

*The case of phonons:
explanatory or
ontological priority*

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Abstract

Recent discussions about the microstructure of materials generally focus on the ontological aspects of the molecular structure. However, there are many types of substances that cannot be studied by means of the concept of molecule, for example, salts. For the quantum treatment of these substances, a new particle, called phonon, is introduced. Phonons are generally conceived as a pseudo-particle, that is, a mathematical device necessary to perform calculations but which does not have a "real" existence. In this context, the aim of this paper will be to analyze the ontological status of phonons. For such purposes we will critically analyze the arguments that would account for the presumed nonexistence of phonons. Finally, having already demonstrated that there are not enough reasons to consider phonons as non-existing entities, we will explore some possibilities that allow us to elucidate their ontological status.

Keywords: Phonons, Quantum Chemistry, Intertheoretical Relationships, Ontological Commitments, Pluralism.

1. Introduction.

* This work is fully collaborative. The order of the names is alphabetical and therefore does not imply priority.

The study of intertheoretical relationships is of particular relevance to the philosophy of chemistry, due to the fact that the close relationships between chemistry and physics affect the independence and autonomy of chemistry as a scientific discipline. The influence that physics has exerted on chemistry from a position of supposed hegemony is manifested, for example, in the modern explanations of the chemical bond proposed since the advent of quantum mechanics in the first half of the twentieth century. These explanations led Dirac to declare in 1929 that quantum mechanics already possessed the power to account for the fundamental principles of chemistry. However, the issue of the effective reduction of chemistry to physics has been much discussed recently by authors such as Eric Scerri (2000, 2011, 2012, 2013), Robin Hendry 2010, Hinne Hettema 2012, Lombardi (2005, 2014), among many others. The main antireductionist arguments stress that physics is incapable of explaining the structure of chemical substances. In particular, they focus on the incompatibility between the fundamental principles of quantum mechanics and the concept of molecular structure used in chemistry (Woolley 1978, 1982, Amann 1992, Sutcliffe and Woolley 2011, 2012, Bishop 2005, Fortin et al., 2017). However, it is important to bear in mind that molecules are not the only type of entities in chemistry; in order to enrich the debate, it is essential to consider other types of chemical entities. One example is the case of salts, which are understood not as “large” molecules, but as a *network*; as we will explain in Section 2, this is a concept completely different from the concept of molecule. As a consequence, although the present work will not specifically delve into the reductionism-anti-reductionist discussion, it will provide new elements for the debate by introducing arguments for the consolidation of the ontological existence of phonons.

Phonons are particles that are appealed to for the quantum treatment of salts. However, phonons are commonly conceived as pseudo-particles. In general, a phonon is considered a mathematical device necessary to perform calculations, but without “real” existence. Some authors classify phonons as quasi-particles, that is, as non-elementary particles that, although can be reduced, on a limited time scale behave as if they were elementary particles (Ladyman 2015).

In this context, the aim of this paper consists in analyzing the ontological status of phonons in the light of the usual arguments by means of which their real existence is denied. For this purpose, in Section 2, we will briefly summarize the way in which salts are traditionally studied; we will point out that, in order to account for certain phenomena, mainly thermal acoustic, it is

necessary to introduce the concept of phonon. In Section 3, we will briefly recall the empirical success that underlies the importance of the concept of phonon at an explanatory and predictive level. In Section 4, we will critically analyze the usual arguments against the real existence of phonons. On this basis, by establishing the analogy between phonons and photons, we will conclude that if the existence of photons is accepted, then the same attitude should be adopted in the case of phonons. Once it is admitted that there are not good reasons to consider phonons as non-existing entities, in Section 5 we will explore some perspectives that will allow us to elucidate their ontological status. Finally, in Section 6, we present our conclusions.

2. The internal structure of crystalline solids.

Substances in the solid state are commonly studied in a different way from how their liquid or gaseous counterparts are treated, mainly due to the magnitude of their components at the molecular level. For example, a macroscopic crystal can very well be described in terms of a single structural unit that extends through the entire crystal. Crystalline materials, as the salts, are those solid substances whose distinctive feature is that their basic structural units have a long-term periodic arrangement.

2.1. The classical description of a crystalline solid.

For conciseness, we will introduce two simplifications that will not harm in any way the conclusions we will arrive at in this work, since the generalization to more complex systems without much difficulty is always possible. On the one hand, we will consider only the so-called monatomic crystals, that is, crystalline solids whose units are composed of a single atom. On the other hand, although a real crystal is understood as a perfectly ordered network in three dimensions, here we will consider only models in one dimension.

