The Limits of Classical Extensional Mereology for the Formalization of Whole–Parts Relations in Quantum Chemical Systems

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Abstract: This paper examines whether classical extensional mereology is adequate for formalizing the whole–parts relation in quantum chemical systems. Although other philosophers have argued that classical extensional and summative mereology does not adequately formalize whole–parts relation within organic wholes and social wholes, such critiques often assume that summative mereology is appropriate for formalizing the whole–parts relation in inorganic wholes such as atoms and molecules. However, my discussion of atoms and molecules as they are conceptualized in quantum chemistry will establish that standard mereology cannot adequately fulfill this task, since the properties and behavior of such wholes are context-dependent and cannot simply be reduced to the summative properties of their parts. To the extent that philosophers of chemistry have called for the development of an alternative mereology for quantum chemical systems, this paper ends by proposing behavioral mereology as a promising step in that direction. According to behavioral mereology, considerations of what constitutes a part of a whole is dependent upon the observable behavior displayed by these entities. Thus, relationality and context-dependence are stipulated from the outset and this makes behavioral mereology particularly well-suited as a mereology of quantum chemical wholes. The question of which mereology is appropriate for formalizing the whole–parts relation in quantum chemical systems is relevant to contemporary philosophy of chemistry, since this issue is related to the more general questions of the reducibility of chemical wholes to their parts and of the reducibility of chemistry to physics, which have been of central importance within the philosophy of chemistry for several decades. More generally, this paper puts contemporary discussions of mereology within the philosophy of chemistry into a broader historical and philosophical context. In doing so, this paper also bridges the gap between formal mereology, conceived as a branch of formal ontology, and "applied" mereology, conceived as a branch of philosophy of science.

Keywords: classical extensional mereology; summative mereology; mereology of quantum chemical systems; mereology of chemical wholes; behavioral mereology

1. Introduction

This paper examines whether classical extensional mereology is adequate for formalizing the whole–parts relation in quantum chemical systems. According to Rafał Gruszczyński and Achille Varzi, "understood as a general theory of parts and wholes, mereology has a long history that can be traced back to the early days of philosophy. [However] as a formal theory of the part-whole relation—or rather, as a theory of the relation of part to whole and of part to part within a whole—it is relatively recent and came to us mainly through the writings of Edmund Husserl and Stanisław Leśniewski" (pp. 409–410, [1]). According to Husserl and many contemporary logicians such as David Lewis, classical extensional mereology captures not only the whole/parts relations within the context

of mathematics and formal ontology but also whole/parts relations in the regional ontologies studied by the sciences.

This paper, however, purports to establish that classical extensional mereology fails to capture whole/parts relations in many of the objects studied by the sciences. Although other philosophers have stressed that classical extensional and summative mereology does not adequately formalize whole–parts relation within the organic wholes and social wholes studied by biology and by the social sciences, such critiques often assume that summative mereology is appropriate for formalizing the whole–parts relation in inorganic wholes such as atoms and molecules. Therefore, this paper will contribute to this debate by establishing that standard extensional mereology cannot adequately describe the relations between atoms and molecules as they are conceptualized in quantum chemistry, since the properties and behavior of such systems are context-dependent and resist attempts at reductionist formalization. This context-dependence, in fact, also includes dependence upon the environment in which the parts and the whole exist and, as in the case of chemistry, the kinds of procedures employed to analyze and synthesize such systems. In fact, philosophers of chemistry have called for the development of an alternative mereology for quantum chemical systems.

This paper proposes behavioral mereology as a promising candidate for the type of non-standard mereology that can accommodate the context-dependent whole/parts relation within quantum chemical systems. According to behavioral mereology, considerations of what constitutes a part of a whole is dependent upon the observable behavior displayed by these entities. Thus, relationality and context-dependence are stipulated from the outset and this makes behavioral mereology particularly well-suited as a mereology of quantum chemical wholes. Although behavioral mereology has not yet been used in the context of quantum chemistry, the paper gives examples of how such a non-summative mereology might be applied to formalize the interdependence of the electronic densities of atoms within molecules, to show that such properties are context-dependent and cannot be formalized in a reductionist manner.

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2. The Fundamental Principles of Standard Summative Extensional Mereology

To the extent that Husserl's work, in the *Logical Investigations* and *Experience and Judgment*, is seminal for the development of mereology as a formal theory of the part–whole relation, it is important to begin this paper by discussing the principles of standard mereology as developed by Husserl, as well as the role that such a mereology fulfills in the context of formal ontology. Gruszczyński and Varzi explain that "[Husserl's work on mereology was] part of a larger project aimed at the development of a general framework for formal ontology" (p. 410, [1]). Husserl understands ontology as a theory of being in the traditional sense, so that "its task is to lay bare the formal structure of what there is no matter what it is . . . For instance, it would pertain to the task of formal ontology to assert that every entity, no matter what it is, is governed by certain laws concerning identity, such as reflexivity, symmetry, or transitivity" (p. 410, [1]). Because identity, reflexivity, and transitivity apply to anything that may exist, they are considered formal. According to Husserl, the whole–parts relation is formal in this same sense because it applies to anything that may exist unless, of course, the thing under

consideration is absolutely monadic. "Parthood seems to apply to entities as different as material bodies (the handle is part of the mug), events (the first act is part of the play), geometrical entities (the point is part of the line), etc. Even abstract entities such as sets, appear to be amenable to mereological treatment" (p. 411, [1]).

Husserl believes that "a purely formal theory of wholes and parts [is] possible" (p. 114, [2]) and serves as the foundation for the mereology of regional ontologies, that is, the specific ontologies to which things belong (for example, physical systems, quantum systems, chemical systems, biological systems, social systems, etc.). Husserl considers that mereology is fundamental to the development of a phenomenology of the formal sciences because he considers pure logical grammar to be "the theory of apophantic forms of complex independent unified wholes of meaning, *Bedeutungskomplexionen*" (p. 16, [3]). He, therefore, devotes a significant part of the second volume of the *Logical Investigations* and of *Experience and Judgement* to developing a formal theory of wholes and parts. According to Thomas Seebohm, the mereology that Husserl develops in the *Logical Investigations* is sufficient for the analysis of "the hyletic correlates of passive synthesis in primordial sensual experience" (p. 19, [3]), that is, first-order wholes. The conclusion reached in the *Logical Investigations* is that the formal ontology of wholes and parts is analogous to the formal ontology of units and manifolds. Therefore, since manifolds are analyzable as additive collections of units, wholes are analyzable as additive collections of parts [2]. Himself a mathematician, Husserl inherits the concept of "manifold" from 19th century mathematical theory, although there is some debate regarding whether he was influenced in this regard by Cantor's set theory (*Mengenlehre*) or by Riemann's topological *Geometrie*.

