Emergence-Free Duality: Phonons and Vibrating Atoms in Crystalline Solids

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Abstract

The crystalline solids admit two models: the one of vibrating atoms and the one of phonons. The model of phonons allows explaining certain properties of crystalline solids that the model of vibrating atoms does not allow. Usually, the model of phonons is assigned to diminished ontological status as quasi-particles. Recently, there has been a proposal to homologate the ontological status of phonons with that of emergent particles, such as photons. In this article, this proposal will be critically examined, and it will be proposed that the model of phonons and the model of vibrating atoms could be considered in ontological parity.

1. Introduction

In the field of physics, solids are classified into two classes: amorphous and crystalline. The distinctive feature of the crystalline solids is that their atoms or molecules are arranged in a lattice pattern. Crystalline solids admit two models: the one of vibrating atoms and the one of phonons. It is known that the model of phonons entails explanatory novelty significantly in comparison with the model of vibrating atoms. For instance, the model of phonons allows the deduction of the heat equation in a very clear and interpretable way. Nonetheless, it is usual in the practice of physics to give to phonons a weakened ontological status, that of quasi-particles. In a paper devoted to analyzing the ontological status of phonons, Alexander Franklin and Eleanor Knox (2018) aim to homologate it with that of other particles usually recognized as emergent, such as photons. In their paper, they employ a particular notion of emergence that includes two distinctive elements: (i) emergence occurs between two levels involving different theories, and (ii) the relationship between these theories is inter-theoretical reduction.

In the current debate on the concept of emergence, Butterfield's notion of emergence compatible with inter-theoretical reduction has gained popularity in recent years. According to Jeremy Butterfield (2011), a theoretical-reducible behavior is emergent if it is novel and

robust with respect to a reducing comparison class. It is important to highlight that while emergence is an ontological notion, reduction is an epistemic notion. Although the precise nature of emergence is still a subject of debate, it generally involves a relation of 'ontological priority' or 'priority in nature' that ontic items in a more fundamental level have with respect to ontic items in a less fundamental one. The priority relation is typically conceived of in terms of ontological dependence or metaphysical grounding by different philosophers (see e. g. Schaffer 2009, Tahko and Lowe 2020). In turn, reduction is a relation that may hold between two theoretical domains. In Nagel-Schaffner's classical account of reduction, the reduced theory is deduced from the reducing theory plus some auxiliary assumptions. Other more recent accounts of reduction usually relax this requirement. While emergence and reduction were usually viewed as opposing theses, Butterfield's account of emergence is characterized by its compatibility with reduction. In fact, it is not a contradiction that a reducible domain may be emergent with respect to the reducing domain, if emergence holds between ontic domains while reduction between the theoretical domains that represent them. According to Butterfield's account, a case of emergence compatible with reduction would be distinguished from a simple reduction case if, for example, the properties or behavior of the entities in the reducible theory exhibit novel and robust features compared to those of the reducing theory.

As is well known, the concept of emergence is broad and encompasses various forms with distinct characteristics. Emergence can be weak or strong, with or without reduction, diachronic or synchronic, etc. (O'Connor 2021.) The version of emergence that Franklin and Knox (2018) employ in their proposal incorporates both reduction and emergence. Therefore, for their description to be considered valid, the case of phonons must involve both reduction and emergence. While the notion of reduction is subject to debate, we argue that it requires acknowledging the existence of a theoretical leap between two descriptions. In the context of physics, this implies the presence of a reducing theory, formulated within a specific mathematical space and including one or more governing equations for its evolution. Additionally, there must be a reduced theory, formulated within its own space and governed by its own equations. These two theories must be distinct so that, when it is somehow possible to derive the equations of the reduced theory from those of the reducing theory, reduction is said to occur. In this sense, we assert that, if this approach is adopted, in the derivation there must be a theoretical leap, from the reducing theory to the reduced one. Within physics, the paradigmatic cases of emergence refer to the relationship between phenomena belonging to different theories. Examples include the emergence of thermodynamics from statistical mechanics, the emergence of classical mechanics from

quantum mechanics, phase transitions, and so on. For this reason, in a very well-known book about emergence and reduction, Robert Batterman (2011) claims that most cases of emergence arise as a result of the use of singular limits (e. g. phase transition). In their paper about the emergence of phonons, Franklin and Knox consider that singular limits make easy to build a case of reduction between theoretical levels but may obscure the novelty that emergent behavior is supposed to have. This is why they are interested in finding a case of emergence that does not make use of singular limits. To fulfil that purpose, they put forward the case of phonons as one of emergence without limits.

There are also cases of intra-domain emergence, in which it is assumed that a single theory can refer to different types of ontic items within a single domain. The distinction between inter-domain emergence and intra-domain emergence has been put forward by Lombardi and Ferreira Ruiz (2018). This distinction between two types of emergences is based on the notion of domain. A domain is understood as a set of phenomena associated with entities whose existence is committed to a given theory. This commitment refers to the fact that each theory is associated with an ontic domain that can be distinct. This domain is characterized, or at least constrained, by the properties of the mathematical space in which each theory is formulated, the specifics of its dynamic equation, the peculiarities of the measurement process it proposes, and so on. In this way, for example, the ontic domain of classical mechanics is distinct from that of quantum mechanics because the mathematical formalism of quantum theory imposes certain characteristics on the entities it describes, such as the existence of incompatible properties, indistinguishability, non-locality, and so forth. Inter-domain emergence is a relation that holds between ontic items belonging to different ontic domains represented by correspondingly different theoretical domains. Consider that ontological priority involved in emergence is an asymmetric, irreflexive and transitive relation that establishes a partial order between different ontic domains. Assuming that each theory refers to a particular ontic domain, it follows that ontological priority between ontic domains requires a leap between the theoretical domains that represent them, that is, two or more relata that supports an asymmetric, irreflexive and transitive inter-theoretical relation. Otherwise, there would be no scientific-informed reason to argue that the different descriptions refer to domains that are not in ontological parity. In this sense, we argue that in Franklin and Knox's description of crystalline solids, there must be a theoretical leap because the inter-domain emergence they propose requires an inter-theoretical relation. In turn, intra-domain emergence is a relation that holds between different types of ontic items that belong to the same ontic domain belonging to the same theory, as for instance, types of properties. Intra-domain emergence does not require an inter-theoretical relation as inter-domain