The simplest model of a crystalline solid is a one-dimensional infinite chain of atoms interconnected by some kind of interaction. Since the chain is infinite and all its links are identical atoms, the chain has a discrete translation symmetry. In turn, by assuming the principle of indifference, the constituent atoms are considered as equidistant in the state of equilibrium. In

this model, when an atom is moved away from its equilibrium position, then a restitutive force will appear on that atom that tends to return it to the equilibrium position. The simplest restitutive force is, as in a spring, proportional to the distance, $F \propto d$. If u_s is the variable that represents the position of the particle s , and given that this particle is bound to its neighbors $s + 1$ and $s - 1$, then the force on it will be

$$F_s = C(u_{s+1} - u_s) - C(u_s - u_{s-1}) \quad (1)$$

where C is a proportionality constant. Once the force is determined, it is introduced into the equations of classical mechanics, for example, into Newton's second law. In this way, a series of differential equations is obtained. If there are N particles in the chain, then N equations of the following form are obtained:

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

where m is the mass of particles and $s = 1, 2, \dots, N$. In principle, if these equations are solved given the initial conditions, the mathematical expression that describes the motion of each atom in time can be computed. Mathematical details are not very important here, but we do want to highlight the picture about the dynamics of solids offered by this model: atoms are linked by interactions that allow them to vibrate about their equilibrium position. In this way, the vibrations in the crystal lattice form waves that propagate through the crystal, by means of which sound and temperature are transported.

2.2. *Quantum solids and the birth of the concept of phonon.*

The problem about the ontological status of phonons arises because the classical description of crystalline solids, offered in the previous section, is not enough to explain the phenomena that can be measured in laboratory. In particular, the dependence of the heat capacity on temperature cannot be explained by the mechanical model. As we will see, in order to account for this kind of phenomena, the introduction of a new entity was required: the phonon.

Let us carefully analyze how phonons are introduced. Since empirical evidence suggests that vibrations are quantized, it is necessary to quantize the model. By assuming that the atoms

only interact with their first neighbors, and on the basis of the fact that the inter-atomic forces are equal to those of the harmonic oscillator, quantizing the model is extremely simple and the Hamiltonian \hat{H} can be written as

$$\hat{H} = \sum_{s=1}^N \frac{1}{2m} \hat{p}_s^2 + \frac{C}{2} (\hat{q}_{s+1} - \hat{q}_s)^2 \quad (3)$$

where \hat{p}_s and \hat{q}_s are the momentum and position operators from s , respectively, and \hat{q}_{s+1} is the position operator from particle $s+1$. Since the total number N of particles is a really huge number, of the order of 10^{23} , solving the Hamiltonian as it is expressed is impossible in practice. As a consequence, a strategy that simplifies the calculation is used. The first step is to make a very specific coordinate change, to the so-called *phononic coordinates*:

$$\hat{Q}_k = N^{-1/2} \sum_{s=1}^N \hat{q}_s e^{-iksa} \quad \hat{P}_k = N^{-1/2} \sum_{s=1}^N \hat{p}_s e^{iksa} \quad (4)$$

where $k = 2\pi n N^{-1} a^{-1}$ and $n = 0, \pm 1, \dots, N/2$. In these coordinates the Hamiltonian is written as a sum of harmonic oscillators that do not interact:

$$\hat{H} = \sum_n \frac{1}{2} (\hat{P}_n^2 + \omega_n^2 \hat{Q}_n^2) \quad (5)$$

where $\omega_n = (2C/m)^{1/2} (1 - \cos(k_n a))^{1/2}$ is the angular frequency of the oscillator n . The result so obtained shows that the system can be represented by the Hamiltonian corresponding to the sum of many independent harmonic oscillators. Therefore, the formalism based on creation and destruction operators originally developed for the harmonic oscillator can be used (Sakurai 1994). In this formalism vibrations can be represented as particles that are created and destroyed, where the quantity of particles increases as a function of the increase of the vibrational magnitude. Thus, some states of the system can be represented by means of a state $|n\rangle$, where n is a integer that represents the number of particles in the system. The creation operator \hat{a}^\dagger , when applied to a state of the system with n particles, returns another state with $n+1$ particles, that is, creates a particle. In turn, the destruction operator \hat{a} destroys a particle.

$$\hat{a}^\dagger |n\rangle = |n+1\rangle \quad \hat{a} |n\rangle = |n-1\rangle \quad (6)$$

On the basis of this representation, the Hamiltonian can be expressed in terms of the creation and the destruction operators as follows:

$$\hat{H} = \sum_k \hbar \omega_k \left(\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right) \quad (7)$$

Although this Hamiltonian is the same Hamiltonian of eq. (3), in this representation the atoms originally introduced to constitute chain no longer appear in the model. The new expression represents a new type of particle called *phonon*. Then, the original mechanical picture can be left aside, to move to a model where there are no atoms in motion, but only phonons. From this perspective, the total energy of the crystal is the sum of the energy of the phonons plus a “vacuum” energy associated with the case in which there are no phonons in the network. Indeed,

$$E = \sum_m \varepsilon_m = \sum_m \hbar \omega_m \left(n_m + \frac{1}{2} \right) = \sum_m \varepsilon^m n_m + \varepsilon_{vacuum} \quad (8)$$

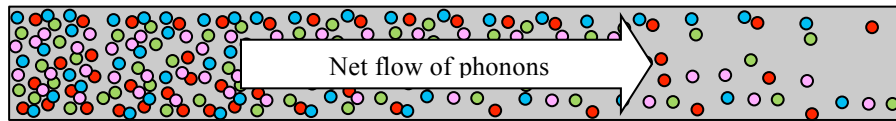
where ε^m is the energy of a phonon whose frequency is ω_m , n_m is the number of phonons whose frequency is ω_m and ε_{vacuum} is the vacuum energy.

