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

Sebastian Fortin

CONICET – Universidad de Buenos Aires, Argentina

Matías Pasqualini

CONICET – Instituto de Investigaciones "Dr. Adolfo Prieto", Universidad Nacional de Rosario, Argentina

Corresponding author: Sebastian Fortin, sfortin@conicet.gov.ar

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Abstract

The crystalline solids admit of 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 a 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 are in ontological parity.

Keywords

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 of 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 the current debate on the notion 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. 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. For that reason, they are interested in finding a case of emergence that does not make use of singular limits. To fill that purpose, they put forward the case of phonons as one of emergence without limits.

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 domain 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 plain-reduction case if the reducible domain has some novel and robust features with respect to the reducing domain.

However, the issue of reduction is probably not an essential feature of emergence, since there are accounts of emergence that preclude reduction. What we believe cannot be dismissed in an account of emergence is the existence of a theoretical leap between descriptions. 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, i. e. two or more relata that support an 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. There also cases of intra-domain emergence (e. g. Matta 2020), in which it is assumed that a single theory can refer to a plurality of ontic domains. These cases do not require a theoretical leap, but at least a kind of asymmetry between descriptions. In what follows, our interest will focus not on whether it is the case that the description of the model of phonons is reducible to the description of the model of vibrating atoms, but only on whether there is a theoretical leap or at least a kind of asymmetry between them.

In this article, we critically assess Franklin and Knox proposal about the emergent status of phonons by pointing out that there is not necessarily a theoretical leap between the descriptions corresponding to the two models of crystalline solids. We argue that, with respect to the model of vibrating atoms, there is not only a classical description but also a quantum description. The same holds true for the phonon model, with both a classical description and a quantum description. We will show that the crucial transition between the description of vibrating atoms and phonons involves a change of variables that does not imply a theoretical leap. As a consequence, we defend that, since the descriptions corresponding to the two different models can be formulated within a single theoretical framework (without a theoretical leap), the case of phonons cannot be built 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 no asymmetry between the descriptions that arise from different TPSs, it is deduced that the case of phonons cannot be constructed as an intra-domain emergence,

unless an external *ad hoc* asymmetry is introduced. We conclude that 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 are on ontological parity with vibrating atoms. The case of phonons is best characterized as one of emergence-free duality where there is no ontological priority between the two models.

In order to reach this goal, the article is structured as follows. In the first section, we review the proposal due to Franklin and Knox about the emergent status of phonons. In the second section we critically assess this proposal. In the third section we embed the case of phonons within the frame of the TPS approach. We end up with some final remarks.

1. 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 there are three conditions for this kind of emergence: novelty, robustness and reducibility. The main argument of their paper is made on the novelty and robustness that the model of phonons is supposed to have. There is not much about reducibility, but it is clear that they assume that there is an inter-theoretical reduction relation between the descriptions. In several passages, they let us believe 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." (Franklin and Knox 2018, p. 2).

Later, 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." (Franklin and Knox 2018, p. 5).

While discussing novelty, they state:

"Knox (2016) argues that novelty might be analyzed as explanatory novelty, and that this explanatory novelty might come about as the result of particular kinds of changes of variable or quantity between theoretical levels. In this section, we'll demonstrate how the phonon example fits into this account." (Franklin and Knox 2018, p. 7).

It is clear that they take the change to phonon variables to amount to a theoretical leap. In the conclusion:

"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" (Franklin and Knox 2018, p. 10).

This passage refers to a leap between descriptions, where two theoretical levels are clearly distinguished.

The authors' insistence on mentioning, in one way or another, that there is a theoretical leap between the description of the model of phonons and the description of the model of vibrating atoms in crystalline solids is perfectly reasonable if one considers that it is a necessary requirement of emergence. However, 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 assume that there is a theoretical leap, but do not consistently argue in favor of that assumption. Their only attempt to justify the assumption is to present an analogy with the case of photons which has its own problems and cannot count as a decisive argument.

Perhaps the assumption that there is more than one theory involved is linked to the way the topic of phonons is often introduced in textbooks. Some mathematical derivations of phonons may lead one to think that there is a theoretical leap between classical and quantum descriptions. In what follows, the deduction of phonons according to Franklin and Knox's account is reconstructed. As a preliminary step, they put forward a simple example of two masses connected to each other and to fixed points by three springs. The equations of motion for the masses are:

$$m\ddot{x}_1 = -kx_1 - k'\left(x_1 - x_2\right) \tag{1}$$

$$m\ddot{x}_2 = -kx_2 - k'\left(x_2 - x_1\right) \tag{2}$$

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

$$\eta_1 = x_1 + x_2$$
$$\eta_2 = x_1 - x_2 \tag{3}$$

By means of the change of variables, equations (1) and (2) are transformed into two decoupled differential equations for two simple harmonic oscillators:

