which is the "true" one is meaningless, much like probing the mind of God through science.

The option for diversity may seem somewhat foreign, however, it is not new in the philosophy of chemistry. Various forms of ontological diversity have been proposed in the general realm (Lombardi 2023) and within the philosophy of chemistry (Fortin et al. 2023, Lombardi 2014, Cordoba et al. 2013, Labarca et al. 2010). Nonetheless, this proposal may be incompatible with the idea that there is a hierarchy of descriptions, one more fundamental than the other. Fortunately, there are other options.



## 5.2 A monist perspective

The alternative is based on the metaphysical stance that one description is more fundamental than the other, such that an ontological priority can be established among different entities (Morganti 2009). In this view, it is necessary to introduce a criterion that allows for the selection of one partition, leading to a single fundamental ontology, and for this reason we call it monistic. Once again, there are two variants, the holistic and the atomistic views.

### 5.2.1 The whole is the legitimate system: Holism

This approach involves adopting a top-down perspective, treating the entire system as the fundamental one. By integrating the holistic nature of quantum mechanics (see Teller 1986, Howard 1989) into the ontology, it posits that the total system constitutes the only “real system,” while phonons and atoms are merely illusions or constructs. It should be noted that this is equivalent to choosing a TPS, since not splitting the system corresponds to a form of decomposition of the Hilbert space (not decomposing it). If this form of holism is carried to its ultimate consequences, it can be asserted that the term 'crystal' refers to the entire quantum system, an entity devoid of components. Regarding energy, the set of allowed energies of the system is related to the nature of the crystal as expressed by the parameters describing it. Just as the energies in the "potential well" do not refer to any fundamental structure, in this case, it is possible to refer to the energies of the crystal without needing to link them to its parts.

The holistic option is well-known in quantum mechanics and, although not the most popular, has many adherents in both the fields of physics and philosophy (Healey 2022). This is because certain situations where a quantum system is divided into parts can lead to paradoxes such as the EPR paradox (Einstein 1935). According to this perspective, a holistic conception of quantum mechanics can clarify controversies surrounding quantum non-separability (Healey 1991).

### 5.2.2 There are fundamental parts: Atomism

This possibility is the most popular, it says that there exists a domain of fundamental particles that serve as the building blocks of a hierarchical reality, from which everything else is constructed bottom-up and derived from them. Typically, cases of emergence and reduction are framed within this approach. In the case of crystals, this perspective entails choosing a partition where the parts constitute the set of basic entities. Since the atomic hypothesis is utilized in many areas of science beyond material physics, the canonical choice is that of vibrating atoms because it is generally understood as the natural choice for constructing a unified description of the

various aspects of nature. This would establish a type of asymmetry between the two descriptions, favoring that of the vibrating atoms. Assuming this, a crystal would be a collection of atoms interacting with each other, arranged in a periodic pattern, and the energy of the system is linked to the coordinated movement of its elements. With regard to phonons, they would possess a diminished ontology, the development of which could be approached from two perspectives. As is common, they could be described as mere computational tools without any form of “real existence.” Alternatively, one could consider attributing to them some kind of derivative ontological status. As demonstrated in Section 4.1, both the vibrating atoms and the phonons belong to the same theoretical domain, which precludes any possibility of discussing reduction. However, phonons might be described as emergent entities, not within an inter-domain emergence framework but rather through some variant of intra-domain emergence (see Lombardi and Ferreira Ruiz 2018, Matta et al. 2020).

Finally, an additional comment is possible. To arrive at this atomistic description, the partition of vibrating atoms was chosen as fundamental. This is reasonable, as it applies to a narrower range of cases and conditions. However, the TPS formalism allows for another possibility, which would be to choose the phonon partition as the fundamental one. Since there are authors who have questioned the arguments supporting the choice of the atomic displacements description as the fundamental one (Accorinti et al. 2023), to complete the range of options, an atomistic variant in which phonons are considered basic entities could also be included.

## **6.- Conclusions**

In this article, we have addressed the study of the ontological status of the entities commonly used to describe crystalline solids and the physical and chemical phenomena associated with them. Since there are two possible descriptions of thermal and acoustic phenomena—vibrating atoms and phonons—it is necessary to examine the relationships between them from an ontological perspective. Traditionally, the description based on vibrating atoms has been regarded as the only legitimate one, relegating phonons to the role of mere computational tools without any ontological relevance. However, recent works have argued that the phonon-based description is sufficiently novel and robust to warrant considering phonons within the conceptual framework of emergence. Still, these are not the only possible approaches to the problem, and in this work we have reviewed the existing emergentist proposal and explored several alternatives.

The importance of phonons in the field of materials science has been highlighted by Franklin and Knox (2018), who show that they meet the requirements of novelty and robustness demanded

by an emergentist description. However, they rely on a special kind of emergence that also involves reduction, and they develop a theoretical framework in which two theories are assumed—one for phonons and another for vibrating atoms. We show that the fundamental step that allows for the transition from the description of vibrating atoms to that of phonons is a change of coordinates. It is thus possible to construct a quantum model of vibrating atoms such that, when a coordinate transformation is applied, a quantum model for phonons is obtained, all within a single theory. Since the shift between descriptions occurs within the same theoretical framework, we argue that it is not accurate to characterize this relation as inter-theoretic emergence. Nor would it be appropriate to speak of reduction, since reduction, as traditionally conceived, requires two distinct theories. This result may challenge the emergentist stance as presented by Franklin and Knox. However, it does not, in itself, constitute an argument against an emergentist description of phonons, since similar arguments could be adapted to support an account of intra-theoretic emergence.