3. Explanation and prediction by means of phonons.

In the previous section we showed that, by means of a series of calculations, it is possible to begin from the Hamiltonian of a system consisting of atoms that vibrate by interacting with their first neighbors, and to arrive to the Hamiltonian of a system composed of phonons. However, the relevance of the model based on phonons, and what makes the question about the ontological issue of phonons so urgent, is the fact that the model is indispensable for the study of the properties of crystalline. In particular, phonons play a central role in explaining the physical and chemical properties of salts. As an example, we present here two simple cases in which the explanatory and predictive power of the concept of phonon can be acknowledged.

3.1. The heat equation.

In the description of crystalline solids, the temperature of the solid is explained microscopically by the presence of phonons; the higher the density of phonons, the higher the temperature. To illustrate this idea, let us consider a metal bar heated at one of its ends and cooled at the other: heat will flow from the hot end to the cold end, producing a temperature gradient. If the phonon model is used for the microscopic explanation, then the situation is described in terms of a source of phonons at the hot end, which travel through the metal bar toward the cold end. In their motion, phonons collide with each other, generating a process of diffusion that ends with the destruction of the phonons at the cold end.



In a metal bar with a hot end (left), where phonons are created, and a cold end (right), where phonons are destroyed, there is a net flow of phonons from the hot end to the cold end. As the density of phonons represents the temperature, the phonon diffusive process explains the temperature gradient along the bar.

In this way, phonons offer a microscopic model of heat flow and temperature gradient based on particles. This model is explanatory simple and very effective, since gives an easy picture of thermal phenomena. In fact, it is surprising that the application of quantum mechanics to crystalline solids ends up recovering a conception of heat similar to that developed by Lavoisier in the thirteenth century with his theory of caloric (Best 2016). In effect, phonons would be a modern and quantized version of the notion of the *substance of heat*.

On the other hand, at the mathematical level, the effectiveness of the model of phonons becomes clear by the fact that it allows deducing the well-known heat equation in a simple way as follows. If collisions are taken into account, the net flow of energy along the longitudinal direction x of the bar is computed as

$$j_U = -\frac{1}{3}Cvl \frac{dT}{dx} \quad (9)$$

where C is the thermal capacity per unit volume, v is the average velocity of the phonons, and l is the average free path of a phonon between collisions (for a detailed analysis of the deduction of the heat equation, see Ashcroft and Mermin 1976). Independently of the details of the derivation,

it is interesting to notice that the constants appearing in the equation, which have no clear interpretation in the traditional view, acquire a precise meaning in the model of phonons: for example, when interpreted in the light of the phonon model, the heat equation shows that there is a directly proportional relation between the velocity of phonons and the propagation of heat

3.2. The heat capacity.

Another interesting example that reinforces the richness and epistemic potential of the concept of phonon is the calculation of the heat capacity of solids. In this case, let us consider that phonons are confined within an isolated crystal without sources or sinks. The system can be thus modeled as an ideal gas of phonons confined in a box. On this basis, the total energy of the crystal can be written as the sum of the energy of each of the phonons

$$E = \sum_m \varepsilon^m \langle n_m \rangle \quad (10)$$

where $\langle n_m \rangle$ is the average occupation number for phonons of energy ε^m , which is given by the Planck distribution

$$\langle n_m \rangle = \frac{1}{e^{\frac{\hbar\omega_m}{k_B T}} - 1} \quad (11)$$

where k_B is the Boltzmann constant and T is the absolute temperature. Then, the specific heat of the crystal $C_{crystal}$ is computed as

$$C_{crystal} = \frac{\partial U}{\partial T} \quad (12)$$

Due to the complexity of the calculation, certain approximations are usually applied. In the case of low temperatures, the Debye approximation is used and the result is proportional to the cube of the temperature (for the details of the derivation, see Kittel 2005)

$$C_{crystal} \propto T^3 \quad (13)$$

In the case of high temperatures, the Einstein approach is used, and the thermal capacity results

$$C_{cristal} \propto \frac{1}{T^2} \frac{e^{\frac{\hbar\omega}{k_B T}}}{\left(e^{\frac{\hbar\omega}{k_B T}} - 1 \right)^2} \quad (14)$$

These equations, deduced from the phononic formalism, fit excellently to the results obtained in the laboratory. For example, the results of the thermal capacity of diamond obtained experimentally are contrasted with the results computed by means of the phononic formalism leading to the above equations. A similar situation occurs with the thermal capacity solid argon. In this case, the agreement between experimental and theoretical results is more than acceptable, it is excellent.

The previous cases are only two of the many applications that show that the phonon formalism is not a mere calculation curiosity; on the contrary, it is a successful model to explain the phenomena associated with solids, which has demonstrate a high empirical success and explanatory power.

