About the concept of electron localization

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Abstract

This article examines the phenomenon of electron localization from a conceptual perspective, without going into technical details. In particular, it analyzes two cases in which electrons are confined to a specific region near one or more atoms, but with different characteristics: electron localization in molecules and in crystalline solids. The features and requirements for localization in each case are discussed, along with their specific interpretative challenges and the various proposals put forward to address them.

Keywords

Pair localization; Anderson localization; Electron density; Emergence.

1.- Introduction

Electron localization, as studied in quantum chemistry, is a phenomenon consisting in the confinement of electrons to a specific region close to an atom or between atoms: electrons are localized in a certain region instead of moving freely throughout space. Although electron localization is manifested in different ways, here we will focus on two cases: molecules and crystalline solids.

The aim of the present article is not to delve into technical matters, but to consider the phenomenon of electron localization from a conceptual point of view. With this purpose, the work is organized in two main parts: Section 2 devoted to molecules and Section 3 devoted to solids. Section 2 will take into account the leading role played by the electron density in the study of electron localization; the aim will be to point out the different interpretations of the concept of electron density, which lead to different ways of conceiving electron localization. In Section 3, the phenomenon of Anderson localization will be considered in order to show that, besides the just mentioned divergences about how electron localization is understood, it involves an additional conceptual issue related to the appeal to limiting procedures. Finally, the paper closes with some concluding remarks.

2.- Electron localization in molecules

In the study of molecular structure, electron localization refers to the concentration of electron density in certain regions of the molecular space. The analysis of the geometrical properties of the electron density (e.g., local maxima, local minima, saddle points) accounts for the chemical features of the molecule. Under certain circumstances, regions of high electron density can be associated with the formation of electron pairs in specific regions of space, thereby providing a quantum description of covalent bonds and lone electron pairs.

Given this relationship between electron localization and electron density, if the concept of electron density is understood, the understanding of the concept of electron localization does not pose any difficulties. The problem is that the interpretation of the concept of electron density is not clear at all.

2.1.- Two interpretations of the concept of electron density

A it is well known, the *electron density* $\rho(\boldsymbol{r})$ of a system of N electrons is computed in terms of the wave function $\psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N,\boldsymbol{s}_1,\boldsymbol{s}_2,\ldots,\boldsymbol{s}_N)$, as the sum of the contributions of each electron, obtained by integrating over the coordinates of the other electrons. Although the mathematical calculation of $\rho(\boldsymbol{r})$ does not pose any difficulty, the definition of the electron density involves passing from an abstract function $\psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N,\boldsymbol{s}_1,\boldsymbol{s}_2,\ldots,\boldsymbol{s}_N)$ on the configuration space of $3N$ spatial dimensions and $2N$ spin dimensions, to a real-valued scalar function $\rho(\boldsymbol{r})$ on a space of three dimensions that, therefore, can be thought as representing the physical space. Although electron density has been deeply studied at the conceptual and mathematical level [1], there is no agreement on the conceptual meaning of the magnitude thus obtained. In particular, two clearly different interpretations can be distinguished:

- According to the *Schrödinger-style charge density interpretation* (*CDI*), the electron density is a density of charge distributed over the entire three-dimensional physical space. In this case the electron density is a physical field, in particular, a *material field* of negative charge. The CDI was the first interpretation to appear: it was formulated by Schrödinger [2] [3], who defined the electron density as a continuous distribution of electricity in the physical space. When it became clear that the wave function could not be conceived of as a physical field in three-dimensional space, Schrödinger's interpretation of the electron density was also rejected in the context of physics. Nevertheless, it was explicitly retrieved in quantum chemistry, in the framework of the Quantum Theory of Atoms in Molecules (QTAIM): for Richard Bader, the electron density acquires materiality since describes the kind of stuff of which atoms and molecules are made (see, e.g., [4]).
- According to the *Born-style probability density interpretation* (*PDI*), the electron density is a probability density. It represents the probability of detecting an electron at a particular point in space. Specifically, $\rho(\boldsymbol{r})$ expresses the probability density of locating an electron

within an infinitesimally small region surrounding a given position $\boldsymbol{r}$. Depending on whether this is interpreted from a realist or instrumentalist point of view, it can mean different things. From a realist point of view, the function $\rho(\boldsymbol{r})$ reflects the chance that the electron actually occupies the position $\boldsymbol{r}$. From an instrumentalist viewpoint, it instead indicates the probability that a measurement would reveal the electron at that position $\boldsymbol{r}$. In both interpretations, the electron density is conceived as a mathematical field describing probabilistic information. This view is the prevailing one in physics, in line with Born's probabilistic formulation of quantum mechanics [5].