To place the phononic coordinate transformation within a broader conceptual framework that has been used to analyze the ontological status of different entities in other domains, we introduce the formalism of Tensor Product Structures. This formalism highlights that both descriptions of the crystal refer to the same total system, differing only in the way the whole is partitioned into parts. Furthermore, it allows us to conclude that, in the absence of an external criterion, it is impossible to select one partition as ontologically privileged. In this way, the adoption of different external criteria allows for conceiving the ontological status of phonons in various ways. Consequently, a range of options becomes available for describing the relationship between phonons and vibrating atoms. In the absence of a criterion, a pluralist ontology is assumed, treating phonons and vibrating atoms on equal footing. With the introduction of a criterion that privileges the total system, a holistic ontology is achieved, leading to the conclusion that phonons and atoms have a derived ontological status or, in its strongest form, lack any ontological correspondence. On the other hand, if a criterion privileging fundamental systems is adopted, an atomistic ontology is assumed, in which one of the descriptions is regarded as fundamental and the other can be consistently derived in a way that aligns with inter-theoretic emergence.

## **Acknowledgements**

This research was partially supported by grants “Tres problemas filosóficos en la fundamentación de la física: Interpretación de la mecánica cuántica, irreversibilidad y relaciones interdisciplinarias” (ID: PIP 11220200100483CO) from CONICET, “Fenómenos irreversibles en

mecánica cuántica desde una perspectiva holista” (ID: PICT-2020-SERIA-00782) from FONCyT and “Relaciones interteóricas entre la mecánica cuántica y otros dominios teóricos” (ID: no number) from the Universidad Austral.

## References

- Accorinti, H., Fortin, S., Herrera, M. and Arriaga, J. A. J. (2023). The case of phonons: explanatory or ontological priority. In Soto, C. (ed.), *Current Debates in Philosophy of Science*. In Honor of Roberto Torretti, Synthese Library, Cham: Springer.
- Andreadakis, F., Dallas, E. and Zanardi, P. (2024). Long-time quantum scrambling and generalized tensor product structures. *Physical Review A*, 109: 052424.
- Ashcroft, N.W. and Mermin, N. D. (1976) *Solid State Physics*. Saunders College, Philadelphia.
- Batterman, R. W. (2011). Emergence, singularities, and symmetry breaking. *Foundations of Physics*, 41(6): 1031-1050.
- Butterfield, J. (2011). Less is different: Emergence and reduction reconciled. *Foundations of Physics*, 41: 1065-1135.
- Castagnino, M., Fortin, S. and Lombardi, O. (2010). Suppression of decoherence in a generalization of the spin-bath model. *Journal of Physics A: Mathematical and Theoretical*, 43: 065304.
- Cordoba, M. and Lombardi, O. (2013). A Kantian perspective for the philosophy of chemistry. In J.-P. Llored (ed.), *The Philosophy of Chemistry: Practices, Methodologies, and Concepts*. Cambridge: Cambridge Scholars Publishing.
- Dagotto, E. (2013). *Nanoscale Phase Separation and Colossal Magnetoresistance*. Berlin: Springer Berlin Heidelberg.
- De Haro, S. (2019). Towards a theory of emergence for the physical sciences. *European Journal for Philosophy of Science* 9: 38.
- Dugić, M. and Jeknić-Dugić, J. (2008). What is «system»: The information-theoretic arguments. *International Journal of Theoretical Physics*, 47: 805-813.
- Einstein, A.; Podolsky, B.; Rosen, N. (1935). Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?. *Physical Review* 47: 777-780.
- Earman, J. (2015). Some puzzles and unresolved issues about quantum entanglement. *Erkenntnis*, 80: 303-337.