For this discussion of Husserlian mereology, we must pay special attention to Husserl's extensive analysis of the notions of dependent parts (or moments) and independent parts (or pieces), since these are both significant features of the Husserlian theory of wholes and parts. Husserl writes, "*Each part that is independent relatively to a whole W we call a Piece (Portion), each part that is non-independent relatively to W we call a Moment (an abstract part) of this same whole W*. It makes no difference here whether the whole itself, considered absolutely, or in relation to a higher whole, is independent or not. *Abstract parts can in their turn have pieces, and pieces in their turn abstract parts*" (p. 29, [4]).

It is important to examine this aspect of Husserl's mereological theory because the question of the reduction of higher-order ontologies to lower-ontologies requires that we examine whether the parts of higher-level wholes are pieces or moments of those wholes. If the parts are pieces of the whole, then reduction is materially possible because the pieces of wholes can exist independently of the whole of which they are parts. On the other hand, if the parts are moments of the whole, then reduction is not materially possible because the parts cannot exist independently of the wholes of which they are parts This is the case because, although the pieces of a whole can exist independently of the whole of which they are independent parts, the moments of a whole cannot exist independently of the wholes of which they are parts. Peter Simons gives an example that can help to illustrate this distinction: "The board which makes up the top of the table is a piece of the table [while] the surface of the table, or its particular individual color-aspect, are moments of it" (p. 115, [2]). This distinction becomes an important component of Husserl's formal ontology because he believes that it extends to all objects in general. He also indicates that he uses the term "part" in the wide sense to include the detachable pieces of a whole, as well as "anything that is a constituent of it, apart from relational characteristics [including] so-called accidents and also boundaries" (p. 120, [5]).

Another element of Husserlian mereology that is significant for the issue of whole–parts reduction is the distinction that he draws between three different types of wholes.[1] The first type of whole is one that is considered in the narrow sense (p. 121, [5]). A "narrow whole" is one wherein entities are joined because of the sorts of entities that they are, without anything else connecting them together, apart from

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[1]   The distinction discussed here is that between narrow wholes, wide wholes, and pregnant wholes. "Narrow whole" and "wide whole" are terms used by Barry Smith to refer to the first two types of wholes described by Husserl, while the term "pregnant whole" is the term used by Husserl himself to refer to the third type of whole.

what Husserl calls a "unifying moment" that is not itself another entity.[2] The entities that form narrow wholes are considered to be pieces, rather than moments, of the whole. This is because, from a formal perspective, the existence of these entities as the sorts of entities that they are is not itself dependent upon the whole of which they may become parts. Although these entities are bound together in the whole due to their intrinsic nature, the whole itself is extrinsically unified (pp. 37–40, [3]).

The second type of whole distinguished by Husserl is one that is considered in the wide sense. A "wide whole" is regarded as a single thing, notwithstanding whether its parts are tightly connected, loosely connected, or widely scattered. Thus, both unities and pluralities can be considered as "wide wholes," since "any plurality may be taken together as something unitary, thereby founding a new higher unity, whose unity is, however, extrinsic to it, in the collective act" (p. 122, [2]). The parts of wide wholes are considered to be pieces since they are independent parts of whatever unity or plurality. From this, it is evident that the parts of wide wholes are to be considered as pieces, since they are independent parts of the unity or of the plurality in which they exist as parts. As a matter of fact, whether a whole is regarded as "wide" or not is the result of a decision, which may or may not be arbitrary, to trace the boundaries of that whole in one place rather than in another. As Simons explains, we may "allow as individuals anything which can possess a (singular) proper name. This will include arbitrary *collectiva*. This liberality is reflected in extensional mereologies by allowing that arbitrary sums of individuals are themselves individuals. The reason for this is . . . that it is not clear in advance where to draw the line between things which are wholes in this widest and weakest sense, and those which have some more intrinsic unity" (p. 122, [2]).

The third type of whole that is identified by Husserl is a "pregnant" whole and this is a more interesting type of whole because it is one in which "a range of contents which are all covered *by a single foundation* without the help of further contents. The contents of such a range we call its parts. Talk of the *singleness of the foundation implies that every content is foundationally connected whether directly or indirectly, with every content* . . . without external assistance" (p. 34, [4]). Unlike narrow and wide wholes, which are mere sums or aggregates of parts and which only have extrinsic unity, pregnant wholes have intrinsic unity. Although their parts are still considered as pieces rather than moments, what distinguishes pregnant wholes from narrow and wide wholes is that the relations between the parts of pregnant wholes are considered as moments. Such relations can be either ideal relations or real relations. Ideal relations are ones that do not alter the parts that they relate and do not imply any real connection between those parts. As an example of this, if entity A is of the same height as entity B, they are in the relation "is the same height as." However, neither A nor B is in any way affected by being in this relation. Because ideal relations are often relations of equivalence and are, therefore, reflexive relations, ideal relations cannot "engender genuine foundation relations" (p. 154, [2]).[3]

On the other hand, real relations are ones that do alter or otherwise affect the parts that they relate. As an example, if a magnet A attracts a metal B, both the magnet and the metal are affected by the relation of magnetic attraction. This example illustrates that the clearest example of a real relation is a relation involving a causal link of some sort (p. 154, [2]). This means that real relations can never be reflexive and can, therefore, serve to engender genuine foundation relations. When they do engender such foundation relations, those relations are considered as moments of the whole of which they unite the parts (p. 154, [2]). Some foundation relations are symmetric and some are asymmetric. Symmetric foundation relations are *two-sided*, or *mutual*, foundations. The relation between color and extension is symmetric because color and extension are mutually founding. Asymmetric foundation relations

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[2] Husserl emphasizes that the "unifying moment" is not itself an entity in order to avoid the regress that is discussed by F.H. Bradley in *Appearance and Reality*. According to Bradley, the regress is generated when a third entity is required to join the first two entities so that "if A and B are bound together by U, then A and U must be bound together by U^1, and so on *ad infinitum*" (p. 121, [2]).