4. The ontological status of phonons.

In the previous sections we have recalled the mathematical derivation of phonons and have stressed their explanatory power. However, such epistemic virtues do not supply sufficient grounds to justify the existence of phonons. Precisely, the anti-realist tradition appeals to the well-known pessimistic meta-induction argument to claim that pragmatic success does not prove the truth of the theory nor, therefore, the effective existence of the entities postulated by it. Aware of this argument, in this section we will try to argue, perhaps not against scientific anti-realism but against a certain type of realism, that if one adopts a realistic attitude in science, there is no reason to consider phonons as non-existing entities. For this purpose, we will follow two strategies: first, we will consider the analogy between phonons and photons, and, second, we will refute the usual arguments by which phonons are commonly considered useful tools but unreal entities.

4.1. Phonon, a cousin of photon.

In Subsection 2.2, we have shown how, by means of a series of calculations it is possible to start from the Hamiltonian of vibrating atoms and to arrive to the Hamiltonian of a system composed of phonons in the following way:

$$\hat{H}_{atoms} + \hat{H}_{int} \xrightarrow{\text{Coordenadas fonónicas}} \sum_m \frac{1}{2} (\hat{P}_m^2 + \omega_m^2 \hat{Q}_m^2) \xrightarrow{\text{op. creación y destrucción}} \sum_m \hbar \omega_m \left(\hat{a}_m^\dagger \hat{a}_m + \frac{1}{2} \right) \quad (15)$$

where $\hat{H}_{atoms} = \sum_{s=1}^N \frac{1}{2m} \hat{p}_s^2$ and $\hat{H}_{int} = \sum_{s=1}^N \frac{C}{2} (\hat{q}_{s+1} - \hat{q}_s)^2$.

This formal operation is highly relevant for the purpose of the present work, due to the complete analogy that can be traced between phonons and photons. In fact, the calculations used to find the phononic Hamiltonian are exactly the same as those used to find the Hamiltonian of photons. Starting from the Hamiltonian of the electric \hat{H}_E and magnetic field \hat{H}_B , we formal strategy in the case of photons is:

$$\hat{H}_E + \hat{H}_B \xrightarrow{\text{Coordenadas fotónicas}} \sum_m \frac{1}{2} (\hat{P}_m^2 + \omega_m^2 \hat{Q}_m^2) \xrightarrow{\text{op. creación y destrucción}} \sum_m \hbar \omega_m \left(\hat{a}_m^\dagger \hat{a}_m + \frac{1}{2} \right) \quad (16)$$

As it easy to see, the formal analogy between the derivation of photons and the derivation of phonons is complete; then, it is legitimate to ask why we phonons are endowed with the fictional or degraded status of quasi-particles. If the procedure of the expression (16) allows us to understand all forms of electromagnetic radiation in terms of particles, why does the procedure of expression (15) not allow us to understand all forms of vibration in a crystal under the same terms? Or, in other words, what are the assumptions that prevent us to say that the temperature and the sound in a crystal are manifestations of the real presence of phonons?

Summing up, in the case of photons, by beginning from the electromagnetic field, certain calculations lead to the expressions that can be easily interpreted in terms of particles named photons. Subsequently, and due to the empirical success of the models based on photons, they acquire the status of real particles. However, in the case of phonons, although exactly the analogous calculations are performed and an equivalent empirical success is reached, the same conclusion is not drawn. In fact, these particles are usually considered as pseudo-particles or quasi-particles (Ladyman 2015, Franklin & Knox 2018). In the following subsections we will

critically assess the reasons that commonly underlie this different attitude. In particular, we will try to elucidate whether the different arguments usually directed against the non-existence of phonons are powerful enough to draw such a conclusion.

4.2. *Two ontologies for matter.*

When a picture and a mathematical formalism to describe the composition of chemical substances is needed, definitely the most popular model is that offered by the usual atomic model, according to which matter is composed of atoms in motion, and in whose context chemical phenomena are explained in terms of atoms and their interaction. An atom is classically conceived as a composite particle whose set of properties includes position and velocity. This idea, when applied to the case of a crystalline solid, leads to the model of the chain of interacting atoms as presented in Section 2. Thus, in order to apply quantum mechanics to a chemical substance under this model, it is necessary to define its Hamiltonian as the Hamiltonian of these component atoms plus the interaction Hamiltonian:

$$\hat{H}_U = \hat{H}_{atoms} + \hat{H}_{int} \quad (17)$$

If some approximations are applied to this Hamiltonian, many natural phenomena can be predicted and explained. For example, the energy levels of a molecule can be computed (Sutcliffe and Woolley 2012).

On the other hand, in Section 2 we presented a different ontology for the case of solid state matter based on the phononic model. According to that model, solids are composed of atoms at rest and phonons in motion. In turn, the Hamiltonian of the phonons plus the interaction Hamiltonian can be defined

$$\hat{H}_U = \hat{H}_{phonons} + \hat{H}'_{int} \quad (18)$$

With these Hamiltonians many natural phenomena can also be predicted and explained. For example, the heat equation can be computed.