emergence does, but it at least requires some kind of asymmetric relation between the descriptions of the two different types of ontic items. Cases of intra-domain emergence have been successfully established in the area of the philosophy of chemistry. For example, in Matta, Lombardi and Jaimes Arriaga (2020) it is argued that electron density arises from the wavefunction as a coarse-grained magnitude within the quantum theory of atoms in molecules (QTAIM) (see also Lombardi and Matta 2022). In this case, both the electronic density and the wave function belong to the domain of quantum mechanics. However, it is argued that the former emerges from the latter in a type of emergence known as intra-domain emergence.

In this article, we critically assess Franklin and Knox proposal about the emergent status of phonons by pointing out that it is possible to derive phonons from vibrating atoms without a theoretical leap. Our interest will not focus on whether it is true that the phonon model's description is indeed reducible to the vibrating atom model's description, but rather on whether there is a theoretical leap as required by the inter-domain emergence proposal as presented by the authors of the paper. Additionally, we will analyze whether it is possible to describe phonons as a case of intra-domain emergence, for which it will be required to identify some form of asymmetry. We will show that the crucial transition between descriptions involves a change of variables that does not imply a theoretical leap. In fact, both the vibrating atom model and the phonon model can be fully developed within a single theoretical domain: quantum mechanics. As a consequence, we defend that, since the descriptions corresponding to the two different models can be formulated within a single theoretical framework, the derivation of phonons that Franklin and Knox propose does not suffice to interpret the case of phonons as one of inter-domain emergence. We also show that the change of variables that mediate between both descriptions amounts to a change of tensor product structure (TPS) within quantum mechanics, thus framing the case of phonons within the so-called TPS approach that has been fruitfully applied elsewhere. Given that there is not a mathematical asymmetry between the descriptions that arise from different TPSs, it follows that the case of phonons cannot be constructed as intra-domain emergence either, unless an external asymmetry is introduced. We conclude that, if only the physics of crystalline solids is considered, phonons do not have a weakened ontological status as quasi-particles, but neither are they emergent particles arising from an allegedly fundamental level, that of vibrating atoms. For us, phonons in crystalline solids should in principle be considered on ontological parity with vibrating atoms. Unless a convincing motivation to introduce an external asymmetry comes into play, the case of phonons is best characterized as one of emergence-free duality, in where there is no ontological priority between the two models.

However, this does not mean that a description formulated in terms of emergence is not possible at all. By introducing an external asymmetry, it is possible to reconstruct an emergentist argument. Nonetheless, as will be seen, the way in which this asymmetry is introduced is not unique, and depending on the criterion used, different ontological hierarchies may be the case.

In order to reach this goal, the article is structured as follows. In Section 2, we review the proposal due to Franklin and Knox about the emergent status of phonons. In Section 3 we critically assess this proposal. In Section 4 we embed the case of phonons within the frame of the TPS approach. We conclude with some final remarks.

2. Phonons and atoms as a case of emergence

In their paper about phonons, Franklin and Knox clearly assume Butterfield's notion of emergence compatible with inter-theoretical reduction sketched above. According to this notion of emergence, three conditions must be satisfied: novelty, robustness and reducibility. The main argument of their paper is made on the novelty and robustness that the model of phonons has. There is not much about reducibility, but, as we show below, it is clear that they assume that there is an inter-theoretical reduction relation between the descriptions.

2.1. Reduction and theoretical leap

As we have mentioned, most of the Franklin and Knox's article focuses on arguing that the novelty and robustness requirements are satisfied. However, their characterization of phonons makes it quite clear that they consider that there are two distinct theories at play and that the phonon phenomenon can be reduced. In several passages, Franklin and Knox affirm that there is a reducible theoretical leap between the descriptions of the two models. Some of these passages are the following.

In the Introduction, when they are explaining the reasons for examining the case of phonons, they state that this case study involves reduction:

> "It's therefore helpful to look explicitly at an example of emergence that does not fit the asymptotic limit mold: our case study will provide an example of a kind of emergence that maintains explanatory novelty even in the face of **reduction**, escaping the tension engendered by the asymptotic analysis [emphasis added]." (Franklin and Knox 2018, p. 2).

In this quote, the authors present their example as a case in which there is reduction. However, they do not indicate which would be the reduced theory and which would be the reducing theory. Later, in Section 3, they suggest that the phonon case includes emergence and reduction:

> "There are those who will define emergence in such a way that phonons do not fall under the definition; any definition (for example Batterman's) that precludes the compatibility of emergence and **reduction** will do this [emphasis added]." (Franklin and Knox 2018, p. 5).

The objective of transcribing these quotes is to make it clear that they assume that phonons are a case of reduction. This is important because the reduction relation implies that there must be two theories involved. Indeed, in the conclusion they refer to two theories, one more fundamental (of the crystal) and another less fundamental (of the phonons). That is, according to them, there is somehow a theoretical leap:

> "Insofar as phonons are also robust under perturbations of the underlying crystal physics, and are described by a **theory that is less fundamental than the basic theory** of the crystal, they are emergent [emphasis added]." (Franklin and Knox 2018, p. 10).

This passage refers to a theoretical leap between descriptions, where two theoretical levels are clearly distinguished. The authors' insistence on highlighting, in various ways, the theoretical leap between the description of the phonon model and the model of vibrating atoms in crystalline solids is perfectly reasonable, considering that it is a requirement for the notion of emergence they discuss. Unfortunately, nowhere in the paper is it made explicit which is the fundamental theory and which is the less fundamental one. We consider that this important point would have deserved a direct and thorough account, a particular section or at least a few paragraphs, instead of passing mentions. They only assume that there is a theoretical leap, but do not consistently argue in favor of that assumption. However, our critique of this work does not require specifying those theories; whether it is classical mechanics, quantum mechanics, or field theory is irrelevant. In the subsequent sections, we will show that both the description of phonons and vibrating atoms naturally fall within a single theory, quantum mechanics. Therefore, a complete description of crystalline solids physics does not require an inter-theoretical relation of some kind between phonons and the atomic lattice.