From a physical viewpoint, the CDI embodies some serious difficulties:

- On the one hand, during measurement, the original distributed charge density must instantaneously, or almost instantaneously, "collapse" to become a charge density represented by a Dirac delta distribution centered at the electron position. This picture leads to two undesirable consequences: (i) collapse should produce highly strong currents, which have never been detected, and (ii) the local conservation of charge is violated during collapse, since charge suddenly disappears from one location to appear at another.
- On the other hand, given two wave functions of a system of many electrons, their corresponding electron densities can be computed. According to quantum mechanics, if the system is in a superposition of those two wave functions, there should exist two different charge densities spread throughout the same three-dimensional physical space (for a detailed criticism, see [6]). In other words, the superposition of wave functions would lead to "superposition" of charge densities, an idea that makes no physical sense.

The PDI, although widely adopted in physics, is not a friendly interpretation in the context of quantum chemistry, in which electron density is endowed with some kind of materiality related to the charge of electrons. It is not clear how a purely mathematical field, dealing with probabilities, can play the key role that electron density plays in quantum chemistry in physically accounting for the central concepts of chemistry.

This dual interpretation of the concept of electron density is immediately reflected in the understanding of electron localization: as the concentration of charge from the CDI perspective, or as the concentration of probability from the PDI perspective.

2.2.- Compatibility through averages

It is important to highlight that these two interpretations generate a conceptual tension when considered together: the CDI and the PDI are, in principle, mutually incompatible, since a given magnitude cannot simultaneously be both a mathematical object and a physical entity. Under the CDI, electron density is understood as a material "cloud" spread across physical space, whereas under the PDI, it is interpreted as an abstract probability. For instance, if the electron density at a specific point in space is 0.9 (in units of electron charge), the PDI would interpret this as a probability of 0.9 that an electron will be detected at that point during a measurement—meaning the electron may or may not be found there. In contrast, the CDI would imply that a certain amount of charge exists at that location independently of whether a measurement is carried out or what its outcome might be.

Despite this conceptual incompatibility, the two interpretations of the concept of electron density usually appear in the literature without distinguishing them. Furthermore, in several cases, the compatibility between the CDI and the PDI is presupposed on the basis of some kind of average strategy.

Sometimes, the electron density is conceived in terms of a *space-average*. It is defined as a measure of the number of electrons per unit spatial volume: the physical space is divided into small cells and each cell is assigned a charge value proportional to the number of electrons it contains. Although this view is more akin to the CDI perspective, the link between charge density and probability is based on assuming that the probability of finding an electron in a given cell is proportional to the number of electrons in that cell. The idea of a "cloud" of electrons can be associated to the CDI only if the number of electrons tends to infinity. Thus, the space-average strategy may approximately work for systems of a high number of electrons; but for systems with few electrons, it is a very difficult strategy to adopt. For this reason, arguments in terms of time-average are more common in the literature.

According to the *time-average* strategy, the electron density represents the mean value of the definite positions of the electron in its motion around the nucleus. This idea had already appeared in Linus Pauling's famous book originally published in 1939: "*We can accordingly describe the normal hydrogen atom by saying that the electron moves in and out about the nucleus, remaining usually within a distance of about 0.5 Å, with a speed that is variable but is of the order of magnitude of* v_0*. Over a period of time long enough to permit many cycles of motion of the electron the atom can be described as consisting of the nucleus surrounded by a spherically symmetrical ball of negative electricity (the electron blurred by a time exposure of its rapid motion).*" [7]. The same strategy is adopted in much more recent works. For instance, in a paper published in a journal of chemical education, the following image is used: "*if a series of measurements could be made of x without disturbing the motion of the particle, the resulting distribution would be* ρ*. The latter would then reflect the motion of the particle in the same way in which the density of the image on a long-exposure photograph reflects the motion of a macroscopic object.*" [8]. The same picture appears in a more recent textbook: "*The rapid motion of electrons causes the sluggish nuclei to 'see' the electrons as a charge cloud rather than as discrete particles*." [9].