Although a relevant empirical success is obtained by the application of the two models, the preference for the atomic hypothesis about the constitution of matter prevails over the phononic

hypothesis in the scientific community. One may ask for the reasons underlying this choice. In the following paragraphs we critically analyze three arguments that can be used to support the usual atomic hypothesis:

- The “*tool argument*” points out that the atomic hypothesis is originally used to introduce phonons (see equation 15). Therefore, phonons must be interpreted as a mere tool that simplifies the calculations that cannot be directly solved in the atomic model.
- The “*supercomputer argument*” claims that we are forced to use the phononic model because we do not have yet sufficient computing power to solve the Schrödinger equation of a crystalline network from first principles. The assumption is that, in the future, when we will count with more powerful computers, we will be able to perform the exact calculations with no need to appeal to phonons.
- The “*explanation argument*” asserts that the usual atomic model, unlike the phononic model, can explain a great variety of phenomena. Due to their different explanatory capacity, both models are not at the same level.

The three arguments are intertwined, since the explanation argument only makes sense either by conceiving phonons as mere calculation tools, or by clinging to the hope that in the near future we will have sufficient computing power to do without phonons. However, for reasons of argumentative clarity, we will treat them independently.

4.3.1. The tool argument.

According to the *tool argument*, on the basis of the model of a chain of atoms that vibrate about their equilibrium position, phonons are introduced with the only purpose of simplifying calculations. In fact, starting from the atoms model was the strategy followed in Section 2 (it is also the way in which phonons appear in the textbooks on the subject; see, e.g., Ashcroft and Mermin 1976, Kittel 2005). However, we followed this strategy only for didactic reasons: since the typical reader is familiar with the idea of atoms in motion, it is easier to begin with a model based on them. The relevant point is that those calculations based on the atomic model are not necessary: it is possible to directly introduce phonons with the Hamiltonian

$$\hat{H} = \sum_k \hbar \omega_k \left(\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right) \quad (19)$$

In other words, the existence of phonons can be postulated from the very beginning, and, with them, the properties of crystalline solids can be explained. When this fact is kept in mind, the tool argument loses its strength: although the calculations are usually presented from atoms to phonons, they can be presented in the opposite direction, such that phonons appear as the fundamental entities.

Our counterargument is further supported by the fact that the Hamiltonian of the atoms in motion can be obtained by departing from the phononic Hamiltonian. This means that, although there is a transformation that turns the atomic Hamiltonian into the phononic Hamiltonian, there is also an inverse transformation that turns the phononic Hamiltonian into the atomic Hamiltonian. Therefore, one might argue that phonons are the fundamental entities and atoms in motion are useful calculation tools for treating in problems that do not involve thermal phenomena. This shows that, since the situation is symmetric, the tool argument cannot be appealed to for supporting the ontological priority of one description matter over the other. It might be taken into account only as a complement in the case that other arguments for the ontological priority of the atoms model were available. If it could be proved, on the basis of other arguments, that the fundamental ontology of matter is one based on atoms in motion, then the tool argument would explain why using phonons is sometimes convenient.

So far we have shown that the two presentation strategies, phonons obtained from atoms and atoms obtained from phonons, are equally legitimate. But this view is valid only in a particular case, the case of non-interacting phonons. In fact, in Section 2, the phonons appearing at the end of the derivation do not interact with each other. This means that the argument that begins by atoms leads to the very idealized case of phonons that do not interact with each other. But, when phonons are used to describe some phenomenon in a crystal in the general case, a *phononic interaction* term is introduced in the phononic Hamiltonian of eq. (19). For example, the dependence of electrical resistivity with temperature is explained by considering that the electrons that move in a conductive material collide with and are dispersed by the phonons of the crystal lattice: the higher the temperature, the more number of phonons in the material, and consequently more collisions occur. The electron-phonon coupling constant is measured in

laboratory, and from this constant the number of phonons surrounding an electron that moves within a crystal is computed: in this way, the type of interaction between the involved particles can be determined (Kittel 2005). This phenomenon is explained by assuming the existence of both electrons and phonons, and by admitting that particles of those these two kinds interact with each other: the interaction Hamiltonian that accounts for this interaction is built in order to account for the results of experiments, as usual in physics. Summing up, the dependence of electrical resistivity with temperature is explained by taking phonons, not atoms, as the starting point.

The same happens in the experiment carried out by Shinen (1963) on magnesium oxide crystals, where a scattering process between phonons can be observed. Shinen describes a situation in which, as a consequence of the cross-linking between two beams of phonons with frequency ω_1 and ω_2 , a third phonon beam is produced with frequency $\omega_1 + \omega_2$. This phenomenon led him to think that, when a phonon with frequency ω_1 collides with a phonon with frequency ω_2 in a scattering process where energy is conserved, a third phonon with frequency $\omega_1 + \omega_2$ is produced. The scattering between the two beams is the consequence of the interaction between phonons; that is, Hamiltonian of phonons must be added an interaction Hamiltonian:

$$\hat{H} = \sum_k \hbar\omega_k \left(\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right) + \hat{H}_{\text{int}} = \hat{H}_{\text{phonons}} + \hat{H}_{\text{int}} \quad (20)$$

The interaction Hamiltonian has the directly interpretation as the Hamiltonian that accounts for the interaction between phonons. Moreover, it is measured in the experiments in laboratory. Only a posteriori, in certain cases the phononic interaction Hamiltonian can be reformulated in the context of the atomic model, that is, it can be computed by means of the introduction of an extra, non-quadratic term in the Hamiltonian of the atomic model given by eq. (3). But even when such a reformulation is possible, the non-quadratic term in the atomic interaction Hamiltonian lacks a direct interpretation: the interaction between atoms represented by that quadratic term has no clear physical meaning. It might be argued that the atomic model is a mere calculation tool and, consequently, the atomic interaction Hamiltonian turns out to be an artifact derived from the real

phononic description. A similar example can be found in Kong *et al.* (2001), where the phonon-electron coupling in magnesium boride crystals is computed.