2.2. Novelty and robustness

We now review their arguments about the novelty and robustness of phononic behavior, which, together with the existence of an inter-theoretical relation or a kind of asymmetry between descriptions, are the conditions for emergence. These two are the points on which the authors have focused, and we believe argued convincingly. Novelty is defined by them in terms of explanatory novelty and robustness is defined as stability with respect to perturbations. First, they settle the issue of novelty. According to them, novelty has to do with abstraction. For them, performing a change of variables (from atomic displacements to normal modes variables, as it is in the case of phonons) involves an abstraction of sorts. However, there is an important difference between Franklin and Knox (2018) and Knox (2016) accounts of the relation of novelty with abstraction. Abstraction in Knox (2016) is construed as if it entailed a loss of information when moving from one description to another, in such a manner that there is a mathematical irreversibility between descriptions. According to Knox (2016) this mathematical irreversibility is important to build a case of novelty in cases where singular limits are performed. Phase transition, for instance, counts as emergent behavior precisely because thermodynamic description abstracts a great deal of information from statistical mechanical description. Abstraction here plays an important role in distinguishing between theoretical levels but also in telling which level is emergent and which is the fundamental one. It is clear that the more detailed description counts as fundamental. However, in Franklin and Knox (2018), in order to fit with the case of phonons, they dispense with mathematical irreversibility and make novel behavior compatible with mathematical equivalent descriptions. They construe 'abstraction' as if the new description (once the change of variables is performed) allows for 'abstractions' not immediately available in the previous description, in the sense that information can be added in new ways, entailing explanatory novelty. In fact, once the change of variables is performed, it is possible to add collisions to the model of phonons. That is, certain anharmonicities that were initially suppressed by the adoption of the harmonic approximation can now be safely reintroduced. This possibility is precisely what allows us to describe a large number of situations that have been observed experimentally.

They also provide arguments to defend robustness of phononic behavior. The description and the dynamics of a robust model of certain phenomena is supposed to be stable with respect to perturbations in the alternative model. As the authors explain, if the model and its dynamics were affected by, for instance, small temperature changes or sudden displacements, then the model at issue would be too fragile and irrelevant for physics. It turns out that the model of phonons is robust in this sense. The very nature of the approximations involved is

the source of its robustness. For example, below Debye temperatures (which are 200 – 500K for most common elements) the harmonic approximation fully holds. For higher temperatures, the approximation is still useful since it is possible to reintroduce anharmonicities leading to phonon-phonon interactions. According to the authors, the model of phonons can be used as long as the crystalline solid remains an approximately rigid structure.

3. Phonons and atoms as a case of duality

We agree with Franklin and Knox that phononic behavior is novel and robust but disagree with the idea that phonons can be interpreted as a case of inter-domain emergence. The point of contention is whether or not there is an inter-theoretical relation (theoretical leap) between the description of the model of phonons and the description of the model of vibrating atoms. We first discuss the alleged inter-theoretical relation required by inter-domain emergence. From our perspective, both descriptions can be framed in the same theoretical domain: quantum mechanics. In contrast, Franklin and Knox seem to frame the description of the model of vibrating atoms and that of phonons in different theories. As a result, they have an allegedly emergent upper-level model that is described by an allegedly reducible theory and an allegedly fundamental lower-level model described by an allegedly reducing theory. However, as we show in this section, it is possible to obtain phonons without introducing a theoretical leap of sorts between descriptions. This point was previously noted by De Haro (2019), who observes that novelty and robustness suffice at most to support what he calls 'epistemic emergence', which he interprets as Franklin and Knox's true thesis under a charitable reading of their work. We agree with De Haro that, in the physics of crystalline solids, we have “only one theory, formulated in different variables” (p. 32).

3.1. A deduction of phonons

As usual in textbooks, we propose a very simple model of vibrating atoms of a crystalline solid, which is a one-dimensional infinite chain of atoms interconnected by a harmonic interaction. In this model, if an atom is not in its equilibrium position, a restoring force exerted by its neighbors tends to bring it into its equilibrium position. The simplest restoring force is proportional to the distance. The force F_s exerted on particle s is defined:

$$F_s = C\left(u_{s+1} - u_s\right) - C\left(u_s - u_{s-1}\right) \tag{1}$$

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 of proportionality. Now it is possible to plug it into classical equations of motion to obtain a series of coupled differential equations. If there are S particles, then there are S equations of the form:

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

where m is the mass of the particles. This simple model offers us a picture of the dynamics of a crystalline solid in which the harmonic interaction between the atoms allows them to vibrate. These vibrations form waves that propagate sound and heat through the crystal lattice. The model of vibrating atoms admits a classical description. In fact, in (2) we have the classical equations of motion that guide the dynamics of this model. But it also admits of a quantum mechanical description, since the evidence indicates that the vibrations are quantized. The Hamiltonian $\hat{H}$ under a quantum description of the model of vibrating atoms reads:

$$\hat{H} = \sum_s \frac{1}{2m}\hat{p}_s^2 + \frac{C}{2}\left(\hat{q}_{s+1} - \hat{q}_s\right)^2 \tag{3}$$

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 $s+1$.