[3] Simons regards the whole notion of a relation that holds between a thing and itself as suspect, especially in cases such as identity, which can only hold between a thing and itself. Thus, Simons considers reflexive relative terms to be "ontologically sterile" since "nothing intrinsically relational is represented" by such terms.

are *one-sided* and an example is the relation between a lake and the dry land that serves as the lake's one-sided foundation.

Husserl discusses these three types of wholes as pertaining to formal ontology. However, if the task of ontology is "to lay bare the formal structure of what there is *no matter what it is*" (p. 410, [1]) and if the task of mereology is to reveal the fundamental principles of that formal structure, then we must resolve the question of what constitutes natural wholes. We must also resolve whether the type of mereology developed in the *Logical Investigations* and in *Experience and Judgment* can adequately describe the whole–parts relations of the objects studied by the special sciences, whose categorial objects belong to the regional ontological spheres of the material world. Because natural wholes or systems are bound together by their causal integrity (p. 150, [2]), we must consider whether the parts of natural wholes or systems are to be considered as pieces (independent parts) or as moments (dependent parts) of those wholes or systems.

When considering objects in the material world, Husserl does not consider the distinction between lower-order and higher-order objects to be absolute because such object are naturally organized in a variety of ways. From one perspective, an object can be viewed as "a natural unity, from another it may coincide with an aggregate of differently organized units, or again be a moment of a greater whole" (p. 150, [2]). However, this relativity between different types of organization "is not the mere imposition of a conceptual scheme on an otherwise unstructured world, but cuts along natural seams in reality" (p. 150, [2]). Therefore, it follows that Husserl considers the parts of both lower-order and higher-order wholes as pieces, rather than as moments, of those wholes. This is precisely what I will contest in my later discussion of quantum chemical systems, because I will argue that the parts of such systems are dependent parts and should, therefore, be considered as moments of those systems.

Rafał Gruszczyński and Achille Varzi point out that "the general applicability of the part-whole relation is controversial … [David] Lewis himself famously argued that entities such as universal *cannot* be structured mereologically, short of unintelligibility" (pp. 409–410, [1]). It is interesting to note that Lewis uses a chemical example to illustrate this point: "Each methane molecule has not one hydrogen atom but four. So, if the structural universal methane is to be an isomorph of the molecules that are its instances, it must have the universal hydrogen as a part not just once, but four times over … But what can it mean for something to have a part four times over?" (p. 34, [6]). The difficulty addressed by Lewis concerns both the limits of mereology and its content. "Consider, for instance, the question of whether there are mereological *atoms* (i.e., entities with no proper parts), or of whether everything is ultimately *composed* of atoms. Clearly any answer to such questions would amount to a substantive metaphysical thesis that goes beyond a 'pure theory of objects as such'" (p. 412, [1]). As Gruszczyński and Varzi claim, "taken together, then, these two sorts of difficulty represent a serious challenge to the idea that mereology can form a genuine piece of formal ontology" (p. 413, [1]).

I am only concerned in this essay with the first difficulty discussed above, rather than the second, and will only be addressing the question of whether Husserl's conception of mereology as formal ontology can also be extended to regional ontologies, as he believed. I will argue that the formal principles of Husserlian mereology do not adequately describe the whole–part relations of the higher-order ontologies with which the special sciences are concerned. I will focus specifically on quantum chemistry, discussing the way in which quantum chemists conceptualize, manipulate, transform quantum systems. This discussion will demonstrate that the manner in which chemists conceptualize subatomic "entities" for the purposes of quantum chemical calculations violates the principles of the summative extensional mereology defended by Husserl and other logicians, such as the contemporary philosopher Kit Fine. More specifically, quantum chemical systems are conceptualized in a manner that violates the standard principles of transitivity, unrestricted composition, and uniqueness of composition. The latter fundamental principle of standard extensional mereology, with which Husserl would agree, has been recently described by Fine as postulating that "the same parts cannot, through different methods of composition, yield different wholes" (p. 138, [7]). Thus, according to this principle, if the same composition of parts is structured differently, then it will yield the same whole

that will display the same properties. I will show later in this essay that the mereology of quantum chemical wholes does not conform to this principle.

Another fundamental principle of extensional mereology that is violated by quantum chemical wholes is the principle, described by David Lewis, that any two or more individuals can constitute a mereological whole. However, inclusion in such a whole does not alter the individuals that are included in that whole (pp. 25–26, [6]). Therefore, the mereological sum or fusion does not have any causal effect in itself, apart from the causal effectiveness of its parts. It will be shown in this essay that the wholes belonging to higher-order regional ontologies, including those belonging to the ontology of quantum chemical wholes, are not adequately described by the aforementioned principles of classical standard mereology, as these have been postulated by Husserl and by contemporary logicians.

3. The Limits of Summative Extensional Mereology for Analyzing the Whole–Parts Relation within Higher-Order Regional Ontologies

The mereological theory that Husserl develops in the *Logical Investigations* and in *Experience and Judgment* focuses on pregnant wholes, that is, first-order wholes that are "held together by unifying foundations" (p. 20, [3]). However, the higher-order wholes that are referred to in natural language are even more complex than the pregnant wholes discussed by Husserl (p. 19, [3]). Such wholes include the solar system and organisms with various degrees of complexity, as well as social groups and communities. These wholes have a greater degree of complexity than the pregnant wholes discussed in Husserl's work because the parts that constitute them are themselves wholes, rather than simple parts. The parts belonging to such wholes are altered both by their relations to the other parts and by their membership in that whole. Since the principles of standard mereology deny any causal efficacy to the mereological sum or to the relations between its parts, standard mereology cannot provide a satisfactory formal account of these types of complex wholes. In fact, Husserl himself admits that his concern is primarily to develop a mereology for the formal ontology of pure logical grammar and then merely assumes that such a mereology would be applicable to categorial objects of a higher order.