Let us consider, for example, a hydrogen atom. The idea of the time-average strategy is that the electron moves very fast around the nucleus so that, in average, it forms a cloud of negative charge surrounding the nucleus. If the physical space is divided into small cells, it is theoretically possible to compute the time the electron spends in each cell. Assuming that the time the electron spends in each cell is proportional to the cell's volume, this volume turns out to be proportional to the probability of finding the electron in that cell. This concept first emerged at the end of the 19th century, when Boltzmann used the motion of particles to explain the appearance of probability in classical statistical mechanics. A key assumption in his theory was the so-called "ergodic hypothesis," which posits that the orbit of the system's representative point in the phase space of microstates eventually passes through all points on the constant energy surface. This principle ensures that the time the system spends in a given region of phase space is proportional to the volume of that region, which, in turn, correlates with the probability of the system being in a microstate within that region.

The average strategies implicitly assume that electrons are particles—similar to the classical particles envisioned by Boltzmann—meaning small objects that occupy specific positions in space. Specifically, the time-average strategy relies on the assumption that electrons follow definite trajectories around the nucleus. In other words, electrons are viewed as individual entities with specific positions and velocities, with the key difference from classical particles being that their behavior is not determined by classical equations of motion, but by an equation that defines their position in a statistical manner. The problem with this view is that it is conflict with the conceptual structure of standard quantum mechanics in the following senses:

- It contradicts the Heisenberg principle, which states that quantum systems cannot have both a definite position and a definite momentum at the same time, and therefore, do not follow definite trajectories in the same way as classical objects.
- The Kochen-Specker theorem [10] establishes that it is impossible to simultaneously assign precise values to all observables of a quantum system while maintaining the functional relationships between commuting observables. This leads to the conclusion that quantum mechanics, as commonly understood, is inherently contextual: definite values can only be consistently assigned to observables within a specific context, which is defined by the observables that share the same eigenbasis [11]. The theorem shows that the fact that some properties of a quantum system cannot be assigned definite values is not a limitation of our knowledge, but rather an ontological feature that arises from the theory's formal structure.
- The quantum realm exhibits striking non-local correlations between the properties of distant, non-interacting systems, as illustrated by the well-known Einstein-Podolsky-Rosen paradox [12]. These EPR correlations connect systems that are too far apart for any light signal to travel between them, yet they still do not permit the transmission of information faster than the speed of light. As a result, quantum non-locality is often interpreted in terms of holism—that is, the idea that certain physical systems behave as unified wholes that cannot be fully understood by analyzing their parts in isolation [13].

- Elementary “particles” are fundamentally indistinguishable from one another—that is, they cannot be individually labeled or distinguished, nor can they be straightforwardly counted when they form collections [14]. This indistinguishability is reflected in the fact that they do not obey Maxwell-Boltzmann statistics; instead, they are described collectively by Bose-Einstein statistics in the case of bosons, or Fermi-Dirac statistics in the case of fermions.

All these characteristics converge on the same conclusion: quantum systems cannot be considered particles in any meaningful sense of the word. Elementary quantum systems do not qualify as individuals in the traditional sense of the term [15]. Indeed, they lack both synchronic and diachronic individuality: they are not identifiable by their location in space and time, nor can they be tracked over time through a continuous trajectory. Furthermore, because they are indistinguishable from one another, they cannot be counted or reidentified when they appear in groups, as is the case with individual objects. Their properties are contextual and inherently indefinite.

The essentially quantum traits that standard quantum mechanics ascribes to quantum systems constitute an obstacle to the time-average strategy. The idea that the electron density represents a kind of mean value of the definite positions occupied by the electron in its motion around the nucleus requires conceiving electrons as particles with individuality and defined trajectories, an ontological picture that is challenged by the standard quantum theory.