The cases described above show that, although in the particular case of non-interacting phonons the position according to which phonons are mere calculation tools might be defended, in the general case such a position becomes untenable. Recall that, according to the tool argument, phonons must be interpreted in an instrumental way since derived from atoms. However, in the case where phonons interact with each other, the roles are reversed: physicists begin with phonons, work with phonons, make experiments with phonons, determine the Hamiltonian interaction of phonons, and finally, just at the end of the process, eventually they translate the obtained results in terms of atoms in motion. In other words, in the generic case, the phonons model is the working methodology, used to pose the problem from the beginning and to design the experiments. Therefore, atoms should be conceived as mere calculation tools without real reference.

Thus, we consider that the analogy between phonons and photons established in Subsection 4.1, and the fact that the phononic hypothesis can be considered as a “first principle”, undermine the defense of the realists who, accepting the existence of photons, maintain a skeptical attitude toward phonons. Therefore, we are faced to the following dichotomy: either we adopt a general instrumentalist view for all entities, or we accept phonons as existing entities.

4.3.2. The supercomputer argument.

This argument insists in that phonons are calculation tools that could be discarded if we had enough computing power to solve the Schrödinger equation of crystals from first principles in an exact way. Let’s consider this new argument in more detail.

Given a quantum system U , according to quantum mechanics it has a Hamiltonian associated \hat{H}_U , and there are many legitimate ways to divide U into parts. In particular, it is always possible to add and subtract an arbitrary \hat{H}_X , so that the original Hamiltonian remains the same:

$$\hat{H}_U = \hat{H}_X - \hat{H}_X + \hat{H}_U = \hat{H}_X + \hat{H}_{\text{int}} \quad (21)$$

where $\hat{H}_{\text{int}} = -\hat{H}_X + \hat{H}_U$. This is a highly artificial but correct procedure, which shows that any Hamiltonian can always be written as a given self-Hamiltonian plus some interaction term. The fact that this can always be done does not mean, as we will see later, that it is always useful.

On the basis of the above remark, the Hamiltonian of a crystal can be quantum-mechanically represented as the Hamiltonian of atoms in motion plus an interaction Hamiltonian, $\hat{H}_U = \hat{H}_{\text{atoms}} + \hat{H}_{\text{int}}$, or as the Hamiltonian of phonons plus an interaction Hamiltonian different from that of the atomic case, $\hat{H}_U = \hat{H}_{\text{phonons}} + \hat{H}'_{\text{int}}$. It is important to note that up to now all the Hamiltonians are exact, since no approximation was introduced yet. In the hypothetical case of having a supercomputer that, following the supercomputer argument, allowed us to obtain exact solutions for systems of many equations, then we could use it to solve the equations based on the atomic Hamiltonian and to calculate, for example, the expectation value of a certain observable \hat{O} . However, nothing prevents us from using the same supercomputer to solve the equations based on the phononic Hamiltonian, and to calculate the expectation value of the same observable \hat{O} . In both cases, because exact Hamiltonians are used and exact solutions are computed, we would obtain exactly the same result.

$$\langle \hat{O} \rangle_{\text{atoms}} = \langle \hat{O} \rangle_{\text{phonons}} \quad (22)$$

Summing up, although it is true that with a supercomputer we can exactly describe any problem with the atomic model, it is also true that we can do the same, and with the same effectiveness, with the phononic model: the supercomputer is neutral in this. Therefore, the asymmetric conclusion drawn by the supercomputer argument, according to which atoms exist but phonons do not, is not acceptable, and the argument loses any strength.

4.3.3. The explanation argument.

According to this argument, the ontological priority of atoms in motion over phonons is due to the fact that, by contrast to the latter, the former explain a large number of phenomena.

Let us recall that the Hamiltonian of any crystalline material can be expressed according to the atomic model and to the phononic model:

$$\hat{H}_U = \hat{H}_{atoms} + \hat{H}_{int} = \hat{H}_{phonons} + \hat{H}'_{int} \quad (23)$$

We have seen that if we had a supercomputer, then we could calculate the exact solutions in both cases, obtaining the same results. But, what happens if we do not have the supercomputer?