$$m\ddot{\eta}_1 = -k\eta_1 \tag{4}$$

$$m\ddot{\eta}_2 = -(k + 2k')\eta_2 \tag{5}$$

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

$$\eta_1 = \alpha_1 e^{i\omega_1 t} + \alpha_1^* e^{-i\omega_1 t} \tag{6}$$

$$\eta_2 = \alpha_2 e^{i\omega_2 t} + \alpha_2^* e^{-i\omega_2 t} \tag{7}$$

Where $\alpha_1, \alpha_1^*, \alpha_2, \alpha_2^*$ are fixed by the initial conditions.

Then, they propose a model much closer to the crystalline solid: a classical arrangement of N basic units with m atoms each. The adiabatic and harmonic approximation are used. The first consists in assuming that the degrees of freedom of the nuclei are independent of the degrees of freedom of the electrons, so the electronic degrees of freedom are not considered. The second consists in assuming that atomic displacements are negligible in comparison with interatomic distances. Thus $3Nm$ displacement variables are obtained with their coupled differential equations, as the arrangement is three-dimensional. After that, a change of variables is performed, which is analogous to what was done for masses on springs (see equation 3). A series of phononic variables q_{kj} representing harmonic oscillators is obtained. From the Lagrangian of the system, a series of decoupled equations of motion are derived:

$$\ddot{q}_{kj} = -\omega_{kj}^2 q_{kj} \tag{8}$$

Franklin y Knox highlight at this point that:

> "the description thus far has been entirely classical, and has given us no reason to think of phonons as resembling particles. For this we need quantum mechanics, specifically, we'd like to perform second quantization on the phonon

mode variables q_{kj} and their associated momenta p_{kj}" (Franklin and Knox 2018, p. 4).

Although not explicitly stated, the mention of the classical nature of the description up to this point seems to indicate that the authors believe that there is a theoretical leap between the description of the model of vibrating atoms and the description of the model of phonons, the former being allegedly classical while the latter is quantum. It is worth noting that, in equations (8), the authors obtained the normal modes variables usually called phonons, but according to them they still do not resemble particles. To obtain particle-like phonons, they reframe the description within quantum mechanics. Specifically, they perform second quantization using creation and annihilation operators to make phonons look like particles. Though reasonable, we think that this theoretical leap is not necessary. The only thing that is needed is the change of variables. A thorough assessment of this point will be the subject of the next section.

We now review their arguments about the novelty and robustness of phononic behavior, which, together with the existence of a theoretical leap 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, to perform 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.

2. 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 are emergent. The point of contention is whether or not there is a theoretical leap or at least a kind of asymmetry between the description of the model of phonons and the description of the model of vibrating atoms. We first discuss the alleged theoretical leap 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 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. But, as we are going to show in this section, it is possible to perform the change of variables after moving to a quantum description of the model of vibrating atoms.

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:

$$F_s = C\left(u_{s+1} - u_s\right) - C\left(u_s - u_{s-1}\right) \tag{9}$$

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:

$$\frac{m}{C}\frac{\partial^2 u_s}{\partial t^2} = u_{s+1} + u_{s-1} - 2u_s \tag{10}$$

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 (10) 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:

$$\hat{H} = \sum_s \frac{1}{2m}\hat{p}_s^2 + \frac{C}{2}\left(\hat{q}_{s+1} - \hat{q}_s\right)^2 \tag{11}$$

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 necessary to perform the change to phonon coordinates. The phonon variables are:

$$\hat{Q}_{k_j} = N^{\frac{-1}{2}}\sum_{s-1}^{S}\hat{q}_s e^{-ik_j sa} \tag{12}$$

$$\hat{P}_{k_j} = N^{\frac{-1}{2}}\sum_{s-1}^{S}\hat{p}_s e^{ik_j sa} \tag{13}$$

where $k_j = 2\pi j N^{-1} a^{-1}$, $j = 0, \pm 1, ..., \dfrac{S}{2}$ and a is the equilibrium distance between atoms. Then we obtain an equivalent expression for the Hamiltonian (11), which is

$$\hat{H} = \sum_j \frac{1}{2}\left(\hat{P}_j^2 + \omega_j^2 \hat{Q}_j^2\right) \tag{14}$$

where $\omega_j = (2C/m)^{\frac{1}{2}}\left(1 - \cos(k_j a)\right)^{\frac{1}{2}}$ is the angular frequency of the oscillator j. By means of this change of variables, it is obtained a different model 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 an interesting consequence of using quantum mechanics to describe the crystalline solid once the change to phonon variables has been performed but second quantization has not been carried out. 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 $n_j = 0, 1, 2, ...$. 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 quanta 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 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

$$E = \sum_j \varepsilon_j = \sum_j \hbar\omega_j\left(n_j + \frac{1}{2}\right) = \sum_j \hbar\omega_j n_j + \varepsilon_{vacuum} \tag{15}$$

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 this view, oscillations are represented as particles. If the oscillation is larger, then there are more particles. This is the core of the phonons description, and this is the movement that precisely allow 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. This shows that though quantum mechanics is necessary to obtain particle-like phonons, creation and annihilation operators are not.