Though this is a quantum model of vibrating atoms, it is not yet a phonon model. To arrive at the phonon model, it will be essential to perform the change to phonon coordinates. The phonon variables are:

$$\hat{Q}_{k_j} = N^{\frac{-1}{2}} \sum_{s-1}^{S} \hat{q}_s e^{-ik_j sa} \tag{4}$$

$$\hat{P}_{k_j} = N^{\frac{-1}{2}} \sum_{s-1}^{S} \hat{p}_s e^{ik_j sa} \tag{5}$$

where $k_j = 2\pi j N^{-1} a^{-1}$, $j = 0, \pm 1, ..., \frac{S}{2}$ and a is the equilibrium distance between atoms. Then we obtain an equivalent expression for the Hamiltonian (3), which is

$$\hat{H} = \sum_j \frac{1}{2}\left(\hat{P}_j^2 + \omega_j^2 \hat{Q}_j^2\right) \tag{6}$$

where $\omega_j = (2C/m)^{\frac{1}{2}}\left(1-\cos\left(k_j a\right)\right)^{\frac{1}{2}}$ is the angular frequency of the oscillator j. By means of this change of variables, a different model is obtained where there are no interacting atoms. Now, the crystalline solid is a sum of non-interacting harmonic oscillators. This is highly convenient, as the solutions of the harmonic oscillator are well-known in the field of quantum mechanics.

Now we are going to delve into some interesting consequences of using quantum mechanics to describe the crystalline solid once the change to phonon variables has been performed. Let us consider the oscillator j once again. Employing the solutions of the harmonic oscillator, it is possible to establish that the energy of the oscillator j is $\varepsilon_j = \hbar\omega_j(n_j + 1/2)$, where $n_j = 0,1,2,\ldots$. Note that there is just one quantum number n_j for this oscillator. Then, it is possible to write the eigenstates of $\hat{H}$ as $\left|\varepsilon_j\right\rangle = \left|n_j\right\rangle$. Since the energy is quantized, if the system is in the state $\left|n_j\right\rangle$ and it transitions to the immediately higher state $\left|n_j + 1\right\rangle$, then the energy is increased in $\hbar\omega_j$. Thus, it is possible to think that every $\hbar\omega_j$ is a quantum of vibration added into the system. In this way, the state $\left|n_j\right\rangle$ represents the number of vibrations with energy $\hbar\omega_j$. Following this idea, it is easy to think of these discrete quantum vibrations as resembling particles, just as quanta of electromagnetic energy are regarded as photons. These new particles are not atoms, they are not electrons, they are not photons; they are something different, and we refer to them as 'phonons'.

Under this quantum description of the model, the total energy of the system is the sum of the energy of the phonons plus the vacuum energy ε_{vacuum}, which is the energy of the crystalline solid when there are no phonons (i. e. when the harmonic oscillators are at rest). The total energy E reads

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

where $\hbar\omega_j$ is the energy of a phonon with frequency ω_j, n_j is the number of phonons with frequency ω_j, and ε_{vacuum} is the vacuum energy. This mathematical maneuver allows us to find the solutions of the system easily and provides an alternative description for the vibrations of a crystalline lattice in which oscillations are represented as particles. If the oscillation is larger, then there are more particles. This is the core of the phonon's description, and this is the movement that precisely allows us to talk about particle-like phonons. If one desires greater elegance, it is possible to use the formalism based on creation and annihilation operators (Sakurai 1994). This formalism also represents vibrations as particles that are created or destroyed as the magnitude of the vibration increases or decreases.

3.2. A single theory: An argument against inter-domain emergence

Let us stress that the description of the model of vibrating atoms in equation (3) and the description of the model of phonons in equation (6) are both at the same theoretical level: quantum mechanics. This means that both descriptions are governed by the Schrödinger equation and belong to the same Hilbert space. Moreover, both descriptions share the same Hamiltonian and the same wave function; the only difference is that they are expressed in different coordinates. The calculations in the previous section show that it is not imperative to appeal to other quantum theories, such as quantum field theory or relativistic quantum field theory, to discuss the relationship between phonons and vibrating atoms. Standard quantum mechanics includes both, and the ontological implications of the coordinate change can be studied within a single theory. In our account, there is not an inter-theoretical relation between descriptions, as Franklin and Knox seem to consider. This indicates that although there are two different descriptions, in principle it is incorrect to think that they belong to a higher-level and a lower-level theoretical domains. If we look at the deduction in detail, we notice that the central step to go from the model of vibrating atoms arranged in a lattice to a model of particle-like phonons is the change of variables. Indeed, within classical mechanics, it is also possible to perform this coordinate transformation without transitioning to the quantum realm. By rewriting equations (2) in phonon variables, decoupled equations of classical oscillators are obtained, and this description is known as classical phonons (Dagotto 2013). In sum, from our perspective, the key that allows us to adopt the model of phonons is the change of variables, not a change of theory.

It should be clear now that the adoption of the model of phonons to represent crystalline solids does not depend on a theoretical leap of sorts. It is perfectly possible to describe both the model of vibrating atoms and of phonons by means of quantum mechanics. It is even possible to describe both models by means of classical mechanics. Of course, under classical description, it is not possible to obtain full explanatory power of the model of phonons. Nonetheless, the mere possibility of framing the descriptions of both models in a single theory (classical or quantum) is enough to disprove the idea that there is inevitably an inter-theoretical relation between the descriptions of the two models. Of course, one can arrange things to make it appear as though there is an inter-theoretical relation between descriptions—by framing the vibrating atoms description within one theory and the phonon description within another. However, these would be ad hoc maneuvers to interpret the case of phonons as one of inter-domain emergence, and they fail to capture the crucial transition from atoms to phonons, which is, as argued, only the change of variables. Consequently, contrary to Franklin and Knox, the case of phonons lacks one of the necessary conditions to

interpret it as a case of inter-domain emergence. Furthermore, the case of phonons as one of inter-domain emergence could not be built even if the assumed notion of emergence rejected reduction, since it is not only the case that the inter-theoretical relation is not one of reduction, but that there is not an inter-theoretical relation at all.