The obstacles that the time-average strategy must face can be surmounted by a change of theoretical perspective [16]. In fact, according to Bohmian Mechanics [17] [18], quantum systems are particles of the same nature as classical ones: they always have definite positions and velocities and, therefore, also definite trajectories. From the Bohmian perspective, then, probabilities are not objective, but only express the ignorance of the observer about the definite positions of the particles. Perhaps the fact that this ontological picture is more akin to the quantum chemistry views partially explains a certain revival of the interest in Bohmian Mechanics for the description of atoms and molecules since the 1980s.

2.3.- How to interpret the concept of electron pair density?

Since electron pairing plays a crucial role in chemistry, the concept of *electron pair density* has been introduced to account for the phenomenon of Lewis-pairing. Analogously to the case of electron density $\rho(\boldsymbol{r})$, the concentration of electron pair density $\rho(\boldsymbol{r}_1, \boldsymbol{r}_2)$ in specific regions of molecular space provides valuable information about chemical bonding: it is through electron pair density that the Lewis model of electronic structure finds its physical expression [19]. It is worth noting that localization indicators such as the Electron Localization Function (ELF), Laplacian maps, and Electron Localization-Delocalization Matrices (LDMs) have found extensive use in recent computational studies. However, again, the question is how to interpret this central concept. In particular, the issue consists in relating the interpretations of $\rho(\boldsymbol{r})$ and $\rho(\boldsymbol{r}_1, \boldsymbol{r}_2)$.

The Schrödinger-style charge density interpretation for the electron density cannot be easily extrapolated to the electron pair density. In fact, $\rho(\boldsymbol{r})$ admits to be conceived as a material field of negative charge distributed over the three-dimensional physical space because it is a function of the three spatial coordinates. On the contrary, $\rho(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is a function of six variables, so cannot be understood as representing a physical field on the spatial dimensions. As a consequence, who adopts a Schrödinger-style interpretation of the electron density is forced to endow the concept of electron pair density with a merely operational meaning in terms of probabilities.

If the Born-style probability density interpretation is conferred to the electron density, it is natural to conceive the electron par density $\rho(\boldsymbol{r}_1, \boldsymbol{r}_2)$ as representing the probability of finding one electron in an infinitesimal volume centered at $\boldsymbol{r}_1$ while another electron is in an infinitesimal volume centered at $\boldsymbol{r}_2$. However, if this probabilistic view is combined with the assumption that electrons are particles, the Born-style interpretation of the electron pair density faces the same difficulties as in the case of the electron density: the concept of particle finds no comfortable place in standard quantum mechanics. The same happens if $\rho(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is interpreted in terms of conditional probabilities as in some papers [20]. If we consider that $\rho(\boldsymbol{r}_1, \boldsymbol{r}_2)$ represents the probability of finding an electron in $\boldsymbol{r}_2$ given that there is another one in $\boldsymbol{r}_1$ it is necessary to adopt the concept of a particle with well-defined position. Therefore, the appeal to the concept of electron pair density to account for electron pairing seems to count as an additional argument in favor of the particle ontological picture offered by Bohmian Mechanics: in the Bohmian context, any probabilistic claim acquires a merely epistemic meaning in terms of the ignorance of the precise position and momentum of the electrons.

Various studies associated with the development of QTAIM have shown that certain chemically relevant properties of the pair density can be explained in terms of the geometric features of the electron density (see, e.g., [20] [21] [22]). In particular, the Laplacian of the electron density $\bar{\nabla}^2\rho(\boldsymbol{r})$, central to QTAIM theory, indicates regions where the density $\rho(\boldsymbol{r})$ is locally concentrated, $\bar{\nabla}^2\rho(\boldsymbol{r}) < 1$, or locally depleted, $\bar{\nabla}^2\rho(\boldsymbol{r}) > 1$. This quantity has been linked to the probability of electron pair formation. Studies such as those by Bader and Heard [20] have demonstrated that the kinetic energy density—derived from the Laplacian—can be interpreted as an indicator of electron localization and pair condensation. This perspective establishes a bridge between chemical topology and the quantum ontological framework underlying electron pairing. From this perspective, the density of pairs does not add any additional difficulty, but problems related to the interpretation of electron density $\rho(\boldsymbol{r})$ remain.