The fact that the relations between the parts of higher-order wholes causally affect those very parts and the fact that the whole itself causally affects the parts that are unified within it are not the only two reasons for why standard extensional mereology cannot adequately describe such wholes. There is, however, another reason that standard mereology cannot provide an adequate description of such wholes. When higher-order wholes are mereologically analyzed, the role played by the environment surrounding such wholes must also be taken into account in the analysis [8].[4] Thus, when one is giving a mereological analysis of biological wholes, "the description of the environment of a species and the ecological relation of the species to the environment is not of immediate significance for the simple recognition of the species of an individual organic being or for the development of taxonomies of organic species. It is, however, of significance for experimental research and for the discovery of causal relations between organisms as concrete wholes (or their parts) and certain properties or aspects of their environments" (p. 245, [3]).

The next section of this paper will show that a description of the environment must also be considered when providing mereological analyses of quantum chemical systems. More precisely, the description of the experimental environment in which such wholes are analyzed, synthesized, or otherwise studied is crucial for the mereological analysis of quantum chemical systems. The question of which mereology is adequate for quantum chemical systems is relevant for the material possibility of reducing chemistry to physics. As recent developments in quantum chemistry suggest, such systems

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[4]   The 19th century French statistician Louis-Adolphe Bertillon called attention to the importance of the relation between an organism and its environment, and he coined the term "mesology" to refer to what he called "la science des milieu" or "the science of environments." The contemporary French geographer, Orientalist, and philosopher Augustin Berque has recently resurrected the focus on mesology as part of a proposal for overcoming modernist reductionism by calling attention to the importance of considering milieu when studying the organism [8].

cannot be analyzed as summative collections of parts and the parts of such systems are to be regarded as moments, rather than pieces, of the whole. Thus, although the reduction of chemistry to physics may remain as an ideal possibility, it will be argued that the reduction of the higher-order ontology of chemistry to the lower-order ontology of physics is not a material possibility.

4. The Limits of Summative Extensional Mereology for Analyzing the Whole–Parts Relation within Quantum Chemical Systems

The autonomy of chemistry as a science and the issue of its reduction to physics have been two of the fundamental questions examined by contemporary philosophy of chemistry. In fact, Eric Scerri claims that the reduction of chemistry to physics is "one of the main areas in which philosophical interest in chemistry should be directed . . . [The question is] whether our current description of chemistry can be reduced to our most fundamental current description of physics, namely quantum mechanics—and with its explanatory consequences" (pp. 214–215, [9]). Since the ontological dependency of chemical properties on fundamental physical states is not in question, the reduction of the material ontological structures of chemical entities to lower-order physical entities remains as an ideal possibility. The remainder of this essay, however, will be concerned with arguing that the reduction in question is not a material possibility precisely because, as with organic wholes, chemical wholes cannot be simply analyzed as mere collections of parts.

Although many philosophers of science have regarded the reduction of chemistry to physics as materially possible [10],[5] contemporary philosophers of chemistry and quantum chemists themselves do not regard the ontological dependency of chemical states upon physical states as undermining the epistemic and heuristic autonomy of chemistry. As Scerri points out, the hope that such a reduction can be carried out

> seems to have been abandoned and . . . all that remains is the possibility for approximate reduction. However, criteria for approximate reduction have not been put forward and the notion remains vague . . . the calculation of the ground state energies of atoms has been achieved to a remarkable degree of accuracy and similarly calculations on small or even medium-sized molecules have given encouraging results. However, whether one can draw the conclusion that chemistry has been reduced rather depends on one's criteria of reduction. If we are to define approximate reduction as has been suggested . . . then it must be concluded that *chemistry is not even approximately reduced to quantum mechanics* (p. 168, [11]).

Doubts regarding the possibility of such reduction were raised as far back as 1939 by Linus Pauling, who claimed that "[a] small part of the body of contributions of quantum mechanics to chemistry has been purely quantum mechanical in character: only in a few cases, for example, have results of direct chemical interest been obtained by the accurate solution of the Schrödinger wave equation . . . The principal contribution of quantum mechanics to chemistry has been the suggestion of new ideas, such as the resonance of molecules among several electronic structures with an accompanying increase in stability" (p. vii, [12]). In fact, several chemical concepts have been shown to resist attempts at reduction.

Two concepts that have resisted reduction are those of valence and bonding. However, there are also serious doubts about the possibility of reducing concepts such as composition and molecular structure precisely because these notions do not represent actual ontological features of the world. In fact, to the extent that the reduction of concepts such as composition and molecular structure is not even possible in principle, such a reduction is both materially and ideally impossible. This is precisely "due to the very nature of the concepts themselves. That is, the concepts of composition, bonding, and molecular structure cannot be expressed except at the chemical level . . . we can calculate

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[5]　　See, for example, Hilary Putnam and Paul Oppenheim [10].

certain molecular properties, but we cannot point to something in the mathematical expressions which can be identified with bonding. The concept of chemical bonding seems to be lost in the process of reduction" (pp. 218–219, [9]). It is also doubtful whether quantum theory can offer much insight that will help us understand these chemical concepts. "[M]any calculations have been extremely sophisticated, designed by some of the foremost researchers in this field to extract a maximum of insight from quantum theory. For simple molecules, outstanding agreement between calculated and measured data has been obtained. Yet, the concept of a chemical bond could not be found anywhere in these calculations. We calculate bonding energies without even knowing what a bond is" (p. 5, [13]).

The physicist and chemist Robert Mulliken, who was one of the pioneers of the molecular orbital theory, stated that "attempts to regard a molecule as consisting of specific atomic or ionic units held together by discrete numbers of bonding electrons or electron-pairs are considered as more or less meaningless, except as approximations in special cases, or as methods of calculation" (p. 55, [14]). According to Mulliken, an atom cannot be said to exist within a molecule. This is because each orbital is delocalized over all the nuclei within the molecule and may contribute either a stabilizing or a destabilizing energy to the total energy of that molecule [15]. He clarifies that "a molecule is here regarded as a set of nuclei, around each of which is grouped an electron configuration closely similar to that of a free atom in an external field, except that the outer parts of the electron configurations surrounding each nucleus usually belong, in part, jointly to two or more *nuclei*" (p. 55, [14]). Therefore, "there is a key semantic shift here from the concept of molecular *orbit* to that of molecular *orbital*" (p. 85, [15]), which takes its meaning from Max Born's probabilistic interpretation according to which the square of a molecular orbital corresponds to the probability density of finding a particular electron within the molecular space. Molecular orbitals have wave functions that contain one electron and that can be delocalized either over all the nuclei or simply over a set of particular nuclei. Thus, "the complete electronic wave function is restricted to one of several types that depend upon the symmetry of the nuclear skeleton" (p. 85, [15]).