The authors also attempt to defend the emergent status of phonons by referencing an analogy: phonons emerge in a similar manner to how quantum particles do with respect to the underlying quantum field. They take this relation to be typically exemplified by photons. About this they state that:

> "The relation that phonons hold to the underlying crystal description is almost identical to the relation that quantum particles hold to the underlying quantum field. And if any inter-theoretic relation betokens an interesting emergence, surely the relationship between quantum particles and the field does." (Franklin and Knox 2018, p. 5).

We stress that, according to the authors, there exists an inter-theoretical relation between an upper-level and a lower-level description, in both the case of phonons and photons. They believe that if it is the case that photons are emergent with respect to the underlying field, then it is also the case that phonons are emergent with respect to the allegedly underlying atomic lattice because of the resembling mathematical derivation. As the authors acknowledge, considering that novelty and robustness of photons and phonons is out of discussion, the only point that could break the analogy is if in both cases there is an analogous inter-theoretical relation between descriptions (p. 5). Here we only suggest that, even in the case of photons, whether there is an inter-theoretical relation should be discussed in more detail. Arguably, both photons description (as well as other quantum particles) and the quantum field description can be framed in quantum field theory, a single theoretical domain. Furthermore, within the realm of the philosophy of quantum field theory, there is ongoing discussion about whether particles or fields constitute the fundamental elements in QFT ontology. As a consequence, it is not clear at all, from a philosophical point of view, if photons should be considered emergent with respect to the quantum field. Franklin and Knox themselves mention this discussion. So, caution here should prevent us from jumping to conclusions. The analogy seems to be too fragile to be considered a decisive argument.

3.3. Regular coordinate transformation and the difference between a theoretical and an external asymmetry

If we accept our previous argument against the inter-domain emergence of phonons, this does not rule out the validity of another type of emergence. Franklin and Knox thesis could be

reformulated if they construed their emergence relation as one of intra-domain emergence. Recall that intra-domain emergence is a relation that holds between different types of ontic items that belong to the same ontic domain, as for instance, types of properties (Lombardi and Ferreira Ruiz 2018). In this type of emergence, both levels under consideration, the upper-level and the lower-level, belong to the same theory. Therefore, they share the ontological characteristics imposed by the equations or mathematical spaces of the theory. If two items, I_1 and I_2, denoted by the terms t_1 and t_2 respectively, are considered to belong to the same theory, then, from an ontic point of view, I_1 and I_2 belong to the same ontic domain, that is associated with the theory in question. In the case of intra-domain emergence, stating that, for example, I_2 emerges from I_1 means that two levels within the same domain can be identified and that the level corresponding to I_2 ontologically depends on the level associated with I_1. From this perspective, it could be the case that 'being a phonon' and 'being a vibrating atom' would be just two different types of properties, belonging to crystalline solids in a single ontic domain and described within a single theoretical domain: quantum mechanics. Nevertheless, even if we accepted this possibility, the mathematical relation between the descriptions of the two models of crystalline solids cannot support the asymmetry that is essential to emergence. In fact, Franklin and Knox themselves consistently argued that descriptions of the models of atoms and phonons are exactly translatable in either direction, since there are no essential idealizations or approximations involved (they are performed before the change of variables). We are quoting this passage in its entirety because it is illustrative:

> "So a complete translation between descriptions is possible in either direction. In this sense, the two descriptions seem to express a duality, rather than a standard reductive relationship. This leads to a question that has been pressed on us by David Wallace: if the relationship here is really one of duality, can one nonetheless talk about novelty and emergence? We think (contra (Knox, 2016)) that the answer, at least to the question with regards to novelty, is yes: explanatory novelty can be displayed even when the descriptive change is entirely reversible. The phonon case demonstrates this. But emergence is plausibly a relation that is, by definition, asymmetric; one cannot both think of phonons as emerging from the crystal lattice and of the crystal lattice as emerging from the phonons. This sounds right to us, and suggests that mere robustness and novelty may not be enough for emergence. We thus may wish to define emergence as a relation that holds between less and more fundamental phenomena" (Franklin and Knox 2018, p. 8).

In this passage, the authors acknowledge that some form of asymmetry is required in the emergentist framework, but unfortunately, they do not discuss what the exact origin of this asymmetry might be. Even by their own lights, it is possible to talk about novelty but not about emergence. In principle, the correct approach is to consider the two models as a duality, as we intend to defend in this article. As previously considered, there is no inter-theoretical relation. As we are considering now, there is no mathematical asymmetry between descriptions: the phonon variables are just linear combinations of the displacement variables and vice versa, as the authors themselves argue. We can go from atoms to phonons or from phonons to atoms. Unlike what happens when we take a mathematical limit, with a change of variables we can go back and forth without loss of information. As a result, if only the physics of crystalline solids is taken into account, the asymmetric relation between phonons and atoms required by emergence cannot be established in this circumstance either. This is even clearer if we take the TPS approach, as we will do in the next section. However, the origin of the asymmetry does not have to be within the mathematical formalism. An external asymmetry to the mathematical formalism can be introduced for various motivations: practicality, metaphysical considerations, greater integration with other areas of science, seeking internal consistency, personal preferences, etc. The introduction of such an asymmetry would allow for grounding a description of phonons in terms of intra-domain emergence. Later, some examples of what possible external asymmetries to consider will be shown. For now, we conclude that, not only is it not possible to construct the phonon case as an emergence between domains, but it is also not possible to construct it as an emergence within a single domain, unless we have a motivation to introduce an external asymmetry.

4. Phonons and atoms from the TPS approach

In this section we will review the concept of TPS and we will apply it to the case of phonons.

4.1. What is a TPS?

A tensor product structure or TPS is a particular way to factorize the Hilbert space into subspaces. The idea behind TPSs can be easily understood as follows. Let us consider a composite quantum system $U = S_1 \cup S_2 \cup S_3 \cup S_4$ with the associated Hilbert space

$$\mathcal{H}_U = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \otimes \mathcal{H}_4 \tag{8}$$

This way of presenting the Hilbert space entails a particular decomposition into subspaces, and therefore, is associated with a particular TPS that we may call, for example, TPS_A.