Actually, the phonon model does not only play the role of simplifying the calculations, but it is also a fundamental element to model and offer explanations about physical phenomena in crystalline solids. It was stressed above that the model of phonons has an explanatory power that the model of vibrating atoms lacks. Let us exemplify this statement. It is the case that the model of phonons allows the deduction of the heat equation. According to the model of phonons, the temperature in a crystalline solid depends on the phonon density, that is, if there is higher density, there is higher temperature. If, for example, we have a metal bar that heats up at one end and cools down at the other, then there is a net flow of heat from one end to the other, producing a temperature gradient. Applying the model of phonons to this example, we have that there is a flow of phonons that can collide with each other. Applying the kinetic theory to colliding phonons, the net flow of energy is obtained

$$j_U = -\frac{1}{3} Cvl \frac{dT}{dx} \qquad (16)$$

where x is the bar longitude, C is volumetric heat capacity, v is the phonons mean velocity and l is the mean free path between collisions (see Ashcroft and Mermin 1976 for details). Thus, the model of phonons provides us with a clear physical interpretation of the constants in the heat equation. For example, using the model of phonons, it is obtained that there is a direct proportionality between the phonons velocity and the heat propagation.

Let us stress that the description of the model of vibrating atoms in equation (11) and the description of the model of phonons in equation (14) are both in the same theoretical level: quantum mechanics. In our account, there is not a theoretical leap 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 there are necessarily 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 (10) in phonon variables, decoupled equations of classical oscillators are obtained, and this description is known as classical phonons (Dagotto 2013). This change of variables appears in Franklin and Knox article (see equations 8). In sum, from our perspective, the key that allow us to adopt the model of phonons is the change of variables, not quantization itself.

It should be clear now that the adoption of the model of phonons to represent crystalline solids does not depend on a theoretical leap from classical mechanics to quantum mechanics. On the one hand, it is perfectly possible to describe both the model of vibrating atoms and of phonons by means of quantum mechanics. On the other hand, 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 necessarily an inter-theoretical leap between the descriptions of the two models. 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 emergence could not be built even if the assumed notion of emergence rejects reduction, since it is not the case that the inter-theoretical relation is not one of reduction, but that there is not an inter-theoretical relation at all.

As we mentioned in Section 1, 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, that is, a theoretical leap, 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 themselves acknowledge, considering than 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.

If our previous argument against the inter-theoretical emergence of phonons is accepted, it still would not rule out any kind of emergence. Franklin and Knox thesis could be reformulated if they construed their emergence relation as one of intra-domain emergence. The distinction between inter-domain emergence and intra-domain emergence has been put forward by Lombardi and Ferreira Ruiz (2018). Inter-domain emergence is a relation that holds between ontic items belonging to different ontic domains represented by correspondingly different theoretical domains. In turn, 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. Intra-domain emergence does not require a theoretical leap as inter-domain emergence does, but it at least require some kind of asymmetric relation between the descriptions of the two different type of ontic items. Cases of intra-domain emergence has been successfully stablished 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 y Matta 2022).

It could be the case that 'being a phonon' and 'being a vibrating atom' would be just two different type-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 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 (even against their own emergentist thesis) 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 symptomatic:

> "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).

It is surprising that they claim that some kind of asymmetric relation is required for emergence and yet they insist on putting forward the case of phonons as one of emergence. Even by their own lights, it is possible to talk about novelty but not about emergence. 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 asymmetry between descriptions: the phonon variables are just linear combinations of the displacement variables and vice versa, as the authors 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, the asymmetric relation between phonons and atoms required by emergence cannot be established in this circumstance either. As a consequence, 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. This is even clearer if we take the TPS approach.

3. Phonons and atoms from the TPS approach

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 $\mathcal{H}_U = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \otimes \mathcal{H}_4$. 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 other 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 and the other is a set of two particles of type B. 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.