In addition to the concepts of valence, bonding, and molecule, there are two additional concepts that defy the possibility of either material or ideal reduction. These are the concepts of molecular shape and of chemical composition. With regard to molecular shape, although this concept does have great heuristic power, it resists reduction even in principle because it is, in fact, a "mere" concept. As such, molecular shape "is metaphorical in virtue of being only chemical . . . Molecules can lack an orientation in three-dimensional space, and a particular shape is dependent on the way that the molecule is picked out in measurement . . . Whether we need to employ the fixed nucleus picture, separate nuclear and electronic 'clouds', or interacting clouds depends on the particular molecule chosen for study, the experimental technique we employ and the questions we ask. As it turns out, there are many different representations of the same property" (pp. 234–248, [16]). With regard to chemical composition, a concept that is related to the concepts of bonding and of molecular structure, it cannot be reduced because "what is physical about a chemical system are its components rather than the system itself [qua chemical system] which possesses emergent (though explainable) properties in addition to physical properties" (p. 210, [17]). Jeffry Ramsey states that "the fundamental idea that molecules are constructed additively of atoms, which retain their essential identity within the molecule, is brought into question" (p. 233, [16]).

The best way to understand the reason why chemical wholes are irreducible to their lower-level physical components is by examining the mereology of chemical systems, for example, the mereology of molecules. The philosopher and psychologist Rom Harré and the philosopher and quantum chemist Jean-Pierre Llored have been pioneers in this area and they explain that "constituent atoms of molecules are not parts of those molecules when we look at the total entity in the light of molecular orbitals. Unlike chair parts which preserve their material properties whether in the chair or on the bench" (p. 73, [18]). It is also debatable whether the concept of molecular can be reduced to the concept of physical component parts without remainder. According to the chemist and philosopher Joseph Earley, we can examine the example of salt and conclude that "Na and Cl ions are not parts of salt lattices

after that salt has been dissolved. Being in the solution determines that the solution will afford salt as a mass substance on the carrying out of certain operations on sea water, and not something else. Thus, they are at best potential material parts of salt" (p. 81, [19]). Earley is here using the concept of "affordance," first introduced into the philosophy of chemistry by Harré, to establish that we must say, not that there is salt as such in the sea, but that the sea affords salt when certain conditions are met and certain procedures are carried out.

In the same way, philosophers of chemistry use the concept of affordance to reinforce Mulliken's point that there are no atoms in molecules by claiming that "molecules afford atoms in the context of certain manipulations as studies of molecular reactivity have shown us. The material content of a molecule can only be a fusion of atomic potentials, not of atoms [and] affordances are not simple conditional properties . . . they incorporate the procedure or method used to display their empirical manifestations . . . the parts of chemical wholes like molecules and atoms are affordances, not themselves concrete entities" (p. 69, [18]). If the parts of the whole (in this case, atoms) are not concrete entities and may even be considered as "ephemeral" individuals, the whole (in this case, molecules) cannot be reducible to those parts. In the case of water, for example, "the swiftly composing and decomposing hydrogen-oxygen structures of which real water is really composed are ephemeral individuals. Water is made up of these beings. As such they are [ontological] constituents of a certain whole" (p. 73, [18]). However, water as a chemical composition cannot be simplistically reduced to these ephemeral individuals.

Earley claims that "most philosophers have yet to recognize that, when components enter into chemical combination, those components do not, in general, maintain the same identity that they would have absent that combination" (p. 89, [19]). H_2O and silver chloride serve as good examples to illustrate Earley's point. Although the property of being H_2O or of being silver chloride "supervenes on the features of the constituent atoms, the features of the atoms on which it supervenes includes features that the atoms have only in virtue of being parts of that compound. The atomic interrelations that give rise to the compound would not obtain if the atoms were parts of a different molecular type" (p. 58, [20]). Therefore, it is chemical reaction networks that define molecules rather than the reverse.[6]

An important issue in philosophical debates regarding emergence and supervenience is whether causal relations between emergent properties and the subvenient base are symmetrical or asymmetrical. If causation occurs only upward from the subvenient base to the emergent properties, then causality is asymmetrical and reduction is materially possible. However, if there is also downward causation from the emergent properties to the subvenient base, then causality is symmetrical and reduction is not materially possible. In the case of quantum chemical systems, the emergent properties of the whole not only display novel causal powers that are not present in the constituent parts but they also specifically display downward causal influence upon those parts. Thus, the causal relations between the whole and the parts in chemical systems is symmetrical, that is, it is neither wholly upwardly nor wholly downwardly directed. Harré and Llored suggest that, in order to best account for this symmetrical causal influence between chemical wholes and their parts, we must appeal to the concept of relationality. This is because, in order to account for the emergent properties of chemical wholes, we must take into account relationality on many different levels, that is, we must take into account the relations between the whole and the parts, the relations of the parts to one another, and the relations of their properties to one another. We must also take into account relation of the whole system to its environment and, if appropriate, to the experimental conditions under which the chemical system is being analyzed or synthesized.

Since standard extensional mereology, by definition, does not take into account relationality, a new type of mereology must be developed that will account for the fact that, when simple individuals enter into complex combinations, they become different kinds of individuals than they were prior to

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becoming parts of such combinations. Thus, the extensional and summative mereology that Husserl believed to be applicable both to formal ontology and to the regional ontologies of higher-order systems, such as chemical wholes, for example, is in fact not adequate for the analysis of such complex systems. In fact, Harré and Llored explain that "the standard mereology for chemical compounds involves the presupposition that just as molecules are ultimate constituents or parts of material things, so atom-cores are parts or constituents of molecules" (p. 133, [21]). Thus, two mereological fallacies are committed when trying to conceptualize electrons as entities. The first of these fallacies involves mistakenly applying a predicate to the parts of a whole when that predicate is designed to ascribe an attribute to the whole only. This is a fallacy because "a holistic predicate is not necessarily a part predicate, the notion of use is crucial because . . . predications are context-sensitive" (p. 133, [21]). The second of these mereological fallacies involves inferring that "substantive products of an analytical procedure are parts of the substance on which the procedure was performed" (p. 134, [21]).