3.- Electron localization in crystalline solids

Electron localization in crystalline solids manifests certain peculiarities that are not present in the case of molecules. Philip Anderson [23] was the first to point out the absence of diffusion of waves in a disordered medium. As well-known, the so-called "*Anderson localization*" is the electron localization in a lattice whose degree of randomness (disorder), due to impurities or defects, is sufficiently large, above a certain critical value. A manifestation of the Anderson localization is the phenomenon of *metal-insulator transition*, which consists in the transition from a metal (a material with good electrical conductivity) to an insulator (a material that is a poor conductor).

Unlike the case of molecules, electron localization in crystalline solids cannot be explained merely by studying the properties of the electron density. On the contrary, in this case localization is the result of the interaction of the electrons with the lattice. Therefore, in addition to the difficulties resulting from the different interpretations of the concept of electron density, here there are certain issues that depend precisely on the properties of the lattice.

3.1.- Limiting procedure and idealization

Since Anderson localization arises as the result of the interaction between the electrons and the "random" lattice, it depends on the features of the lattice: its degree of disorder and its dimension. In a one-dimensional or two-dimensional lattice, it can be proved that the resistivity grows exponentially with the number N of sites in the lattice: the solid becomes a perfect insulator in the limit $N\to\infty$. In other words, the metal-insulator transition is a phase transition that arises in the thermodynamic limit. However, since infinite systems do not exist, this theoretical procedure is an approximation or an idealization. But, which of the two?

Although acknowledging that, in science, the terms 'approximation' and 'idealization' are commonly used without a clear distinction and even interchangeably, John Norton [24] proposes the following distinction:

- An *approximation* is an inexact description of a target system.
- An *idealization* is a real or fictitious system, distinct from the target system, some of whose properties provide an inexact description of some aspects of the target system.

For example, if a property of a target system is represented by a power series, an approximation consists in retaining only the first term of the series as an approximated description of the target system's property, whereas an idealization is the strategy of replacing the target system with an ideal system whose property is exactly described by the first term of the series. The distinction between the two strategies is relevant when limits are involved, because limits can be badly behaved. For example, the ratio between of the area to the volume of a sphere is $3/r$, and goes to zero as the radius r goes to infinity; however, zero area-to-volume ratio is not a property of a limit system because a “sphere” of infinite radius is not a sphere at all. Therefore, not always an approximation can be promoted to an idealization.

Since statistical mechanics describes systems with a huge number of components, the operation of letting this number go to infinity is pervasive in the field. In fact, calculations with very large but finite number of components do not give the expected results: “*The physical systems to which the thermodynamic formalism applies are idealized to be actually infinite* […] *This idealization is necessary because only infinite systems exhibit sharp phase transitions. Much of the thermodynamic formalism is concerned with the study of states of infinite systems*.” [25]. “*The existence of a phase transition requires an infinite system. No phase transitions occur in systems with a finite number of degrees of freedom*.” [26]. The replacement of the target system by a system with an infinite number of components is an idealization. What makes the idealization admissible is the assumption that the ideal infinite system provides a sufficiently good description of the large but finite target system. It is important to stress that such admissibility arises from comparing the calculations on the ideal infinite system with the measurements on the real finite target system, because calculations on a finite model do not yield to the expected results, especially regarding phase transitions.

The above quotes, referred to the thermodynamic behavior of statistical systems, perfectly apply to the case of Anderson localization. In fact, the metal-insulator transition is a phase transition which, although observed in finite real systems, can only be accounted for in idealized systems with infinite lattices. Therefore, independently of how the electron density is interpreted, in this case it is necessary to recognize the conceptual oddity that consists in obtaining results in idealized systems that are substantially different from real systems. However, some think that the role played by infinite limits in idealization is a mark of the objective emergence of new behavior.

3.2.- Emergence of new behavior

The idea of emergence came-up in the late-nineteenth and early-twentieth centuries with British emergentism, as an antireductionist stance [27]. However, the rest of twentieth century, under the strong influence of positivism, was marked by reductionism. It was only during the last decades of the century that the notion of emergence has “reemerged” [28].