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 11) to the quantum description of the model of phonons (see the Hamiltonian in equation 14), 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 $\mathcal{H}_T$:

$$\mathcal{H}_T = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes ... \otimes \mathcal{H}_N = \overset{N}{\underset{j=1}{\otimes}} \mathcal{H}_j \tag{17}$$

Equation (17) 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:

$$\hat{p}_1 = \hat{p}(x_1) \otimes \hat{I}(x_2) \otimes ... \otimes \hat{I}(x_N) \tag{18}$$

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:

$$\hat{o}_1 = \hat{o}(x_1) \otimes \hat{I}(x_2) \otimes ... \otimes \hat{I}(x_N) \tag{19}$$

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:

$$\hat{h}_{1y2} = \hat{h}(x_1) \otimes \hat{I}(x_2) \otimes ... \otimes \hat{I}(x_N) + \hat{I}(x_1) \otimes \hat{h}(x_2) \otimes ... \otimes \hat{I}(x_N) \tag{20}$$

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

$$\hat{H} = \sum_{j=1}^{N} \frac{1}{2m} \hat{p}_j^2 + \frac{C}{2}\left(\hat{q}_{j+1} - \hat{q}_j\right)^2 \tag{21}$$

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

$$\hat{Q}_{k_j} = N^{\frac{-1}{2}} \sum_{s-1}^{S} \hat{q}_s e^{-ik_j sa} \tag{22}$$

$$\hat{P}_{k_j} = N^{\frac{-1}{2}} \sum_{s-1}^{S} \hat{p}_s e^{ik_j sa} \tag{23}$$

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

$$\left[\hat{P}_k, \hat{Q}_k\right] = i\hbar\delta_{k,k'} \tag{24}$$

$$\left[\hat{P}_k, \hat{P}_{k'}\right] = \left[\hat{Q}_k, \hat{Q}_{k'}\right] = 0 \tag{25}$$

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

$$\hat{H} = \sum_k \frac{1}{2}\left(\hat{P}_k^2 + \omega_k^2 \hat{Q}_k^2\right) \tag{26}$$

Then new quantum systems with coordinates $\tilde{x}_k$ (22) and (23) 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

$$\bigotimes_k \tilde{\mathcal{H}}_k = \tilde{\mathcal{H}}_{-\frac{N}{2}} \otimes \tilde{\mathcal{H}}_{-\frac{N}{2}+1} \otimes ... \otimes \tilde{\mathcal{H}}_{\frac{N}{2}} = \mathcal{H}_T \tag{27}$$

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 obtained shows that the system can be represented with a Hamiltonian that expresses the sum of many independent harmonic oscillators (26). That is to say,

$$\hat{H} = \sum_k \hat{H}_k \tag{28}$$

where

$$\hat{H}_k = \hat{I}(\tilde{x}_1) \otimes ... \otimes \hat{I}(\tilde{x}_{k-1}) \otimes \hat{\tilde{h}}(\tilde{x}_k) \otimes \hat{I}(\tilde{x}_{k+1}) \otimes ... \otimes \hat{I}(\tilde{x}_N) \tag{29}$$

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

$$\varepsilon_{n_k} = \hbar\omega_k\left(n_k + \frac{1}{2}\right) \tag{30}$$

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

$$\hat{\tilde{h}}(\tilde{x}_k)\left|\varepsilon_{n_k}^{(k)}\right\rangle = \varepsilon_{n_k}\left|\varepsilon_{n_k}^{(k)}\right\rangle \tag{31}$$

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 $\hat{n}_k(\tilde{x}_k)$

$$\hat{n}_k(\tilde{x}_k)\left|\varepsilon_{n_k}^{(k)}\right\rangle = n_k\left|\varepsilon_{n_k}^{(k)}\right\rangle \tag{32}$$

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

$$|E\rangle = |N\rangle = \left|n_{-\frac{N}{2}}\right\rangle \otimes \left|n_{-\frac{N}{2}+1}\right\rangle \otimes ... \otimes \left|n_{\frac{N}{2}}\right\rangle = \underset{k}{\otimes}|n_k\rangle \tag{33}$$

In this step, the TPS was not changed, just another label was used for these states. Now, it is possible to go to the creation and annihilation formalism to have a description more similar to that of field theory, but it is not necessary, the phonons are already there.

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$_V$) or 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. 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 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 emergentism, a kind of asymmetry would necessarily 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.

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 there is not necessarily a theoretical leap or 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, as Franklin and Knox intend to do. We have also shown that it is not only the case that there is not an inter-theoretical relation but there is not any kind of asymmetric relation between descriptions that would have allowed 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 of the crystalline solid. 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.

We conclude that 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 are on ontological parity with vibrating atoms. 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 ontology of properties for quantum mechanics (Lombardi y Castagnino 2008, da Costa, Lombardi y Lastiri 2013, da Costa y Lombardi 2014). But this is the subject of future work.

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