According to this TPS, there are four particles with some mass, some charge, some spin, etc. The mathematics of Hilbert space allow us to decompose space $\mathcal{H}_U$ in another way, for example $\mathcal{H}_U = \mathcal{H}_i \otimes \mathcal{H}_{ii}$. Now, the same total Hilbert space is the tensor product of other Hilbert spaces. In this TPS_B, the system is composed of two particles $U = S_i \cup S_{ii}$. Then, we have another number of particles, other mass, other charge, other spin, etc. When we consider the system from a bottom-up perspective, we can think that these are two very different systems. One is a group of four particles of type A, as the eq. (8) suggest, and the other is a set of two particles of type B, since the decomposition $\mathcal{H}_U = \mathcal{H}_i \otimes \mathcal{H}_{ii}$ have two factors. However, although the subsystems are very different, the whole system is exactly the same. At this point it is possible to ask, what is the correct composition of system U? Are there two particles or four? According to the TPS approach there is no privileged decomposition, but there are two equivalent descriptions of the same system. By 'TPS approach' we understand a line of research carried out by several authors, in which the relativity of certain notions closely linked to quantum formalism with respect to the previous specification of a tensor product structure for a system has been considered. Thus, notions such as the entanglement of quantum states or the separability between subsystems have been reviewed from this approach with interesting results.

Let us briefly mention some results achieved within this approach. Zanardi (2001) and Dugić and Jeknić (2006, 2008) emphasize the relativity of the notion of separability between subsystems. Zanardi (2001) tries to avoid the ambiguity that the notion of separability has with respect to the set of available partitions by selecting those subalgebras of operators that represent a set of operationally accessible observables. These represent 'real' subsystems against 'virtual' subsystems, whose observables could not be measured. Dugić and Jeknić (2006) strive to find criteria that allow distinguishing 'real' and 'virtual' subsystems from the approach of quantum decoherence (2006) and quantum information (2008). However, to the extent that such criteria cannot receive a precise formulation at the moment, the authors recognize that not only the notion of separability between subsystems but also the very notion of system should be relativized. Harshman and Wickramasekara (2007) emphasized the variety of TPSs that a system can admit, highlighting among them those that allow each particular subsystem to undergo global symmetry transformations and dynamic transformations. The first are called by the authors symmetry-invariant TPSs and the second the dynamically invariant. These would be TPSs of particular interest because the subsystems defined by them respect the symmetries of the Galileo group and have a unitary dynamic evolution. Earman (2005) emphasizes the relativity and even ambiguity of the notion of entanglement, since the entanglement of the state of a system defined by its algebra of

observables is necessarily entangled with respect to a certain decomposition of the algebra into subalgebras. A quantum state can be entangled with respect to a particular decomposition and factorable with respect to others. As long as there is no criterion that defines which decomposition should be preferred over the others, the notion of entanglement cannot escape, according to the author, from a radical ambiguity. More recently, Fortin and Lombardi (2022) applied this approach to study the relativity of the notion of entanglement in case of indistinguishable particles, concluding that indistinguishability should be considered no longer as a relation between particles but between properties. In turn, Pasqualini and Fortin (2022) studied the ontological status of composite bosons or cobosons: although generally regarded as mere quasi-particles, the authors argue that cobosons should be considered on ontological parity with fermions that compose them.

4.2. TPSs view and the case of phonons

Now let us apply the TPS approach to the case of phonons. Since there is a bijective transformation that leads from the quantum description of the model of vibrating atoms (see the Hamiltonian in equation 3) to the quantum description of the model of phonons (see the Hamiltonian in equation 6), it is possible to show that these quantum descriptions correspond to two different TPSs. The quantum description of the model of atomic nuclei interacting via the harmonic oscillator potential is built as follows. Let be the atomic nucleus j, which constitutes the quantum system S_j and is represented in Hilbert space $\mathcal{H}_j$. The group of N atomic nuclei constitute the total quantum system $S_T = S_1 \cup S_2 \cup ... \cup S_N$ and is represented in the Hilbert space $\mathcal{H}_T$:

$$\mathcal{H}_T = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes ... \otimes \mathcal{H}_N = \bigotimes_{j=1}^{N} \mathcal{H}_j \tag{9}$$

Equation (9) is an expression of $\mathcal{H}_T$ as a Tensor Product Structure that we will call TPS_V, corresponding to N vibrating atoms. This is manifested in the fact that the individual properties of each nucleus can be represented with the same tensor structure. For example, the momentum operator of nucleus 1 is represented as:

$$\hat{p}_1 = \hat{p}(x_1) \otimes \hat{I}(x_2) \otimes ... \otimes \hat{I}(x_N) \tag{10}$$

Where $\hat{p}(x_1)$ is the momentum operator expressed with the coordinates x_1 of nucleus 1, $\hat{I}(x_2)$ is the identity operator expressed with the coordinates x_2 of nucleus 2 and so on. That is, the operator $\hat{p}_1$ is written as a tensor product in which there is an operator other than the

identity in the first term and identities in the rest of the terms. In general, any nucleus 1 observable will have the form:

$$\hat{o}_1 = \hat{o}(x_1) \otimes \hat{I}(x_2) \otimes ... \otimes \hat{I}(x_N) \tag{11}$$

On the other hand, there are collective observables that do not correspond to any individual particle but are associated with global properties, such as the operator associated with the joint energy of nuclei 1 and 2:

$$\hat{h}_{1y2} = \hat{h}(x_1) \otimes \hat{I}(x_2) \otimes ... \otimes \hat{I}(x_N) + \hat{I}(x_1) \otimes \hat{h}(x_2) \otimes ... \otimes \hat{I}(x_N) \tag{12}$$