If, as it is the case, we do not have the supercomputer, then we are forced to introduce some kind of approximations. The most common approaches are always variations of the traditional perturbation theory (Ballentine 1990), which requires that the self-Hamiltonian is much larger than the interaction Hamiltonian. Therefore, the requirement to apply the perturbation theory to the Hamiltonian in the atomic model is that $\hat{H}_{atoms} \gg \hat{H}_{int}$: if this requirement is met, then approximate solutions can be obtained and the expectation value $\langle \hat{O} \rangle_{atoms}$ of a certain observable \hat{O} can be computed. Analogously, the requirement to apply the perturbation theory to the Hamiltonian in the phononic model is that $\hat{H}_{phonons} \gg \hat{H}'_{int}$: once again, if this requirement is met, then approximate solutions can be obtained and the expectation value $\langle \hat{O} \rangle_{phonons}$ of the same observable \hat{O} can be computed. However, unlike what happens in the case of the exact solution presented in the previous section, in this case the results are not the same:

$$\langle \hat{O} \rangle_{atoms} \neq \langle \hat{O} \rangle_{phonons} \quad (24)$$

This is due to the fact that the two expectation values are obtained by means of approximate solutions. Therefore, one result may be better than the other, and this can only be decided experimentally. Precisely, in general the perturbation theory cannot be applied to the two Hamiltonians, since the requirements $\hat{H}_{atoms} \gg \hat{H}_{int}$ and $\hat{H}_{phonons} \gg \hat{H}'_{int}$ in general cannot be satisfied at the same time. As a consequence, in the generic case the atomic model or the phononic model can be applied, but not both.

The above remark means that, although it is true that without a supercomputer assisting us the atomic model is successful in many cases, it is also true that in many other cases it does not work. In the case of thermal processes, the phononic model must be used, not by whim, but by necessity. It does not matter that the list of applications of the atomic model is longer than that of the phononic model: they complement each other since both are indispensable when the goal is to

explain all phenomena. In fact, when one model cannot be applied, the other applies. The phononic model is essential because the atomic model is not universally applicable.

The explanation argument might gain strength if it received additional theoretical support from the other two arguments previously considered. However, this does not happen because, as we have shown, they are not adequate or effective to deny the existence of phonons.

5. Therefore, phonons exist. But how do they exist?

Up to this point we have argued that there are good reasons to accept phonons as really existing entities. However, there is still a long way to understand the effective ontological status of phonons. In the current philosophical literature, the prevailing realist position about phonons relies on emergentism. For instance, in the paper “Are there individuals in physics, and if so, what are they?”, James Ladyman conceives phonons as quasi-particles, where quasi-particles are entities with a finite life time and therefore always related to a limited time scale (2015: 202). On the other hand, although in the line of Ladyman’s proposal, Alexander Franklin and Eleanor Knox (2018) develop in their paper “Emergence without limits: the case of phonons” develop a purely emergentist proposal to understand the case of phonons. From their perspective, the fundamental entities inhabit a basal level, from which the entities that cannot be explained from the behavior of the basal level emerge. Phonons are entities that emerge from the basal level populated by atoms.

Although the emergentist view is very appealing, it faces a serious difficulty. The particular case of phonons, as Franklin and Knox (2018) themselves admit, is a strange kind of emergence. Usually, at least in physics, the emergence scheme is supported by the fact that the concepts of the involved theories are linked by some singular or asymptotic limit. It is precisely those kinds of limit what introduces the asymmetry indispensable for emergence. In fact, in spite of the many conceptions about emergence, everybody accepts that emergence is an asymmetric relation: if A emerges from B, then B does not emerge from A. In the case of phonons, by contrast, there are no limits relating the atomic model and the phononic model. Furthermore, as explained in detail in the previous section, the two models stand in symmetric relations in several senses. Whereas

there is a transformation that turns the atomic Hamiltonian into the phononic Hamiltonian, there is also an inverse transformation that turns the phononic Hamiltonian into the atomic Hamiltonian. Although it is true that a supercomputer could exactly solve any problem with the atomic model, it is also true that it could do the same, and with the same effectiveness, with the phononic model. In turn, the atomic model is successful in many cases but does not work in many others, precisely in those where the phononic model is successful. Given the strong parallelism between the two models, where does the asymmetry required by emergence come from?

Of course, conceiving phonons as entities emergent from atoms is not a contradictory stance. However, the ontological priority of atoms over phonons is introduced as a metaphysical assumption, which is supported neither by the formal theory of phonons nor by the experimental practice in physics. Therefore, those who want to avoid those non-scientifically founded metaphysical assumptions may prefer a pluralist perspective that rejects hierarchical relations between levels.

Scientific pluralism, in its ontological version, has been proposed by several authors such as Dupré (1993), Cartwright (1994, 1999), Chakravarty (2011), and Lombardi and Pérez Ranzanz (2014). Despite this, the pluralist perspective is in general very resisted in the scientific community, and even by many philosophers of science. Although scientific practice witnesses an increasing proliferation of models configured from theoretical principles in conflict (Hendry 1998), or even incompatible models applied to the same system of study, a reductionist, monistic and universalist view prevails in science, as a product of what Scerri (2000) called the “imperialism of physics”.

The roots of this situation can be found in the fact that the traditional philosophy of science was constituted as a field of inquiry by taking the evolution of physics as its model, that is, a discipline characterized by trying to provide a unified and integral vision of the world. This may explain the widespread tendency of trying to explain the multiplicity of existing things by means of an economic and simple ontology. However, not only regarding the interdisciplinary relations the reductionist project has faced insurmountable obstacles as a consequence of the impossibility of translating the concepts coming from different scientific disciplines. Also within physics itself similar obstacles appear. It is in this context that pluralism becomes strong because, as Chang

asserts, the best reason to be pluralist is that it is not very likely that we will achieve an accurate theory that meets all our needs; and if it is not so, maintaining multiple systems makes much sense (Chang 2012: 20).