- Fortin, S., Labarca, M. and Lombardi, O. (2023). On the ontological status of molecular structure: is it possible to reconcile molecular chemistry with quantum mechanics?, *Foundations of Science*, 28: 709-725.
- Fortin, S. and Lombardi, O. (2016). A top-down view of the classical limit of quantum mechanics, in R. E. Kastner, J. Jeknic-Dugic y G. Jaroszkiewicz (eds.), *Quantum Structural Studies: Classical Emergence from the Quantum Level*, pp. 435-468, London: World Scientific Europe, London.
- Fortin, S. and Lombardi, O. (2021). Is the problem of molecular structure just the quantum measurement problem? *Foundations of Chemistry*, 23: 379-395.
- Fortin, S. and Lombardi, O. (2022). Entanglement and indistinguishability in a quantum ontology of properties, *Studies in History and Philosophy of Science* 91: 234-243.
- Fortin, S., Lombardi, O. and Martinez Gonzalez, J. C. (2017). The relationship between chemistry and physics from the perspective of Bohmian mechanics. *Foundations of Chemistry*, 19: 43-59.
- Fortin, S. y Pasqualini, M. (2025), “Emergence-Free Duality: Phonons and Vibrating Atoms in Crystalline Solids”, *Foundations of Physics* 55: 24.
- Franklin, A. and Knox, E. (2018). Emergence without limits: The case of phonons, *Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics*, 64: 68-78.
- Franklin, A., Seifert, V. (2024). The problem of molecular structure just is the measurement problem. *The British Journal for the Philosophy of Science*, 75:31-59.
- Harshman, N. L., Wickramasekara, S. (2007). Tensor Product Structures, Entanglement, and Particle Scattering. *Open Systems and Information Dynamics*, 14: 341–351.
- Healey, R. (1991). Holism and Nonseparability, *Journal of Philosophy*, 88: 393-421.
- Healey, R. and Gomes, R. (2022). Holism and Nonseparability in Physics, *The Stanford Encyclopedia of Philosophy*, Spring 2022 Edition, Edward N. Zalta (ed.), URL = <https://plato.stanford.edu/archives/spr2022/entries/physics-holism/>
- Howard, D. (1989). Holism, separability, and the metaphysical implications of the Bell experiments. In Cushing, J. and McMullin, E. (Eds.), *Philosophical consequences of quantum theory*, pp. 224-253, Notre Dame: University of Notre Dame Press.

- Kittel, C. (2005). *Introduction to Solid State Physics*. 8th Edition, New York: John Wiley & Sons.
- Knox, E. (2016). Abstraction and its limits: Finding space for novel explanation. *Noûs*, 50(1), 41-60.
- Labarca, M. and Lombardi, O. (2010). Why orbitals do not exist? *Foundations of Chemistry*, 12: 149-157.
- Lombardi, O. (2014). “The ontological autonomy of the chemical world: facing the criticisms.” In E. Scerri and L. McIntyre (eds.), *Philosophy of Chemistry: Growth of a New Discipline*, Boston Studies in the Philosophy and History of Science. Dordrecht: Springer.
- Lombardi, O. (2023). A Kantian-rooted pluralist realism for science. In: Soto, C. (ed.) *Current Debates in Philosophy of Science*. Synthese Library, vol 477. Cham: Springer.
- Lombardi, O. and Ferreira Ruiz, M. J. (2019). Distinguishing Between Inter-domain and Intra-domain Emergence. *Foundations of Science* 24, 133–151.
- Lombardi, O. and Castagnino, M. (2008), A modal-Hamiltonian interpretation of quantum mechanics. *Studies in History and Philosophy of Modern Physics* 39: 380-443.
- Lombardi, O., Fortin, S., Ardenghi, J. S. and Castagnino, M. (2010). *Introduction to the Modal-Hamiltonian Interpretation*, New York: Nova Science Publishers Inc.
- Lombardi, O., Fortin, S. and Castagnino, M. (2012). The problem of identifying the system and the environment in the phenomenon of decoherence. In H. W. de Regt, S. Hartmann and S. Okasha (eds.). *European Philosophy of Science Association (EPSA). Philosophical Issues in the Sciences Volume 3*, pp. 161-174, Berlin: Springer.
- Matta, C.F., Lombardi, O. and Jaimes Arriaga, J. (2020). Two-step emergence: the quantum theory of atoms in molecules as a bridge between quantum mechanics and molecular chemistry. *Foundations of Chemistry* **22**, 107–129.
- Martinez Gonzalez, J. C., Fortin, S. and Lombardi, O. (2019). “Why molecular structure cannot be strictly reduced to quantum mechanics. *Foundations of Chemistry*, 21: 31-45.
- Morganti, M. (2009), Ontological Priority, Fundamentality and Monism. *Dialectica*, 63: 271-288.
- Nagel, E. (1961). *The structure of science. Problems in the logic of scientific explanation*. New York: Harcourt, Brace & World
- Pasqualini, M. and Fortin, S. (2022). Trans-statistical Behavior of a Multiparticle System in an Ontology of Properties. *Foundations of Physics* 52, 70.

- Sakurai, J.J. (1994). *Modern Quantum Mechanics*. Revised Edition, Addison-Wesley Publishing Company, Reading, MA.
- Schaffner, K. F. (2013). Ernest Nagel and reduction. *Journal of Philosophy*, 109, 534–565.
- Teller, P. (1986). Relational Holism and Quantum Mechanics. *The British Journal for the Philosophy of Science*, 37: 71-81.
- Weisberg, M., Needham, P. and Hendry, R. (2016). Philosophy of chemistry. In E. N. Zalta (ed.), *The Stanford Encyclopedia of Philosophy*,  
 URL= <https://plato.stanford.edu/archives/win2016/entries/chemistry>
- Zanardi, P. (2001). Virtual Quantum Subsystems. *Physical Review Letters*, 87: 077901.
- Zanardi, P., Lidar, D. and Lloyd, S. (2004). Quantum Tensor Product Structures are Observable Induced. *Physical Review Letters*, 92: 060402.