This operator cannot be written as a tensor product, but it is a sum of tensor products. The total Hamiltonian $\hat{H}$ is written as:

$$\hat{H} = \sum_{j=1}^{N} \frac{1}{2m} \hat{p}_j^2 + \frac{C}{2} \left(\hat{q}_{j+1} - \hat{q}_j \right)^2 \tag{13}$$

where $\hat{p}_j$ and $\hat{q}_j$ are the momentum and position operators of the particle j and $\hat{q}_{j+1}$ is the position operator of the particle $j+1$. This is the Hamiltonian of a chain of particles, in this case vibrating atoms, that interact at first neighbors. As there is interaction between neighbors, it is not possible to write the Hamiltonian as the sum of independent Hamiltonians of isolated particles. If now we change to phonon variables, we have to define the operators

$$\hat{Q}_{k_j} = N^{\frac{-1}{2}} \sum_{s-1}^{S} \hat{q}_s e^{-ik_j sa} \tag{14}$$

$$\hat{P}_{k_j} = N^{\frac{-1}{2}} \sum_{s-1}^{S} \hat{p}_s e^{ik_j sa} \tag{15}$$

It can be shown that these operators can be interpreted as position and momentum operators of new particles since they satisfy the canonical commutation relations

$$\left[\hat{P}_k, \hat{Q}_k \right] = i\hbar \delta_{k,k'} \tag{16}$$

$$\left[\hat{P}_k, \hat{P}_{k'} \right] = \left[\hat{Q}_k, \hat{Q}_{k'} \right] = 0 \tag{17}$$

In these coordinates the Hamiltonian is written as a sum of harmonic oscillators that do not interact:

$$\hat{H} = \sum_k \frac{1}{2}\left(\hat{P}_k^2 + \omega_k^2 \hat{Q}_k^2\right) \tag{18}$$

Then new quantum systems with coordinates $\tilde{x}_k$ (14) and (15) are defined. The independent oscillator k constitutes the quantum system $\tilde{S}_k$ and is represented in the Hilbert space $\tilde{\mathcal{H}}_k$. Since this change of variables is a simple discrete Fourier transform from which normal coordinates are obtained, it can be shown that

$$\bigotimes_k \tilde{\mathcal{H}}_k = \tilde{\mathcal{H}}_{-\frac{N}{2}} \otimes \tilde{\mathcal{H}}_{-\frac{N}{2}+1} \otimes ... \otimes \tilde{\mathcal{H}}_{\frac{N}{2}} = \mathcal{H}_T \tag{19}$$

That is, it is the same Hilbert space $\mathcal{H}_T$ but factored into another tensor product structure, that is, it is another TPS, the TPS$_P$.

The result shows that the system can be represented with a Hamiltonian that expresses the sum of many independent harmonic oscillators (18). That is to say,

$$\hat{H} = \sum_k \hat{H}_k \tag{20}$$

where

$$\hat{H}_k = \hat{I}\left(\tilde{x}_1\right) \otimes ... \otimes \hat{I}\left(\tilde{x}_{k-1}\right) \otimes \hat{\tilde{h}}\left(\tilde{x}_k\right) \otimes \hat{I}\left(\tilde{x}_{k+1}\right) \otimes ... \otimes \hat{I}\left(\tilde{x}_N\right) \tag{21}$$

and $\tilde{h}\left(\tilde{x}_k\right)$ is the energy of the oscillator k. This energy is quantized and can take the following values

$$\varepsilon_{n_k} = \hbar\omega_k\left(n_k + \frac{1}{2}\right) \tag{22}$$

where $n_k = 0,1,...,\infty$ that corresponds to each eigenstate $\left|\varepsilon_{n_k}^{(k)}\right\rangle$ such that

$$\hat{\tilde{h}}\left(\tilde{x}_k\right)\left|\varepsilon_{n_k}^{(k)}\right\rangle = \varepsilon_{n_k}\left|\varepsilon_{n_k}^{(k)}\right\rangle \tag{23}$$

This means that when the oscillator k is at the level n_k, it has energy ε_{n_k}. At this point it is possible to notice the fact that the energy levels are equally spaced. This allows us to think of the state $\left|\varepsilon_{n_k}^{(k)}\right\rangle$ of the system k in such a manner that it represents a system of n_k phonons each one with energy $\hbar\omega_k$ that inhabit an empty space with vacuum energy $\frac{\hbar\omega_k}{2}$ so that the energy of the set is $\varepsilon_{n_k} = n_k\hbar\omega_k + \frac{\hbar\omega_k}{2}$.

Thus, it is understood that the total energy is the sum of the energy of these particles (called phonons) plus the energy of the vacuum. The eigenstates of the Hamiltonian $\hat{\tilde{h}}(\tilde{x}_k)$ are also eigenstates of the particle number operator $\hat{n}_k(\tilde{x}_k)$

$$\hat{n}_k(\tilde{x}_k)\left|\varepsilon_{n_k}^{(k)}\right\rangle = n_k\left|\varepsilon_{n_k}^{(k)}\right\rangle \tag{24}$$

Then, we will name the eigenstates of the energy directly by the number n_k, so that $\left|\varepsilon_{n_k}^{(k)}\right\rangle = |n_k\rangle$. This can be done for each of the oscillators, so that the eigenstates of the total Hamiltonian can be expressed as

$$|E\rangle = |N\rangle = \left|n_{-\frac{N}{2}}\right\rangle \otimes \left|n_{-\frac{N}{2}+1}\right\rangle \otimes \ldots \otimes \left|n_{\frac{N}{2}}\right\rangle = \bigotimes_k |n_k\rangle \tag{25}$$

In this step, the TPS was not changed, just another label was used for these states. In this way, we obtain the phonon description of the system as a result of a change of TPS.

We conclude this section pointing out that the change to phonon variables amounts to a change of TPS and therefore that the model of vibrating atoms and the model of phonons correspond to two different ways of dividing the system. As a new result of the TPS approach, we obtain that a crystalline solid is a system composed of vibrating atoms with respect to a certain tensor product structure (TPS_V) and it is a system composed of phonons with respect to another tensor product structure (TPS_P). Different but equivalent models of the same composite system within the same theoretical framework arise in relation to two different but equivalent TPSs. As defended in the TPS approach, from a mathematical point of view there is no reason to assign priority to one of the two partitions. More generally, it is reasonable to suggest that in principle all descriptions that arise as a result of taking different TPSs correspond to domains that are in ontological parity. To argue that one of these cases is a case of emergence, a kind of asymmetry would have to be introduced through the application of some external criterion. As long as no such criterion is provided, our proposal about the ontological parity of these domains should be preferred.