At present, after many years of discussion, there are almost as many conceptions of emergence as authors who address the issue. Nevertheless, there is a certain consensus about the fact that the general notion of emergence conjoins two apparently opposed features: *dependence* and *autonomy*. It mediates between extreme forms of dualism, which reject the dependence over the micro-level, and reductionism, which rejects the autonomy of the macro-level [29]. Moreover, in relation to the lower level domain from which they arise, emergents are usually characterized as novel, unpredictable, unexplainable and/or irreducible on the basis of said lower level domain. As Anderson himself claims in his famous paper “More is different,” the word ‘emergence’ expresses the idea that the whole is not merely greater than but essentially different from the sum of the parts [30].

A point that has been repeatedly emphasized is the association of emergence with the presence of a singular limit relation between the basal and the upper-level description [31] [32] [33]. The limit of a function is singular when the value of the function at the limit is different than its value as the parameter approaches the limit. When the function describes the behavior of a system, the singular limit implies that the system’s behavior in the limit is qualitatively different from its behavior for finite values of the parameter. In Anderson’s terms: “*The essential idea is that, in the so-called N→∞ limit of large systems (on our own, macroscopic scale), it is not only convenient but essential to realize that matter will undergo mathematically sharp, singular “phase transitions” to states in which the microscopic symmetries, and even the microscopic equations of motion, are in a sense violated.*” [30].

It is not surprising that Anderson, reflecting on his scientific work, recognized the importance of singular limits in the description of phase transitions and emergent behaviors. In fact, the phenomenon of localization that he discovered leads to the metal-insulator phase transition, in which the insulator behavior of the system emerges when the size of the lattice goes to infinity. From this perspective, the idealization involving infinite lattices is not a conceptual problem, but rather is precisely the mark of the novel behavior. It is in this sense that “more is different”: “*The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear.*” [30].

4.- Concluding remarks

As anticipated in the Introduction, the perspective of the present article was essentially epistemological: the purpose was to point out the issues involved in the phenomenon of electron localization when considered from a conceptual viewpoint.

On the one hand, the understanding of electron localization in molecules, central to account for many chemical facts, depends on the way in which the concept of electron density is interpreted. However, the interpretation of such a concept is not univocal, and the different interpretative perspectives have their peculiar difficulties.

On the other hand, electron localization in crystalline solids, which is a collective phenomenon, leads to a phase transition that arises in the limit of infinite lattices. For this reason, such a transition can be conceived in terms of the emergence of novel and irreducible properties. The conceptual difficulty lies, in this case, in justifying the predictive success of a model of infinite size, when real systems are always finite.

Although this work does not does not offer technical results, we hope that it will contribute to the way in which quantum chemists understand their own theoretical practices, under the assumption that conceptual clarification is an important resource for scientific development.

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References

[2] Schrödinger, E. (1926a). "Quatisierung als Eigenwertproblem (Vierte mitteilung)". *Annalen der Physik*, **81**: 437-490. English translation in E. Schrödinger, *Collected Papers on Wave Mechanics*, 1928. London and Glasgow: Blackie & Son Limited.

[3] Schrödinger, E. (1926b). "An undulatory theory of the mechanics of atoms and molecules". *Physical Review*, **28**: 1049-1070.

[4] Bader, R. F. W. and Matta, C. F. (2013). "Atoms in molecules as non-overlapping, bounded, space-filling open quantum systems". *Foundations of Chemistry*, **15**: 253-276.

[5] Born, M. (1926). "Zur Quantenmechanik der Stoßvorgänge." *Zeitschrift für Physik*. **37**: 863-867.

[6] Allori, V., Goldstein, S., Tumulka, R., and Zanghì, N. (2011). "Many worlds and Schrödinger's first quantum theory". *The British Journal for the Philosophy of Science*, **62**: 1-27.

[7] Pauling, L. (1960). *The Nature of the Chemical Bond*. Ithaca: Cornell University Press (first edition 1939).

[8] Nelson, P. (1990). "How do electrons get across nodes?". *Journal of Chemical Education*, **67**: 643-647.

[9] Levine, I. N. (2014). *Quantum Chemistry*. Boston: Pearson, 7th edition.

[10] Kochen, S. and Specker, E. (1967). "The problem of hidden variables in quantum mechanics." *Journal of Mathematics and Mechanics*, **17**: 59-87.

[11] Martínez González, J. C., Fortin, S., and Lombardi, O. (2019). "Why molecular structure cannot be strictly reduced to quantum mechanics". *Foundations of Chemistry*, **21**: 31-45.