Furthermore, in the context of quantum chemical calculations, chemists conceptualize subatomic "entities" in ways that violate the principles of transitivity, unrestricted composition, and uniqueness of composition, which are all fundamental principles of standard extensional mereology. If we recall Fine's claim regarding composition, if the same parts were to be structured differently, they would yield the same whole with the same properties as the original composition. We also recall from our discussion above that, according to Lewis, a mereological fusion had no distinctive causal effectiveness apart from the causal effectiveness of its parts and that the inclusion of parts in a mereological sum or fusion does not alter those parts [6]. However, quantum chemical systems violate both of these fundamental principles of standard mereology. Quantum chemists consider the principle of uniqueness of composition to be "unintuitive and inadequate to those rules for chemical parts-whole reasoning that are required to accommodate the role of chemical entities in structures, such as atoms in 'polyatomic' ions. [Quantum chemists] are likely to question the relevance of transitive mereology whenever the whole molecule and the parts are co-dependent and relative to a specific environment or action" (p. 159, [22]). It is interesting to note that Fine himself admits that mereology must recognize relationships in a manner that does not conflate the properties of parts with the relations between parts.

The mereology of structured and complex wholes such as chemical systems must accommodate the fact that such systems "generally have causal efficacy in virtue of their 'connectivity'—in addition to the causal powers of their constituent atoms" (p. 9, [23]). The connectivity of chemical systems contributes to a large number of their properties, such as optical activity and chirality. For example, "Levorotatory amino acids are nutritious [but] the corresponding dextrorotatory amino acids are poisonous—although both sorts of molecules have exactly the same component parts" (p. 9, [23]). Besides accounting for optical activity and chirality, the structural arrangement and connectivity of chemical systems also account for the phenomenon of isomerism. This phenomenon was first discovered by Friedrich Woehler, in 1827, as he was preparing cyanic acid and noticed that, even though its elemental composition was identical to that of fulminic acid, its properties were entirely different. This discovery called into question the dominant mereological conception of chemical composition of that time, which embraced the idea that difference in chemical properties was only accounted for by difference in composition, without taking structure and connectivity into account.

5. Behavioral Mereology: A Promising Alternative for the Mereological Description of Quantum Chemical and Other Higher-Order Wholes

Clearly, the standard summative mereology proposed by philosophers such as Husserl, Lewis, Simons, and other logicians cannot adequately capture the whole–parts relations both of organic wholes but also of the inorganic wholes studied by quantum chemistry. However, a recent proposal was made by Brendan Fong, David Jaz Myers, and David Spivak for a type of non-standard mereology, called "behavioral mereology," that would better capture the whole–parts relation in higher-order wholes, such as those discussed in this paper. The behavioral mereology proposed by Fong, Myers, and Spivak is an approach to mereology "in which systems and their parts are known only by the types

of behavior they can exhibit . . . Given a behavior on one part, we can consider all possible extensions to the whole, and subsequently ask how those extensions restrict to behaviors of other parts. In this way one part may constrain another" (pp. 1–2, [24]). Once the notion of parthood is construed as being dependent on the observable behavior displayed by parts and wholes, context-dependence must be stipulated from the outset. Behavioral mereology incorporates context-dependence by considering "the relationship between various parts of a whole in terms of how behavioral constraints are passed between them, and [gives] an inter-modal logic that generalizes the usual alethic modalities in the setting of symmetric accessibility" (p. 1, [24]).

The starting point of this proposal is that parthood displays a kind of behavioral coherence. When one part is affected, other parts are affected, as is the whole that is constituted by those parts. Thus, being a part of a whole entails a restriction on possible behaviors and, in general, the behavior of a part is constrained both by the parts around it and by the corresponding whole. "A whole then has the property that it coordinates constraints—or said another way, it enables constraints to be *passed*–between parts" (p. 1, [24]). A behavior of X is simply something that X does, but there is no intentionality implied here. Since the term "behavior" does not imply intentionality, this constraint coordinating property is not merely found in organic wholes such as animals and ecosystems but also in inorganic wholes such as a cup of water. Thus, the movements ("behavior") of the water in the cup are constrained by the movements ("behavior") of the cup and the behavior of a person's brain constrains the behavior of the person's muscles.

In addition to considering the interdependence between parts and parts and between parts and whole, behavioral mereology also takes into consideration the environment surrounding the whole and how that environment also constrains behaviors. For example, because the behavior of a person's muscles changes that person's relation to the environment and because the environment constrains the person's senses, it follows transitively that the person's muscle-behavior constrains her sense-behavior. Consequently, one can think of the whole "person" system as providing a context for the passage of constraints between the parts of the person, and this gives rise to a lattice structure on the corresponding category of parts.

Fong, Myers, and Spivak specifically emphasize that behavioral mereology remains "agnostic to the topos [thus] providing maximal generality" (p. 1, [24]). For the sake of keeping the language simple, Fong, Myers, and Spivak develop the logic of behavioral mereology from a set theoretic point of view, by choosing to work in the "set of sets and functions" topos, but they also repeatedly emphasize that their arguments "are valid in any topos[7] . . . As a consequence, [their] logic retains its character as a logic of constraint passing across a wide variety of semantics. One possibly valuable notion of semantics is that it captures a notion of time [since] behavior is best conceived as occurring over time" (p. 16, [24]). They add that they "won't need to settle on what precisely a behavior type is, so long as [they] can reason about it logically . . . A topos can be understood as a system of variable sets [which can vary in time and/or in space] or according to different observers . . . Thus a *behavior type* is simply a set whose elements are regarded as possible behaviors of a system" (pp. 1–2, [24]).

This proposal implies a decidedly non-reductionist conception of the whole–parts relation and what makes it especially promising as a mereology of not only organic wholes, but also of quantum chemical systems, is that it takes into consideration the way in which the behavior of one part affects the behavior of other parts, and also the way in which the behavior of the whole, as a whole, affects the behavior of its individual parts. Thus, "given a system for which B_S is its set of possible behaviors, we define a part to be a quotient of B_P, i.e., a surjection of $B_S \twoheadrightarrow B_P$ from the behavior type. This surjection describes how a behavior of the entire system determines a behavior of the part, and any behavior of

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7 The only qualification that Fong, Myers, and Spivak make to this claim is for Proposition 18 of their system, which states: "Assuming Boolean logic, compatibility and ensurance are de Morgan duals." This proposition is valid for the topos under consideration, which is the Set of sets and functions, and for all Boolean toposes. But it is clearly not valid for non-Boolean toposes such as quantum chemical wholes, organic wholes, ecosystems, or other complex or higher-order wholes.

the part qua part must extend to the behavior of the whole . . . Given a behavior on one part, we can consider all possible extensions to the whole, and subsequently ask how those extensions restrict the behaviors of other parts. In this way one part may constrain another" (pp. 1–2, [24]).