4.3. TPSs and the external asymmetries

At first glance, the most natural criterion when choosing a privileged partition that defines the fundamental entities would be the following. The concept of the atom, described as an entity that can move and interact with other atoms, is widely used in various fields outside of solid-state physics, while the concept of the phonon is used in a more restricted domain. This asymmetry in applicability, coupled with the advantages of proposing an ontology that is

compatible with that of other theories and areas of science, leads one to think that proposing vibrating atoms as more fundamental is the natural choice. However, before comparing the theory with other areas of knowledge, quantum mechanics has several internal ontological problems that have been studied for decades by physicists and philosophers, such as contextuality, non-separability, indistinguishability, the measurement problem, etc. (see Bub 1997; Lombardi and Dieks 2016.) These studies have led to different interpretative proposals for the theory, which provide quantum mechanics with a peculiar ontology that distinguishes it from other areas of science. Thus, concluding that atoms are more widely used in other fields may not be the best choice from the perspective of the internal coherence of quantum mechanics. The introduction of an external asymmetry is not neutral from an interpretative viewpoint, that is, each interpretation of quantum theory is associated with an ontology that proposes a different type of criterion.

If we choose to adopt an external criterion, we have several options available, each of which yields different results. For instance, one might consider the model of atoms to be more fundamental and phonons emergent, given that the atomic model has much wider applicability in physics than the phonon model. However, other criteria are also possible. For example, under the modal-Hamiltonian interpretation of quantum mechanics (Lombardi and Castagnino 2008; Lombardi, Fortin, Ardenghi and Castagnino 2010; Lombardi and Dieks 2024), where the energy of quantum systems always has a definite value, the Composite Systems Postulate establish that "A quantum system represented by S:($\mathfrak{O}$,H), with initial state $\rho_0 \in \mathfrak{O}'$, is composite when it can be partitioned into two quantum systems S_1:($\mathfrak{O}_1$,H_1) and S_2:($\mathfrak{O}_2$,H_2) such that (i) $O=O_1\otimes O_2$, and (ii) $H=H_1\otimes I_2+I_1\otimes H_2$ (where I_1 and I_2 are the identity operators in the corresponding tensor product spaces). In this case, we say that S_1 and S_2 are subsystems of the composite system $S=S_1\cup S_2$. If the system is not composite, it is elemental." Then, according to this interpretation, the TPS in which subsystems do not interact holds ontological priority. This is because the interpretation applies its actualization rule to the most fine-grained partition in where subsystems have time-independent Hamiltonians. Subsystems in coarse-grained partitions possess actual properties that result from the composition of the properties of subsystems in the fundamental partition. Applying this criterion to the case under discussion, we would have a scenario of intra-domain emergence in which phonons are more fundamental (since in the presented case they do not generally interact, while vibrating atoms are dependent (since they certainly interact). Entering into the details of the different possible criteria is not the objective of this paper, but it could also be mentioned that from a holistic interpretation (Healey and Gomez 2022), the fundamental system with an associated ontology would be the crystal as a whole. Other interpretations

based on decoherence would consider the privileged basis, which is the one that minimizes the production of entropy. Bohmian versions prioritize the entities that give rise to trajectories in physical space.

In summary, the TPS approach demonstrates a formal mathematical parity between the descriptions of phonons and vibrating atoms. Thus, if one considers only the quantum mechanics formalism that describes crystalline solids, without introducing any external elements, the results presented in this work invite us to regard phonons and vibrating atoms as ontologically on par. In contrast, if one accepts the introduction of external criteria to the formalism, it becomes possible to induce an asymmetry between the descriptions, enabling an account in terms of intra-domain emergence or another type of ontological hierarchy. However, depending on the type of asymmetry introduced, the choice of which level is fundamental may vary.

Final remarks

In this article, we evaluate the ontological status of the model of phonons with respect to the model of vibrating atoms in crystalline solids. We demonstrate that it is possible to derive phonons without giving rise to an inter-theoretical relation between the descriptions of the two models, in a manner that prevents to build the case of phonons as one of inter-domain emergence. We have also shown that, considering only the physics of crystalline solids, it is not only the case that there is not an inter-theoretical relation but there is not any kind of mathematical asymmetric relation between descriptions that would allow to build the case of phonons as one of intra-domain emergence. That point has been reinforced by showing that the change to phonon variables amounts to a change of the tensor product structure that is adopted to decompose the whole system. In such a manner, we framed the case of phonons within the so-called TPS approach that has been previously applied to other physical situations.

While the arguments above do not mean that an emergent description of phonons is completely ruled out, our contribution in this regard is that, without invoking external criteria, an understanding of phonons as an emergent phenomenon cannot be sustained. Perhaps it is possible to introduce some type of asymmetry that grounds an intra-domain emergence. At this point, it must be emphasized that the ontological status of phonons will depend on the external asymmetry adopted. Though it is common to consider the model of atoms more fundamental due to its wider applicability, according to other criteria, phonons could be considered fundamental relative to vibrating atoms.

In sum, we conclude that without external criteria, phonons do not have a weakened ontological status as quasi-particles, but neither are they emergent particles arising from an allegedly fundamental level, that of vibrating atoms. For us, the case of phonons is best characterized as one of an emergence-free duality where there is no ontological priority between the two models. We believe that the case of phonons as one of a duality (as well as other cases that can be framed in the TPS approach) could be ontologically clarified by the adoption of the modal ontology of properties for quantum mechanics (Lombardi and Castagnino 2008, da Costa, Lombardi and Lastiri 2013, da Costa and Lombardi 2014). But this is the subject of future work.

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