[12] Einstein, A., B. Podolsky, and N. Rosen (1935). “Can quantum-mechanical description of physical reality be considered complete?” *Physical Review*, **47**: 777-780.

[13] Healey, R. and Gomes, H. (2022). “Holism and nonseparability in physics”. In E. N. Zalta and U. Nodelman (eds.), *The Stanford Encyclopedia of Philosophy* (Winter 2022 Edition), URL = https://plato.stanford.edu/archives/win2022/entries/physics-holism/.

[14] French, S. (2019). “Identity and individuality in quantum theory”. In E. N. Zalta (ed.), *The Stanford Encyclopedia of Philosophy* (Winter 2019 Edition), URL = https://plato.stanford.edu/archives/win2019/entries/qt-idind/.

[15] Lombardi, O. (2023). “Not individuals, nor even objects: On the ontological nature of quantum systems”. Pp. 45-77 in J. R. B. Arenhart and R. W. Arroyo (eds.), *Non-Reflexive Logics, Non-Individuals, and the Philosophy of Quantum Mechanics*. Cham: Springer, Synthese Library.

[16] Fortin, S. and Lombardi, O. (2024). “What is the electron density?” *Foundations of Chemistry*, **26**: 371-383.

[17] Bohm, D. (1952). “A suggested interpretation of the quantum theory in terms of ‘hidden’ variables”. *Physical Review*, **85**: 166-179, 180-193.

[18] Dürr, D., Goldstein, S., and Zanghì, N. (2013). *Quantum Physics without Quantum Philosophy*. Berlin: Springer.

[19] Matta, C. F., Ayers, P. W., and Cook, R. (2024). *Electron Localization-Delocalization Matrices, Lecture Notes in Chemistry*. Cham: Springer Nature.

[20] Bader, R. W. F. and Heard, G. L. (1999). “The mapping of the conditional pair density onto the electron density”. *Journal of Chemical Physics*, **111**, 8789-8797.

[21] Gillespie, R. J., Bayles, D., Platts, J., Heard, G. L. and Bader, R. F. W. (1998). “The Lennard-Jones function: a quantitative description of the spatial pairing of electrons as determined by the exclusion principle”. *Journal of Chemical Physics A*, **102**, 3407-3414.

[22] Matta, C. F., Hernández-Trujillo, J. and Bader, R. F. W. (2002). “Proton spin-spin coupling and electron delocalization”. *Journal of Chemical Physics A*, **106**, 7369-7375

[23] Anderson, P. W. (1958). “Absence of diffusion in certain random lattices.” *Physical Review*, **109**: 1492-1505.

[24] Norton, J. (2012). “Approximation and idealization: Why the difference matters.” *Philosophy of Science*, **79**: 207-232.

[25] Ruelle, D. (2004). *Thermodynamic Formalism.* 2nd Edition. Cambridge: Cambridge University Press.

[26] Kadanoff, L. (2000). *Statistical Physics: Statics, Dynamics and Renormalization*. Singapore: World Scientific.

[27] McLaughlin, B. (1992). “The rise and fall of British emergentism.” Pp. 49-93 in A. Beckermann, H. Flohr, and J. Kim (eds.), *Emergence or Reduction? Essays on the Prospects of Nonreductive Physicalism*. New York: de Gruyter.

[28] Cunningham, B. (2001). “The reemergence of ‘emergence’.” *Philosophy of Science*, **68**: S62-S75.

[29] O’Connor, T. (2021).”Emergent properties.” In E. N. Zalta (ed.), *The Stanford Encyclopedia of Philosophy* (Winter 2021 Edition), URL = https://plato.stanford.edu/archives/win2021/entries/properties-emergent/,

[30] Anderson, P. W. (1972). “More is different.” *Science*, **177**: 393-396.

[31] Rueger, A. (2006). “Functional reduction and emergence in the physical sciences.” *Synthese*, **151**, 335-346.

[32] Batterman, R. (2002). *The Devil in the Details: Asymptotic Reasoning in Explanation, Reduction, and Emergence*. Oxford: Oxford University Press.

[33] Batterman, R. (2005). “Critical phenomena and breaking drops: Infinite idealizations in physics.” *Studies in History and Philosophy of Modern Physics*, **36**: 225-244.