If we ask what a P-behavior means for the other parts of S, Fong, Myers, and Spivak introduce operators for the formal inter-associated concepts of *compatibility* and *ensurance*. So, for example, if a person has P-behavior "rapid heart rate," we can ask what this means for the legs of that person. Once we introduce compatibility, we can say that the person's exertion of her muscles, let's say due to running away from a bear, are compatible with her having P-behavior "rapid heart rate." Thus, a list of compatible behaviors can be obtained that restricts the behaviors of S to its parts. The right adjoint of compatibility is *ensurance*, which corresponds to a relation called *determination*. Informally, we can say that while the person not moving is compatible with her having a rapid heart rate, strenuous exertion would ensure this. So, the Q-behavior "strenuous exertion" is said to determine the P-behavior "rapid heart rate."

To provide an example of how behavioral mereology may be a promising mereological approach for formalizing the whole–parts relations in quantum chemical systems, I return to Mulliken's claim that "A molecule is here regarded as a set of nuclei, around each of which is grouped an electron configuration closely similar to that of a free atom in an external field, except that the outer parts of the electron configurations surrounding each nucleus usually belong, in part, jointly to two or more *nuclei*" (p. 55, [14]). Let us consider a simple case of a polyatomic molecule that contains two nuclei and see how Mulliken quantum chemical population analysis interprets holistically the wave function ψ. After this, I will propose a way in which behavioral mereology can help us make sense of this holistic interpretation.

For this example, if we begin with a polyatomic molecule, using Mulliken's notation for the linear combination of two atomic orbitals is

$$\phi = c_r \chi_r + c_s \chi_s. \tag{1}$$

This equation seems to imply that the whole belonging to the molecular level is reducible to the electrons and nuclei that belong to the more fundamental level. However, adopting Max Born's probabilistic interpretation of the term "orbital," "the square of a molecular orbital corresponds to the probability density of finding a particular electron within the molecular space" (p. 86, [15]). Therefore, from the standpoint of Mulliken's holistic interpretation, the correct equation must go beyond the linear combination of the two atomic orbitals and incorporate "the overlap in the space region that corresponds to the intersection of each atomic space" (p. 86, [15]). Once the net atomic population and the overlap population are considered and the sums are simplified, Mulliken's expression is

$$N = Nc_r^2 + Nc_s^2 + 2Nc_r c_s S_{rs}. \tag{2}$$

Mulliken's interpretation of the weighting coefficients c_r^2 and c_s^2 means that the weighing coefficients, multiplied by the number of electrons that can be assigned to that particular molecular orbital, represent the part of the electron density that belongs to nucleus 1 or to nucleus 2. On the other hand, the term $2Nc_r c_s S_{rs}$ represents "the overlap population" and expresses the part of the electronic density that refers to the two atomic functions *at the same time* and, thus, to the *whole molecule*. The electronic density of the overlap population provides crucial information about the "strength" of the chemical bond. For instance, in the case of the molecule LiH (lithium hydride), Mulliken establishes that (1) a first fraction, equal to 0.111 of the whole electronic charge, "belongs" to the hydrogen atom; (2) another fraction, equal to 0.641, belongs to the lithium; and (3) the last but not the least fraction, equal to 0.248, belongs to both the hydrogen and the lithium (pp. 1833–1840, [25]). As a consequence, the overlap population between any set of two related *nuclei* depends upon the whole molecule. In other words, when one wants to study a local bond between particular *atoms* in the molecule, one has to integrate the characteristic of belonging to the whole molecule into the calculation. *The whole and the*

parts are thus co-defined. There is no room for reductionism here because quantum chemists must take both of these elements into consideration [15].

It is, therefore, clear that a summative mereological approach cannot succeed in formalizing the whole–parts relation in such cases. On the other hand, the behavioral mereology proposed by Fong, Myers, and Spivak would have much better success, particularly with regard to mereologically formalizing the overlap population in which the electronic densities of the two nuclei "intersect," affecting both each other and the entire molecule. If the electronic density of either the hydrogen atom or the lithium atom is altered, the electronic density of the other will be changed, as will the electronic density of the overlap population. Although attempting an actual mereological formalization would extend beyond the scope of this essay, one can provide a narrative account of how such a formalization could be developed. Applying the terms of behavioral mereology to the example of LiH, the quotient of B_P would describe the behavior (electronic density) of the overlap population. The P-behavior of the lithium atom (electronic density 0.641) affects the Q-behavior of the hydrogen atom (the electronic density 0.111) and vice versa, since these compatible behaviors constrain each other and affect the behavior of the overlap population (electronic density 0.248). How each of these behaviors affects the others is ensured or determined by the behavior (electronic density 1) of the whole molecule.

The fact that behavioral mereology accommodates interdependency between the parts within a whole, as well as the interdependency between the whole and its parts and how all of these factors constrain each other, is a promising step toward formalizing the mereology of higher-order wholes, both organic and inorganic, and the whole–parts relations within complex systems. Behavioral mereology also supplies a way of formalizing the mereological relations within *autopoietic* systems, that is, systems whose behavior ensures their organizational integrity, which, in turn, ensures compatibility with their environments. Thus, organic wholes are autopoietic within their ecological niches and, if we consider ecosystems the parts of which include preys and predators, an autopoietic part A is one that constrains an internal model, that is, a subpart that sits in isomorphism with the environment E. In order to ensure compatibility between A and E, A must behave to maintain its isomorphism and this entails perception and action. Because A is not omniscient, Fong, Myers, and Spivak suggest abandoning the Boolean topos of set theory and framing A's behavior in terms of approximate Bayesian inferences. As Karl Friston has recently argued, Bayesian modelling optimizes descriptions of biological self-organization and "internal states (and their [Markov] blanket) will appear to engage in active Bayesian inference" (p. 1, [26]). So, for example, "internal states will appear to respond to sensory fluctuations based on posterior beliefs about underlying fluctuations in external states. We can formalize this notion by associating these beliefs with a probability density over external states $q(\psi|\lambda)$ that is encoded (parametrized) by internal states (p. 4, [26]). However, although approximate Bayesian inference successfully frames autopoietic systems, the Bayesian model may not be appropriate for quantum chemical systems and this is an area worthy of further exploration. Thus, although the Boolean topos of set theory should be abandoned, the specific way in which this is done will depend on the specific topos under consideration, whether that topos is preys and predators in a given ecosystem or quantum chemical systems in an experimenter's laboratory.