Carwright does not advocate only for an epistemic pluralism; by taking seriously what scientific practice suggests, she asserts: “as appearances suggest, we live in a dappled world, a world rich in different things, with different natures, behaving in different ways. The laws that describe this world are a patchwork, not a pyramid ” (Carwright 1999: 01). In agreement with this pluralist stance, although from a slightly different philosophical approach, Olimpia Lombardi and Ana Rosa Pérez Ransanz ascribe to a Kantian-inspired ontological pluralism that retain the realist requirement of a correspondentist conception of truth: “rejecting metaphysical realism does not imply rejecting truth as correspondence. (...) a Kantian-rooted realism is able to preserve a notion of truth as correspondence” (Lombardi and Pérez Ransanz 2012, p. 50). From this perspective, the simultaneous existence of incompatible entities and/or properties can be asserted whenever it is done from different conceptual schemes. In continuity with certain fundamental aspects of Carnap’s position (1950), and inspired by Putnam (1981), the authors assume that the question of what really exists only makes sense in an internal framework, in the context of the ontological domain defined by a scientific successful theory. Thus, the theories of science do not describe a transcendental reality that waits to be discovered as it is in itself. On the contrary, each scientifically successful conceptual scheme constitutes its own ontology, so the problem “is not to establish what actually exists; the problem is to accept that what we call ‘object’ is constituted within our categorical scheme, thus it is an «object for us»” (Lombardi and Pérez Ransanz 2012: 23). Whereas a monist and reductionist position only accepts a single reality, the pluralist position implies not only that there is no absolute reality, but that there are multiple realities relative to the conceptual schemes of the different successful theories of science.

The present discussion about phonons is not the first time that ontological pluralism is considered in the field of chemistry. According to a traditional reductionist view, eminently anti-pluralist, the entities raised by chemistry, although with some explanatory efficiency, are merely apparent since resulting from an approximate description of the only true world described by quantum physics. However, the reductionist position disagrees with the effective scientific

practice. For instance, incompatible assumptions coexist in quantum chemistry, coming from structural chemistry and quantum mechanics, and none of them are dispensable. In particular, certain concepts of classical structural chemistry, such as the notion of molecular structure, are so essential for chemical practice that even when a mathematical reduction were possible, the resources of structural chemistry would still be absolutely indispensable. The case of optical isomerism, in turn, shows that even if we could calculate the exact Hamiltonian of a system, from such information we would not be able to obtain the precise structure that allows us to differentiate the dextrorotatory from the levorotatory molecules (for more details see Lombardi 2014, Fortin, Lombardi and Martínez González 2017, 2018a, 2018b). Ontological pluralism faces this situation by admitting that quantum chemistry is an autonomous discipline with its own ontology (see Lombardi y Labarca 2005, 2010)

On the basis of the arguments developed in the previous sections, the case of phonons can also be interpreted in a pluralistic philosophical framework, so that both the phononic and the atomic descriptions, even if incompatible with each other, are equally valid in their respective contexts. If a supercomputer existed, any system could be described with both models. And in the actual case in which such a supercomputer does not exist, the two descriptions remain equally valid in their respective fields of application. Therefore, both descriptions of reality must be accepted as equally valid.

From a pluralistic perspective, scientific ontology is context-dependent. In certain contexts, we should admit an ontology of mobile atoms since it allows us to explain a series of phenomena. But assuming such an interpretation in certain explanatory contexts should not limit or cancel other interpretive contexts. The phononic picture of reality, according to which atoms are at rest and many phenomena are the result of the motion of phonons, is another non-exclusive successful interpretation. As Cartwright claims, “all evidence points to the conclusion that I really like –that Nature is not reductive and single-minded. It is rich and diverse” (1994: 361).

6. Conclusions.

The main aim of this work has been to discuss the ontological status of phonons, usually discredited in physics as mere calculation tools. For this purpose, first we recalled the epistemic virtues of such entities, not only their explanatory power but also their interpretive capability with respect to certain phenomena that remain obscure from other theoretical views.

Then we argued that there are not good reasons to conceive phonons as non-existing entities. To reach this goal we first established an analogy between photons and phonons, so that anyone who accepts photons as existing entities should also accept phonons in the same sense. Second, we examined three arguments that are often used to explain the ontological primacy of atoms over phonons: the *tool argument*, the *supercomputer argument* and the *explanation argument*. By showing the weaknesses of those arguments, we undermined the views of those who, from a realist position, nevertheless deny the real existence of phonons.

Finally, having already rejected the reductionist position, we considered two possible ways of interpreting the ontological status of phonons. On the one hand, the emergentist perspective proposed by certain authors for the case of phonons is faced to the difficulties derived from the symmetric relations linking the atomic and the phononic models, which turn the asymmetry of emergence into a metaphysical postulate. On the other hand, ontological pluralism have the resources to cope with the conceptual problems derived from the case of phonons, with no need to postulate a hierarchical relationship between the different domains of reality.

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