6. Conclusions

In spite of the goal of logicians such as Husserl to develop a mereology that would capture the whole–parts relation in a formal manner and that would do so regardless of the entities being described, "there is a growing consensus that this is the best one can say, and that mereology is best understood as a theory—or a plurality of theories—whose fundamental truths do not reflect the properties of the part-whole relation itself but the nature of the entities to which it applies" (p. 16, [3]). Thus, the kind of mereology that accounts for the summative wholes considered by Husserl in the context of formal ontology is not the same kind of mereology that must be used when the objects under consideration are of a different type. The mereology used must be appropriate to the type of objects being considered.

It is clear from the above discussion that quantum chemical systems are clearly not mere sums of parts and cannot be reduced without remainder to the parts that constitute them, because such complex systems have emergent properties that are novel and that are not themselves reducible to the properties of the parts. Additionally, once we closely examine the way in which molecules, atoms, and subatomic parts are conceptualized, we see that quantum chemists conceive of chemical wholes in terms of connectivity and relationality at different levels of chemical organization that co-define each other. Thus, a non-summative and non-extensional mereology must be developed that is capable of accounting for these co-constituting and co-defining relational features of chemical wholes and parts. Additionally, such a mereology must consider the constituent parts of chemical wholes as dependent moments of the whole, rather than as independent pieces, precisely because the parts and the whole are co-dependent and co-define each other. Furthermore, a proper mereology of chemical wholes must also account for the way in which the experimental environment (or milieu) also contributes to constituting the whole–parts relation.

This kind of non-standard mereology challenges the assumptions of summative extensional mereology that the parts are not causally affected by the whole or that the relations between the parts have no causal effect on the properties of the whole. However, in order for us to succeed in developing a mereology that successfully accounts for the co-dependence of chemical parts and whole, we must alter the way in which we conceptualize chemical systems, taking our cue from the way in which the experimental practice and calculations of quantum chemists must always take into account different levels of organization, connectivity, and interdependence as they synthesize, analyze, and study quantum chemical systems. As has been discussed in this essay, quantum chemists have established that neither atoms nor molecules can be simplistically described as being entity-like or as having clear boundaries in the manner of traditional representations, such as the "ball and stick" model that is still used for purely pedagogical purposes. As a matter of fact, Harré and Llored emphasize that "it is a mistake to treat electrons as constituents of anything" (p. 9, [23]). Therefore, the standard summative extensional mereology advanced by logicians such as Husserl, Leśniewski, Fine, and Lewis cannot adequately meet the requirements for describing the whole–parts relations of regional ontologies such as the one studied by quantum chemists, which is concerned with "such structured entities as molecules, where the whole is not merely the sum of its parts" (p. 303, [27]).

There has been considerable attention paid recently to reconceptualizing mereology to better account for the distinctive parts/whole relations that are studied within the various natural and social sciences. Notable examples of this work include Claudio Calosi and Pierluigi Graziani's important collection *Mereology and the Sciences: Parts and Wholes in the Contemporary Scientific Context* [28], which includes a contribution by Harré and Llored focusing on the mereology of chemistry [29], and individual works such as Robert Prentner's article "Chemistry, Context, and Objects of Thought" [30]. However, although all of these authors have given a negative account of extensional, summative mereology as inappropriate to describe quantum chemical systems, logicians and mathematicians have not yet explicitly responded to philosophy of chemistry's call for the development of an alternative mereology specifically for describing quantum chemical systems. Yet, to the extent that Fong, Myers, and Spivak's proposal is intended to help us understand what gives complex wholes the quality of being cohesive and closed, it is a promising step in this direction.

In fact, behavioral mereology is very well adapted to explain the concept of "affordance" in the philosophy of chemistry as it has been applied by Harré, Llored, and Earley. Thus, one can say that salt being a part of sea water is context-dependent, in that sea water will "behave" in a particular manner, that is, it will "afford" salt, under certain conditions and when certain procedures are carried out. Another virtue of behavioral mereology is that, because it remains topos agnostic, it avoids unnecessary ontological commitments. This permits behavioral mereology to accommodate seemingly contradictory claims regarding the presence of atoms in molecules. Therefore, it can capture the Hund–Mullikan theory of molecules, once the claim that nuclei are part of a molecule is interpreted in the theoretical context of wave-function-based quantum chemistry, as claiming that molecules afford

an understanding in terms of a collection of nuclei and electrons. As well, behavioral mereology can accommodate Richard Bader's Quantum Theory of Atoms in Molecules (QTAIM), which regards atoms as constituent of molecules, by incorporating the theoretical context of electron density calculations.

The topos agnosticism and resistance to unnecessary ontological commitments makes behavioral mereology appropriate for the type of "interventionalist" or "pragmatist" conception of science that has been defended by philosophers such as Bas Van Fraassen, Ian Hacking, and Larry Laudan. Furthermore, although a detailed discussion of the following point would extend beyond the scope of this essay, it is important to emphasize the need for developing non-summative and non-extensional mereologies to analyze the whole–parts relations in the regional ontologies studied by other natural sciences, especially those sciences that are concerned with organic and complex systems, such as biochemistry, biology, and the human and social sciences. The logic of constraint upon which behavioral mereology is structured inherently emphasizes the co-dependency of the parts, the co-dependency of parts and whole, and the co-dependency of the whole and its environment. By incorporating the latter mesological consideration, behavioral mereology moves a step beyond other proposed non-summative alternatives to classical extensional mereology. However, as the authors themselves admit, "the logic of constraint passing between parts is essential . . . but perhaps not sufficient. The question of what additional structures need to be added or considered in order to construct a viable notion of a [whole] remains future work" (p. 16, [24]).

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